



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:16 AM EDT

PDB ID : 6CIE  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with N-(1-(2-(Ethyl(methyl)amino)ethyl)-1,2,3,4-tetrahydroquino-lin-6-yl)thiophene-2-carboximidamide  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : 2018-02-23  
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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

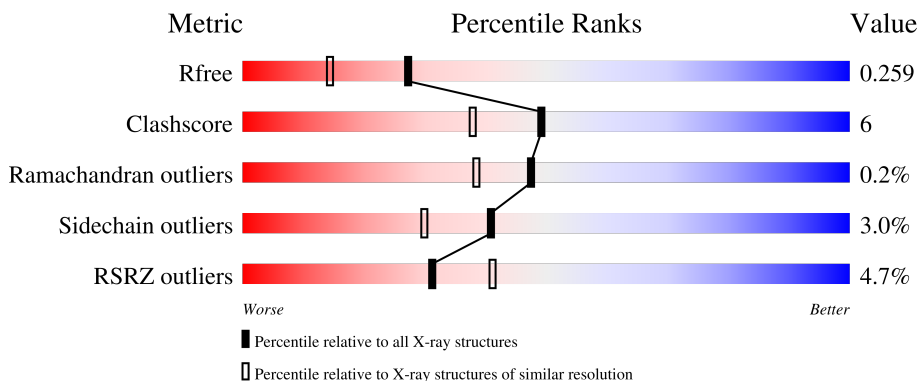
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13763 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
			Total	C	N	O	S			
1	A	401	Total 3215	C 2047	N 566	O 586	S 16	0	2	0
1	B	402	Total 3220	C 2051	N 566	O 587	S 16	0	3	0
1	C	401	Total 3209	C 2044	N 563	O 586	S 16	0	2	0
1	D	402	Total 3215	C 2048	N 565	O 586	S 16	0	2	0

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



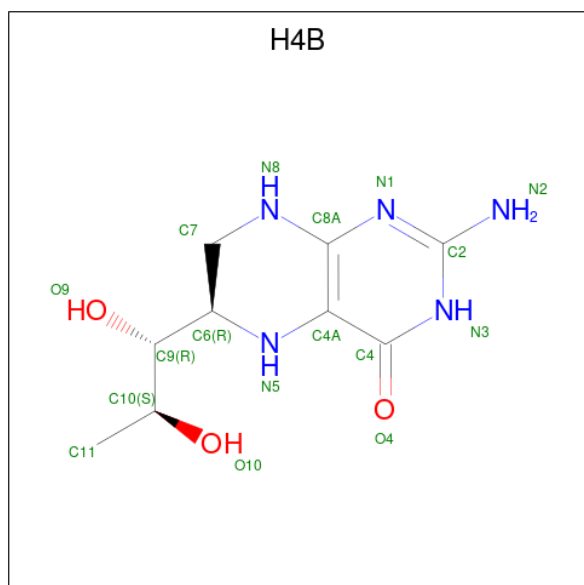
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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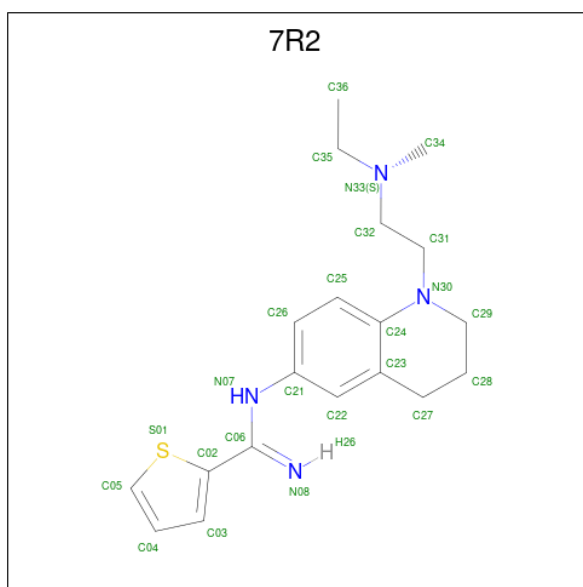
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



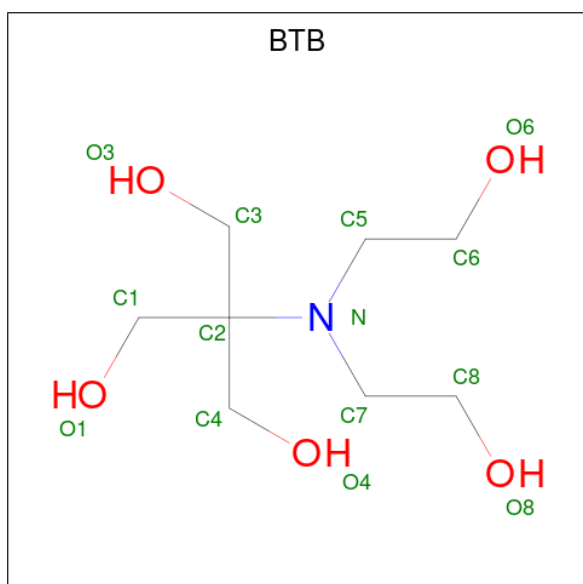
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-(1-{2-[ethyl(methyl)amino]ethyl}-1,2,3,4-tetrahydroquinolin-6-yl)thiophene-2-carboximidamide (three-letter code: 7R2) (formula:  $C_{19}H_{26}N_4S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			24	19	4	1		
4	B	1	Total	C	N	S	0	0
			24	19	4	1		
4	C	1	Total	C	N	S	0	0
			24	19	4	1		
4	D	1	Total	C	N	S	0	0
			24	19	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	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	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		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is CHLORIDE ION (three-letter code: 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 (three-letter code: 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	C	1	Total Gd 1 1	0	0

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

- Molecule 10 is water.

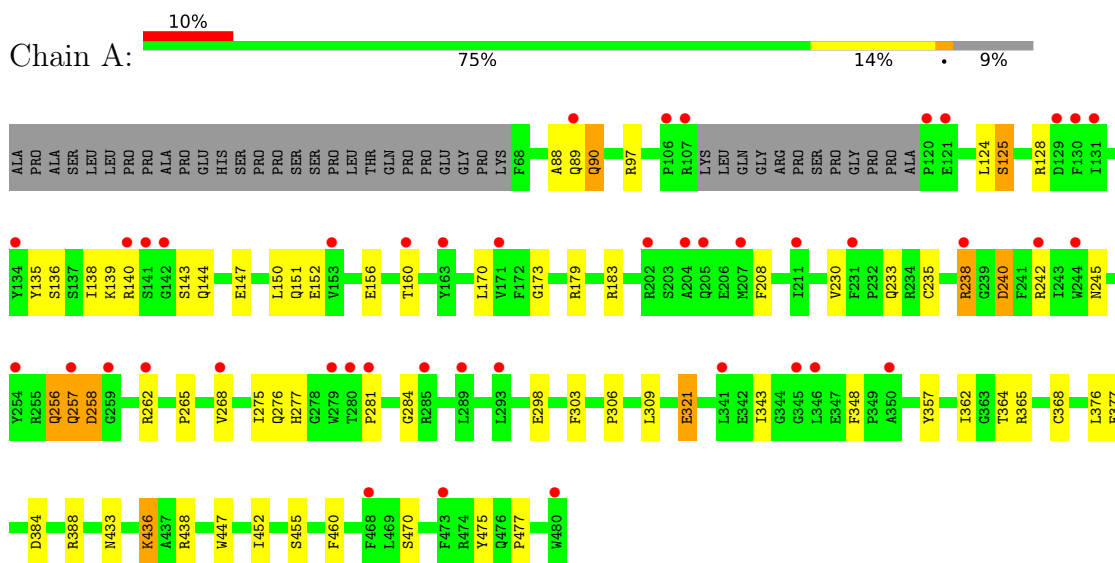
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	58	Total 58	O 58	0	0
10	B	113	Total 113	O 113	0	0
10	C	86	Total 86	O 86	0	0
10	D	135	Total 135	O 135	0	0



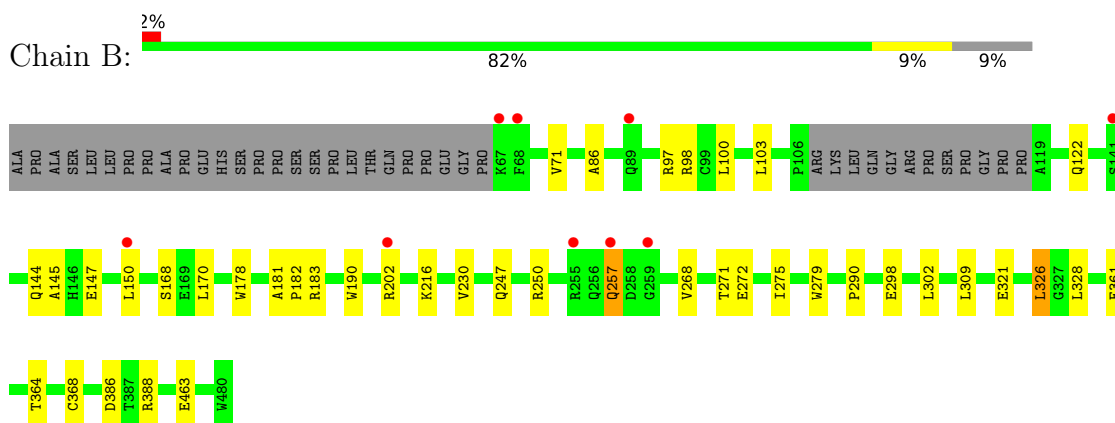
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

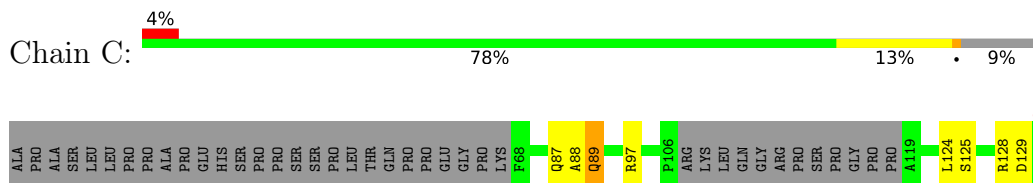
- Molecule 1: Nitric oxide synthase, endothelial

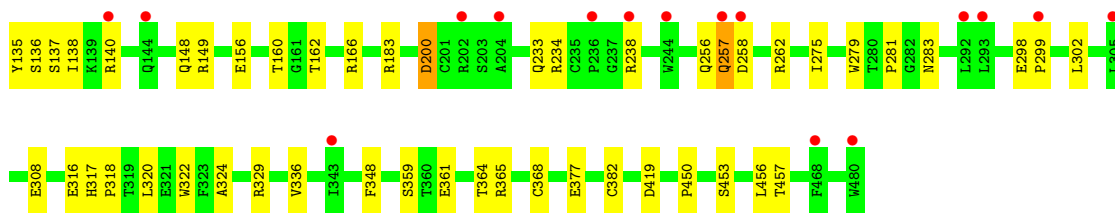


- Molecule 1: Nitric oxide synthase, endothelial

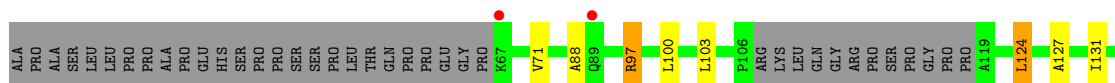
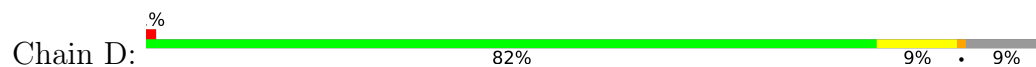


- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.52Å 152.23Å 108.80Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	45.99 – 1.95 45.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.99-1.95) 99.9 (45.99-1.95)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, $R_{free}$	0.212 , 0.262 0.208 , 0.259	Depositor DCC
$R_{free}$ test set	7097 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtrriage
Anisotropy	0.871	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: CL, BTB, GD, H4B, HEM, 7R2, ZN, GOL

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	0.34	0/3313	0.51	0/4513
1	B	0.40	0/3321	0.54	0/4525
1	C	0.36	0/3307	0.50	0/4507
1	D	0.42	0/3313	0.54	0/4514
All	All	0.38	0/13254	0.52	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	47	0
1	B	3220	0	3127	27	0
1	C	3209	0	3109	34	0
1	D	3215	0	3121	24	0
2	A	43	0	30	7	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	0	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	24	0	0	0	0
4	B	24	0	0	1	0
4	C	24	0	0	2	0
4	D	24	0	0	0	0
5	A	42	0	56	10	0
5	B	42	0	56	8	0
5	C	42	0	56	8	0
5	D	28	0	37	7	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	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	58	0	0	2	0
10	B	113	0	0	1	0
10	C	86	0	0	3	0
10	D	135	0	0	0	0
All	All	13763	0	12876	155	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 (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLN:OE1	10:A:601:HOH:O	1.93	0.84
1:C:128:ARG:O	1:C:132:ASN:ND2	2.16	0.79
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.01	0.79
1:C:183:ARG:HB2	2:C:501:HEM:HBD2	1.66	0.77
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.67	0.75
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.68	0.73
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.71	0.73
1:C:257:GLN:NE2	10:C:601:HOH:O	2.20	0.72
1:A:433:ASN:HA	1:A:436:LYS:HE3	1.72	0.72
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.72	0.72
1:B:298:GLU:OE2	5:B:505:BTB:N	2.24	0.71
1:C:128:ARG:NH1	1:C:129:ASP:OD1	2.27	0.68
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.75	0.68
5:D:505:BTB:O4	5:D:505:BTB:O1	2.09	0.67
1:C:200:ASP:OD1	1:C:200:ASP:N	2.25	0.65
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.08	0.64
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.78	0.64
1:B:183:ARG:HB2	2:B:501:HEM:HBD2	1.78	0.64
1:C:382:CYS:HA	5:C:504:BTB:H12	1.80	0.63
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.80	0.63
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.79	0.63
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.81	0.62
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.84	0.60
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.84	0.60
1:A:238:ARG:HH21	1:A:240:ASP:HA	1.67	0.59
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.84	0.59
1:A:183:ARG:HB2	2:A:501:HEM:HBD2	1.84	0.59
1:C:298:GLU:HG3	1:C:299:PRO:HD2	1.83	0.59
1:D:233:GLN:O	1:D:238:ARG:NH2	2.36	0.59
1:D:298:GLU:CD	5:D:505:BTB:H42	2.24	0.58
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.85	0.58
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.86	0.58
1:A:147:GLU:O	1:A:151:GLN:NE2	2.25	0.57
1:C:160:THR:HG23	1:C:162:THR:H	1.70	0.56
1:B:170:LEU:HD21	1:B:230:VAL:HG11	1.88	0.55
1:C:133:GLN:NE2	10:C:604:HOH:O	2.28	0.55
1:A:321:GLU:H	1:A:321:GLU:CD	2.09	0.55
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.89	0.54
1:A:384:ASP:HB3	10:C:601:HOH:O	2.08	0.54
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.20	0.54
1:B:147:GLU:HA	1:B:150:LEU:HD12	1.89	0.53
1:B:321:GLU:OE1	5:B:504:BTB:H82	2.09	0.53
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.90	0.53
1:B:216:LYS:HB2	1:B:309:LEU:HD11	1.91	0.53
1:D:271:THR:O	1:D:275:ILE:HG12	2.08	0.53
5:A:506:BTB:O3	5:A:506:BTB:O1	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:O	10:A:602:HOH:O	2.19	0.53
1:C:262:ARG:NH1	1:C:283:ASN:O	2.41	0.53
1:A:125:SER:HA	1:A:128:ARG:HD2	1.91	0.52
1:A:388:ARG:HA	5:A:505:BTB:H81	1.91	0.52
1:C:97:ARG:HG2	1:D:88:ALA:HB3	1.91	0.52
1:A:447:TRP:CE3	2:A:501:HEM:HBA2	2.45	0.52
1:B:361:GLU:OE1	4:B:503:7R2:N07	2.42	0.51
5:A:505:BTB:O3	5:A:505:BTB:O1	2.23	0.49
1:A:256:GLN:HG3	1:A:258:ASP:CG	2.33	0.49
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.94	0.49
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.48	0.49
1:A:276:GLN:O	1:A:277:HIS:ND1	2.45	0.49
1:C:257:GLN:O	1:C:257:GLN:HG3	2.11	0.49
1:A:156:GLU:O	1:A:160:THR:OG1	2.31	0.49
1:A:258:ASP:OD1	1:A:258:ASP:N	2.45	0.49
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.25	0.49
1:A:388:ARG:HG2	5:A:505:BTB:H82	1.95	0.48
1:C:361:GLU:OE1	4:C:503:7R2:N07	2.46	0.48
1:B:71:VAL:HG13	1:B:463:GLU:HB2	1.95	0.48
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.49	0.48
1:C:156:GLU:O	1:C:160:THR:HG22	2.14	0.48
1:A:298:GLU:OE2	5:A:506:BTB:O8	2.19	0.47
1:C:377:GLU:OE2	5:C:505:BTB:O1	2.29	0.47
2:A:501:HEM:HBA1	2:A:501:HEM:CHA	2.44	0.47
1:B:144:GLN:NE2	1:B:145:ALA:H	2.13	0.47
1:A:173:GLY:HA3	1:A:343:ILE:HD13	1.97	0.47
1:C:364:THR:O	1:C:368:CYS:HB2	2.14	0.47
1:D:298:GLU:OE1	5:D:505:BTB:O6	2.28	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.15	0.47
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.51	0.46
5:C:506:BTB:H71	5:C:506:BTB:H32	1.41	0.46
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.97	0.46
5:C:504:BTB:O8	5:C:504:BTB:O6	2.30	0.46
1:B:326:LEU:CD1	5:C:504:BTB:H41	2.45	0.46
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.97	0.45
1:D:100:LEU:HB3	1:D:103:LEU:HD22	1.97	0.45
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.51	0.45
1:A:447:TRP:HE3	2:A:501:HEM:HBA2	1.79	0.45
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.97	0.45
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.97	0.45
1:A:179:ARG:NH2	1:A:438:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.51	0.45
1:A:306:PRO:HB2	1:A:309:LEU:HB2	1.99	0.45
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.52	0.45
5:D:505:BTB:H51	5:D:505:BTB:H32	1.72	0.45
5:B:505:BTB:O3	5:B:505:BTB:H51	2.16	0.45
1:C:148:GLN:OE1	1:C:166:ARG:NH2	2.50	0.45
1:D:262:ARG:NH1	1:D:283:ASN:O	2.50	0.45
5:D:504:BTB:H12	5:D:504:BTB:H72	1.68	0.45
1:A:377:GLU:OE1	5:A:505:BTB:H11	2.17	0.45
1:C:359:SER:OG	1:C:419:ASP:HA	2.17	0.45
5:B:506:BTB:H11	5:B:506:BTB:H72	1.56	0.44
1:C:124:LEU:O	1:C:128:ARG:HG2	2.17	0.44
1:C:132:ASN:O	1:C:136:SER:OG	2.30	0.44
1:B:250:ARG:NH2	10:B:606:HOH:O	2.51	0.44
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.51	0.44
1:A:88:ALA:HB3	1:B:97:ARG:NH1	2.33	0.44
1:A:135:TYR:HA	1:A:138:ILE:HG12	1.99	0.44
1:A:256:GLN:OE1	1:A:257:GLN:N	2.45	0.43
1:B:268:VAL:O	1:B:272:GLU:HG3	2.17	0.43
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.53	0.43
1:B:257:GLN:HA	1:B:257:GLN:OE1	2.18	0.43
5:B:506:BTB:H51	5:B:506:BTB:H32	1.45	0.43
1:C:275:ILE:HD11	1:C:281:PRO:HB3	2.00	0.43
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.99	0.43
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.53	0.43
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.54	0.43
5:A:505:BTB:H11	5:A:505:BTB:H51	1.46	0.43
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.53	0.43
5:C:505:BTB:H41	5:C:505:BTB:H72	1.50	0.43
5:D:505:BTB:H52	5:D:505:BTB:H81	1.62	0.43
2:A:501:HEM:HBA1	2:A:501:HEM:HHA	2.01	0.43
1:A:152:GLU:O	1:A:156:GLU:HB2	2.18	0.43
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.58	0.42
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.84	0.42
5:A:505:BTB:H41	5:A:505:BTB:H72	1.38	0.42
1:D:455:SER:HA	1:D:460:PHE:CG	2.54	0.42
5:B:504:BTB:H32	5:B:504:BTB:H51	1.73	0.42
1:C:336:VAL:HG23	4:C:503:7R2:C03	2.49	0.42
1:D:127:ALA:O	1:D:131:ILE:HG12	2.20	0.42
1:A:89:GLN:HB3	1:A:90:GLN:H	1.50	0.42
1:A:262:ARG:HE	1:A:284:GLY:HA2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:506:BTB:H72	5:A:506:BTB:H42	1.77	0.42
1:C:135:TYR:CD1	1:C:138:ILE:HD11	2.55	0.42
5:A:504:BTB:H51	5:A:504:BTB:H32	1.66	0.42
1:C:89:GLN:H	1:C:89:GLN:HG2	1.63	0.42
1:A:97:ARG:NH2	1:B:86:ALA:O	2.53	0.42
1:A:140:ARG:HA	1:A:140:ARG:HD3	1.81	0.42
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.42
1:B:326:LEU:HD11	5:C:504:BTB:H41	2.02	0.42
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	2.02	0.41
1:A:364:THR:O	1:A:368:CYS:HB2	2.21	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.93	0.41
1:C:382:CYS:HA	5:C:504:BTB:H32	2.03	0.41
1:A:135:TYR:CD1	1:A:138:ILE:HD11	2.56	0.41
5:B:505:BTB:H42	5:B:505:BTB:H72	1.58	0.41
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.02	0.41
1:D:140:ARG:HH12	1:D:145:ALA:HB3	1.86	0.41
1:A:242:ARG:NH1	1:A:477:PRO:O	2.46	0.41
1:A:256:GLN:HG3	1:A:258:ASP:OD1	2.20	0.41
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.55	0.41
1:A:265:PRO:HA	1:A:268:VAL:HG23	2.03	0.41
1:B:279:TRP:HB2	1:B:302:LEU:HD21	2.01	0.41
1:D:243:ILE:HG21	1:D:337:SER:HB2	2.02	0.41
1:B:271:THR:O	1:B:275:ILE:HG13	2.21	0.40
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.20	0.40
5:B:505:BTB:O4	5:B:505:BTB:O1	2.23	0.40
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.57	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	399/440 (91%)	377 (94%)	20 (5%)	2 (0%)	29	17
1	B	401/440 (91%)	391 (98%)	10 (2%)	0	100	100
1	C	399/440 (91%)	381 (96%)	17 (4%)	1 (0%)	41	30
1	D	400/440 (91%)	390 (98%)	10 (2%)	0	100	100
All	All	1599/1760 (91%)	1539 (96%)	57 (4%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	A	143	SER
1	A	144	GLN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/373 (92%)	329 (96%)	14 (4%)	30	18
1	B	344/373 (92%)	337 (98%)	7 (2%)	55	48
1	C	342/373 (92%)	329 (96%)	13 (4%)	33	21
1	D	343/373 (92%)	335 (98%)	8 (2%)	50	42
All	All	1372/1492 (92%)	1330 (97%)	42 (3%)	41	28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	124	LEU
1	A	125	SER
1	A	136	SER
1	A	235	CYS
1	A	238	ARG
1	A	240	ASP
1	A	245	ASN

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	257	GLN
1	A	258	ASP
1	A	321	GLU
1	A	436	LYS
1	A	470	SER
1	B	98	ARG
1	B	122	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	202	ARG
1	B	257	GLN
1	B	326	LEU
1	C	87	GLN
1	C	125	SER
1	C	137	SER
1	C	140	ARG
1	C	149	ARG
1	C	200	ASP
1	C	234	ARG
1	C	238	ARG
1	C	256	GLN
1	C	257	GLN
1	C	258	ASP
1	C	308	GLU
1	C	329	ARG
1	D	71	VAL
1	D	97	ARG
1	D	124	LEU
1	D	230	VAL
1	D	255	ARG
1	D	257	GLN
1	D	262	ARG
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	C	506	-	13,13,13	0.41	0	7,16,16	0.59	0
5	BTB	D	504	9	13,13,13	0.34	0	7,16,16	0.75	0
5	BTB	B	506	-	13,13,13	0.34	0	7,16,16	0.41	0
2	HEM	B	501	1	41,50,50	1.53	8 (19%)	45,82,82	1.89	13 (28%)
3	H4B	C	502	-	16,18,18	0.87	0	11,26,26	2.57	5 (45%)
5	BTB	D	505	-	13,13,13	0.48	0	7,16,16	0.75	0
4	7R2	D	503	-	26,26,26	1.13	4 (15%)	26,35,35	2.05	3 (11%)
4	7R2	A	503	-	26,26,26	1.08	3 (11%)	26,35,35	1.75	3 (11%)
4	7R2	C	503	-	26,26,26	1.11	3 (11%)	26,35,35	1.84	3 (11%)
3	H4B	B	502	-	16,18,18	0.91	0	11,26,26	2.59	5 (45%)
3	H4B	A	502	-	16,18,18	0.83	0	11,26,26	2.60	6 (54%)
5	BTB	A	505	-	13,13,13	0.49	0	7,16,16	1.03	1 (14%)
7	GOL	A	508	-	5,5,5	0.35	0	5,5,5	0.51	0
2	HEM	D	501	1	41,50,50	1.47	7 (17%)	45,82,82	1.81	12 (26%)
4	7R2	B	503	-	26,26,26	1.21	2 (7%)	26,35,35	1.89	4 (15%)
2	HEM	A	501	1	41,50,50	1.51	6 (14%)	45,82,82	1.69	9 (20%)
3	H4B	D	502	-	16,18,18	0.86	0	11,26,26	2.58	5 (45%)
5	BTB	C	505	-	13,13,13	0.63	0	7,16,16	0.96	0
2	HEM	C	501	1	41,50,50	1.61	6 (14%)	45,82,82	1.61	9 (20%)

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	0.37	0	7,16,16	0.55	0
7	GOL	C	508	-	5,5,5	0.35	0	5,5,5	0.38	0
5	BTB	C	504	9	13,13,13	0.35	0	7,16,16	0.78	0
5	BTB	B	505	-	13,13,13	0.51	0	7,16,16	0.73	0
5	BTB	B	504	9	13,13,13	0.43	0	7,16,16	0.78	0
5	BTB	A	506	-	13,13,13	0.35	0	7,16,16	0.29	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	C	506	-	-	5/21/21/21	-
5	BTB	D	504	9	-	5/21/21/21	-
5	BTB	B	506	-	-	7/21/21/21	-
2	HEM	B	501	1	-	2/12/54/54	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	D	505	-	-	10/21/21/21	-
4	7R2	D	503	-	-	3/11/25/25	0/3/3/3
4	7R2	A	503	-	-	4/11/25/25	0/3/3/3
4	7R2	C	503	-	-	5/11/25/25	0/3/3/3
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	505	-	-	15/21/21/21	-
7	GOL	A	508	-	-	4/4/4/4	-
2	HEM	D	501	1	-	2/12/54/54	-
4	7R2	B	503	-	-	4/11/25/25	0/3/3/3
2	HEM	A	501	1	-	4/12/54/54	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	C	505	-	-	10/21/21/21	-
2	HEM	C	501	1	-	4/12/54/54	-
5	BTB	A	504	9	-	7/21/21/21	-
7	GOL	C	508	-	-	3/4/4/4	-
5	BTB	C	504	9	-	3/21/21/21	-
5	BTB	B	505	-	-	6/21/21/21	-
5	BTB	B	504	9	-	3/21/21/21	-
5	BTB	A	506	-	-	6/21/21/21	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-CAC	3.98	1.56	1.47
2	C	501	HEM	C3C-C2C	-3.80	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.79	1.35	1.40
2	C	501	HEM	C3C-CAC	3.69	1.55	1.47
2	A	501	HEM	C3C-CAC	3.53	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.47	1.35	1.40
4	B	503	7R2	C06-N07	-3.40	1.32	1.39
2	C	501	HEM	FE-ND	3.36	2.13	1.96
2	D	501	HEM	C3C-CAC	3.22	1.54	1.47
2	A	501	HEM	FE-NB	3.09	2.12	1.96
2	C	501	HEM	CAB-C3B	3.02	1.55	1.47
2	A	501	HEM	CAB-C3B	2.98	1.55	1.47
2	B	501	HEM	CAB-C3B	2.95	1.55	1.47
4	B	503	7R2	C21-N07	-2.94	1.35	1.41
4	D	503	7R2	C06-N07	-2.91	1.33	1.39
2	D	501	HEM	CAB-C3B	2.84	1.55	1.47
2	C	501	HEM	CAA-C2A	2.84	1.56	1.52
2	D	501	HEM	FE-NB	2.82	2.10	1.96
4	C	503	7R2	C21-N07	-2.82	1.35	1.41
4	A	503	7R2	C21-N07	-2.80	1.36	1.41
2	B	501	HEM	FE-NB	2.79	2.10	1.96
4	A	503	7R2	C02-C06	2.77	1.49	1.45
4	C	503	7R2	C02-C06	2.65	1.49	1.45
4	D	503	7R2	C21-N07	-2.65	1.36	1.41
2	B	501	HEM	C3C-C2C	-2.58	1.36	1.40
4	C	503	7R2	C06-N07	-2.57	1.33	1.39
4	A	503	7R2	C06-N07	-2.52	1.33	1.39
4	D	503	7R2	C02-C06	2.34	1.49	1.45
2	A	501	HEM	CAA-C2A	2.33	1.55	1.52
2	D	501	HEM	CMD-C2D	2.31	1.55	1.50
2	C	501	HEM	FE-NB	2.28	2.08	1.96
2	B	501	HEM	CAA-C2A	2.23	1.55	1.52
2	D	501	HEM	CAA-C2A	2.22	1.55	1.52
2	B	501	HEM	CMB-C2B	2.09	1.55	1.50
2	D	501	HEM	FE-ND	2.06	2.07	1.96
2	B	501	HEM	CMD-C2D	2.04	1.55	1.50
2	B	501	HEM	CHB-C1B	2.04	1.40	1.35
2	A	501	HEM	CMD-C2D	2.03	1.55	1.50
4	D	503	7R2	C04-C05	2.01	1.40	1.34

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	7R2	C04-C05-S01	-7.36	107.01	112.98
4	C	503	7R2	C04-C05-S01	-7.16	107.17	112.98
4	A	503	7R2	C04-C05-S01	-7.15	107.18	112.98
4	B	503	7R2	C04-C05-S01	-6.19	107.96	112.98
3	C	502	H4B	C8A-C4A-C4	5.69	119.63	114.57
3	A	502	H4B	C8A-C4A-C4	5.67	119.60	114.57
3	D	502	H4B	C8A-C4A-C4	5.29	119.27	114.57
3	B	502	H4B	C8A-C4A-C4	5.25	119.23	114.57
2	D	501	HEM	C4C-CHD-C1D	4.80	128.89	122.56
2	C	501	HEM	C4B-CHC-C1C	4.66	128.71	122.56
2	B	501	HEM	C3B-C2B-C1B	4.51	109.83	106.49
4	C	503	7R2	C28-C29-N30	-4.37	102.52	111.05
2	B	501	HEM	CBA-CAA-C2A	-4.33	105.24	112.62
4	D	503	7R2	C28-C29-N30	-4.16	102.92	111.05
2	C	501	HEM	C1B-NB-C4B	4.16	109.37	105.07
4	B	503	7R2	C28-C29-N30	-3.99	103.27	111.05
4	D	503	7R2	C23-C24-N30	-3.96	118.58	121.62
2	A	501	HEM	C1B-NB-C4B	3.79	108.98	105.07
4	B	503	7R2	C23-C24-N30	-3.71	118.78	121.62
2	D	501	HEM	C3B-C2B-C1B	3.58	109.14	106.49
2	D	501	HEM	C4D-ND-C1D	3.45	108.64	105.07
4	B	503	7R2	C31-N30-C29	3.45	123.91	116.71
2	B	501	HEM	C4D-ND-C1D	3.40	108.59	105.07
2	A	501	HEM	C3B-C2B-C1B	3.37	108.98	106.49
3	B	502	H4B	N1-C2-N3	-3.29	120.26	125.42
2	A	501	HEM	C4B-CHC-C1C	3.28	126.89	122.56
2	D	501	HEM	CBA-CAA-C2A	-3.27	107.04	112.62
3	A	502	H4B	C4-C4A-N5	3.14	121.75	119.12
3	D	502	H4B	N1-C2-N3	-3.14	120.50	125.42
3	D	502	H4B	C2-N3-C4	3.12	120.89	115.93
2	B	501	HEM	C1B-NB-C4B	3.09	108.27	105.07
2	D	501	HEM	CMA-C3A-C4A	-3.07	123.75	128.46
2	A	501	HEM	C4A-C3A-C2A	3.04	109.11	107.00
2	A	501	HEM	C4D-ND-C1D	3.03	108.20	105.07
2	B	501	HEM	C4C-CHD-C1D	2.97	126.47	122.56
3	B	502	H4B	C2-N1-C8A	2.96	121.18	114.54
2	A	501	HEM	C4C-CHD-C1D	2.93	126.42	122.56
3	B	502	H4B	C2-N3-C4	2.92	120.57	115.93
3	C	502	H4B	N1-C2-N3	-2.91	120.86	125.42
2	B	501	HEM	CMC-C2C-C3C	2.81	129.93	124.68
2	D	501	HEM	CMC-C2C-C3C	2.78	129.89	124.68
3	C	502	H4B	C2-N3-C4	2.75	120.30	115.93
2	B	501	HEM	C4B-CHC-C1C	2.71	126.14	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	N1-C2-N3	-2.69	121.20	125.42
2	D	501	HEM	C1B-NB-C4B	2.68	107.84	105.07
2	C	501	HEM	C4A-C3A-C2A	2.67	108.86	107.00
3	A	502	H4B	C2-N3-C4	2.67	120.17	115.93
3	D	502	H4B	C4-C4A-N5	2.67	121.36	119.12
3	B	502	H4B	C4-C4A-N5	2.65	121.34	119.12
2	D	501	HEM	C4B-CHC-C1C	2.64	126.05	122.56
3	C	502	H4B	C2-N1-C8A	2.63	120.44	114.54
2	C	501	HEM	C3B-C2B-C1B	2.63	108.44	106.49
2	B	501	HEM	C2B-C1B-NB	-2.62	106.73	109.84
3	A	502	H4B	C2-N1-C8A	2.61	120.39	114.54
3	D	502	H4B	C2-N1-C8A	2.59	120.33	114.54
2	B	501	HEM	C2D-C1D-ND	-2.57	106.80	109.88
2	B	501	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
2	B	501	HEM	CHD-C1D-ND	2.51	127.16	124.43
2	C	501	HEM	C4D-ND-C1D	2.46	107.62	105.07
3	A	502	H4B	N2-C2-N3	2.45	121.06	117.25
2	D	501	HEM	C3D-C4D-ND	-2.42	107.47	110.17
2	C	501	HEM	C2B-C1B-NB	-2.40	107.00	109.84
2	A	501	HEM	C2B-C1B-NB	-2.39	107.01	109.84
2	D	501	HEM	CBD-CAD-C3D	-2.37	106.04	112.63
4	A	503	7R2	C23-C24-N30	-2.35	119.81	121.62
4	C	503	7R2	C31-N30-C29	2.31	121.54	116.71
2	B	501	HEM	CHC-C4B-C3B	2.25	128.01	124.57
2	A	501	HEM	CHC-C4B-C3B	2.24	128.00	124.57
2	C	501	HEM	C3D-C4D-ND	-2.22	107.70	110.17
3	C	502	H4B	C4-C4A-N5	2.18	120.95	119.12
2	C	501	HEM	CMA-C3A-C4A	-2.17	125.14	128.46
2	C	501	HEM	CHC-C4B-C3B	2.15	127.86	124.57
2	A	501	HEM	C3D-C4D-ND	-2.13	107.80	110.17
2	B	501	HEM	C4A-C3A-C2A	2.11	108.46	107.00
2	D	501	HEM	C2B-C1B-NB	-2.10	107.35	109.84
5	A	505	BTB	O3-C3-C2	-2.05	105.82	111.44
4	A	503	7R2	C32-C31-N30	-2.04	103.74	114.42
2	D	501	HEM	C4A-C3A-C2A	2.03	108.41	107.00

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C2A-CAA-CBA-CGA
4	C	503	7R2	C31-C32-N33-C35
4	C	503	7R2	C36-C35-N33-C34
4	D	503	7R2	C36-C35-N33-C34
5	A	504	BTB	C3-C2-C4-O4
5	A	505	BTB	O1-C1-C2-C3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C4-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-C5
5	A	505	BTB	C4-C2-N-C7
5	A	506	BTB	O1-C1-C2-C3
5	A	506	BTB	O1-C1-C2-C4
5	A	506	BTB	O1-C1-C2-N
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	B	504	BTB	O1-C1-C2-C3
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
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	B	506	BTB	C3-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C7
5	C	506	BTB	C8-C7-N-C5
5	D	504	BTB	C3-C2-C4-O4

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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	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C8-C7-N-C5
7	C	508	GOL	O1-C1-C2-C3
4	B	503	7R2	C31-C32-N33-C35
5	C	504	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
5	B	505	BTB	N-C5-C6-O6
5	B	505	BTB	N-C7-C8-O8
4	A	503	7R2	N30-C31-C32-N33
7	A	508	GOL	O1-C1-C2-C3
7	A	508	GOL	C1-C2-C3-O3
5	C	505	BTB	N-C7-C8-O8
2	B	501	HEM	C2A-CAA-CBA-CGA
2	D	501	HEM	C2A-CAA-CBA-CGA
7	A	508	GOL	O1-C1-C2-O2
7	A	508	GOL	O2-C2-C3-O3
7	C	508	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
5	C	504	BTB	N-C7-C8-O8
4	D	503	7R2	C36-C35-N33-C32
4	B	503	7R2	C36-C35-N33-C34
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	B	506	BTB	C1-C2-C4-O4
5	C	506	BTB	C1-C2-C3-O3
5	D	504	BTB	C1-C2-C4-O4
4	B	503	7R2	C32-C31-N30-C24
4	A	503	7R2	C32-C31-N30-C29
4	B	503	7R2	C32-C31-N30-C29
4	C	503	7R2	C32-C31-N30-C29
5	A	504	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	N-C2-C3-O3
5	B	504	BTB	O1-C1-C2-N
5	B	506	BTB	N-C2-C4-O4
5	C	505	BTB	C4-C2-N-C5
5	C	506	BTB	N-C2-C3-O3
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
5	D	504	BTB	N-C5-C6-O6
5	C	506	BTB	N-C7-C8-O8
7	C	508	GOL	O2-C2-C3-O3
5	B	506	BTB	N-C7-C8-O8
4	A	503	7R2	C36-C35-N33-C34
4	D	503	7R2	C31-C32-N33-C34
5	A	505	BTB	C3-C2-C4-O4
5	B	504	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-C3
5	C	506	BTB	C4-C2-C3-O3
5	A	504	BTB	N-C7-C8-O8
4	C	503	7R2	N30-C31-C32-N33
4	C	503	7R2	C32-C31-N30-C24
4	A	503	7R2	C31-C32-N33-C35

There are no ring outliers.

19 monomers are involved in 52 short contacts:

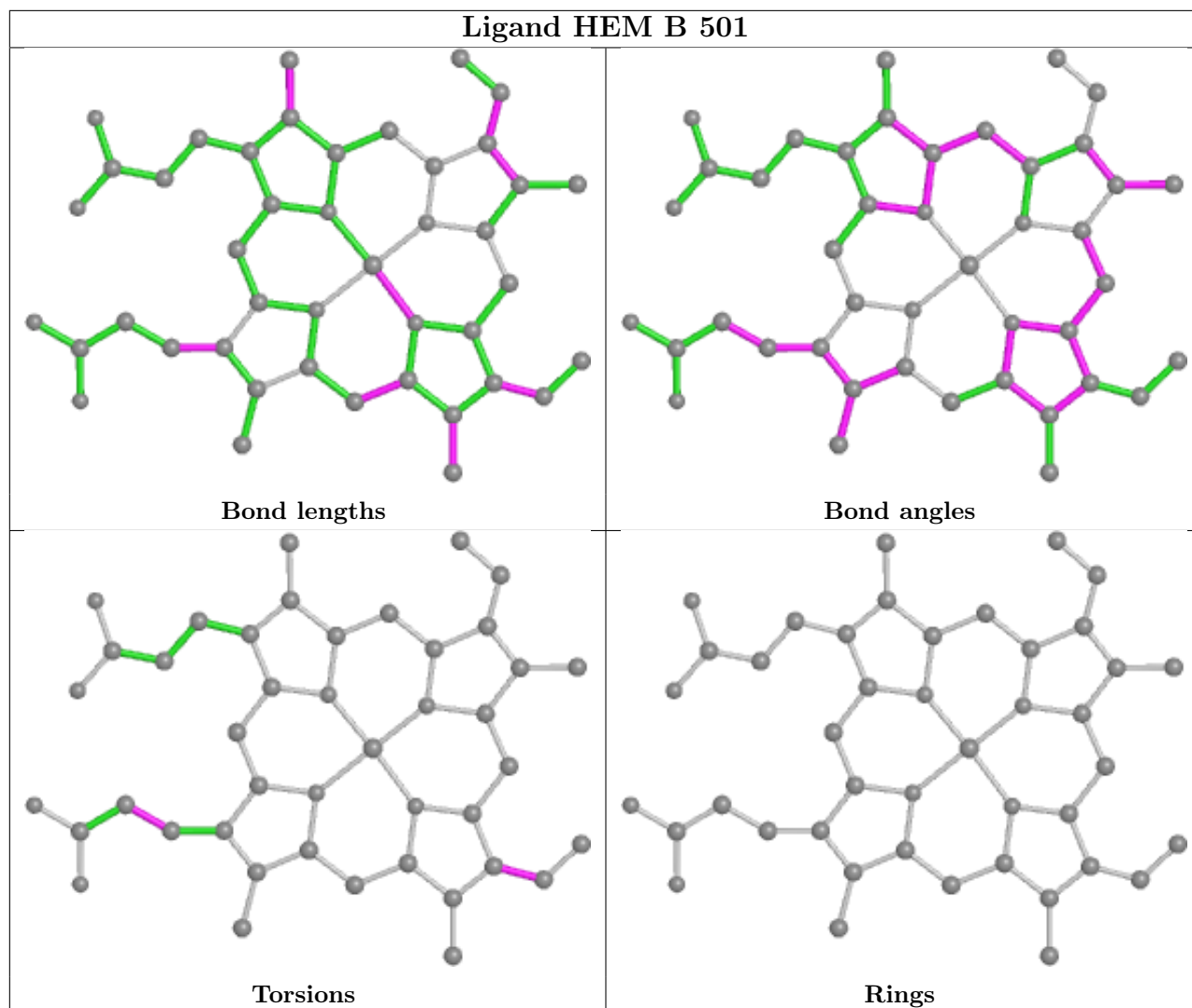
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	506	BTB	1	0
5	D	504	BTB	2	0
5	B	506	BTB	2	0
2	B	501	HEM	3	0
3	C	502	H4B	1	0
5	D	505	BTB	5	0
4	C	503	7R2	2	0
3	A	502	H4B	1	0
5	A	505	BTB	6	0
2	D	501	HEM	1	0
4	B	503	7R2	1	0

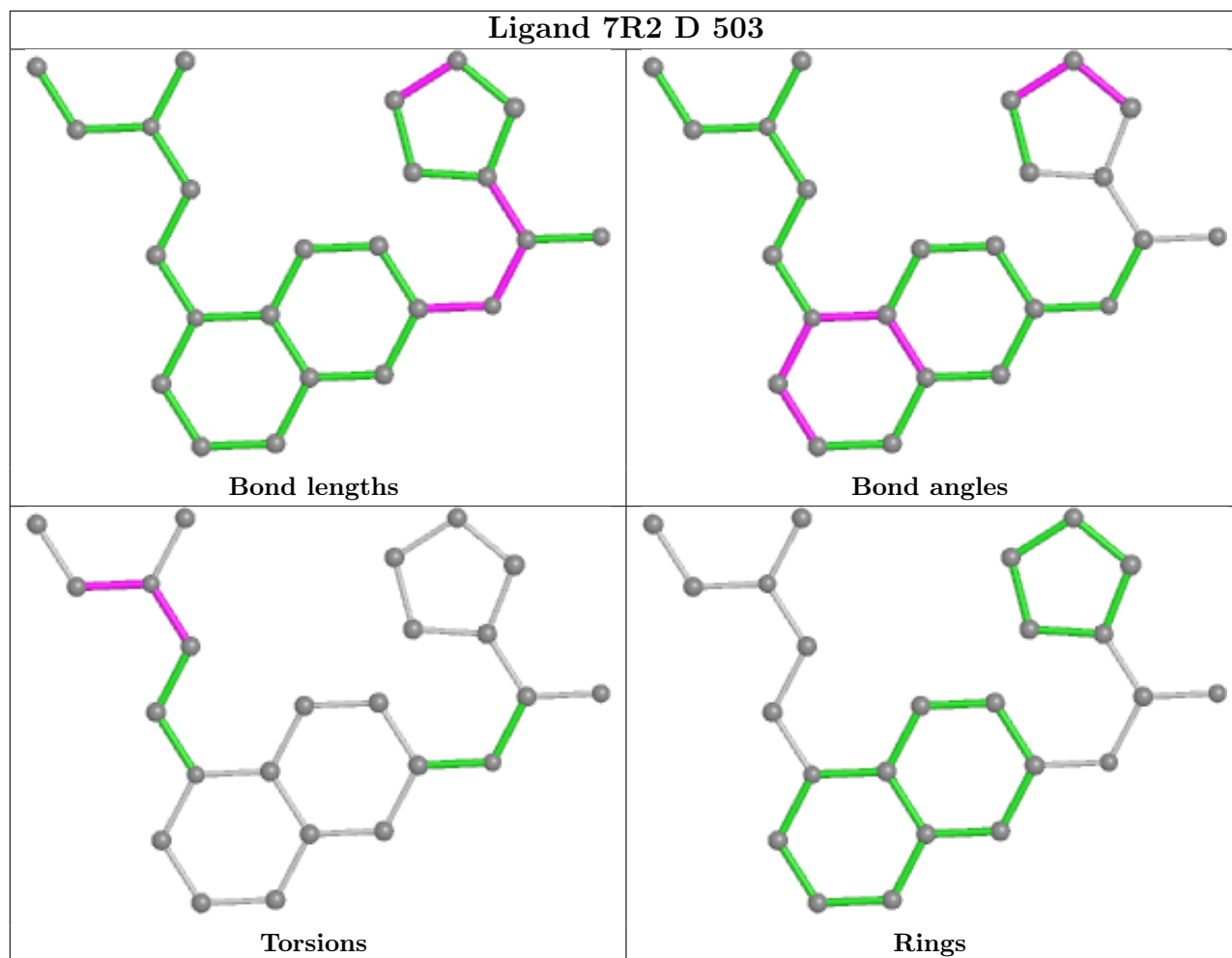
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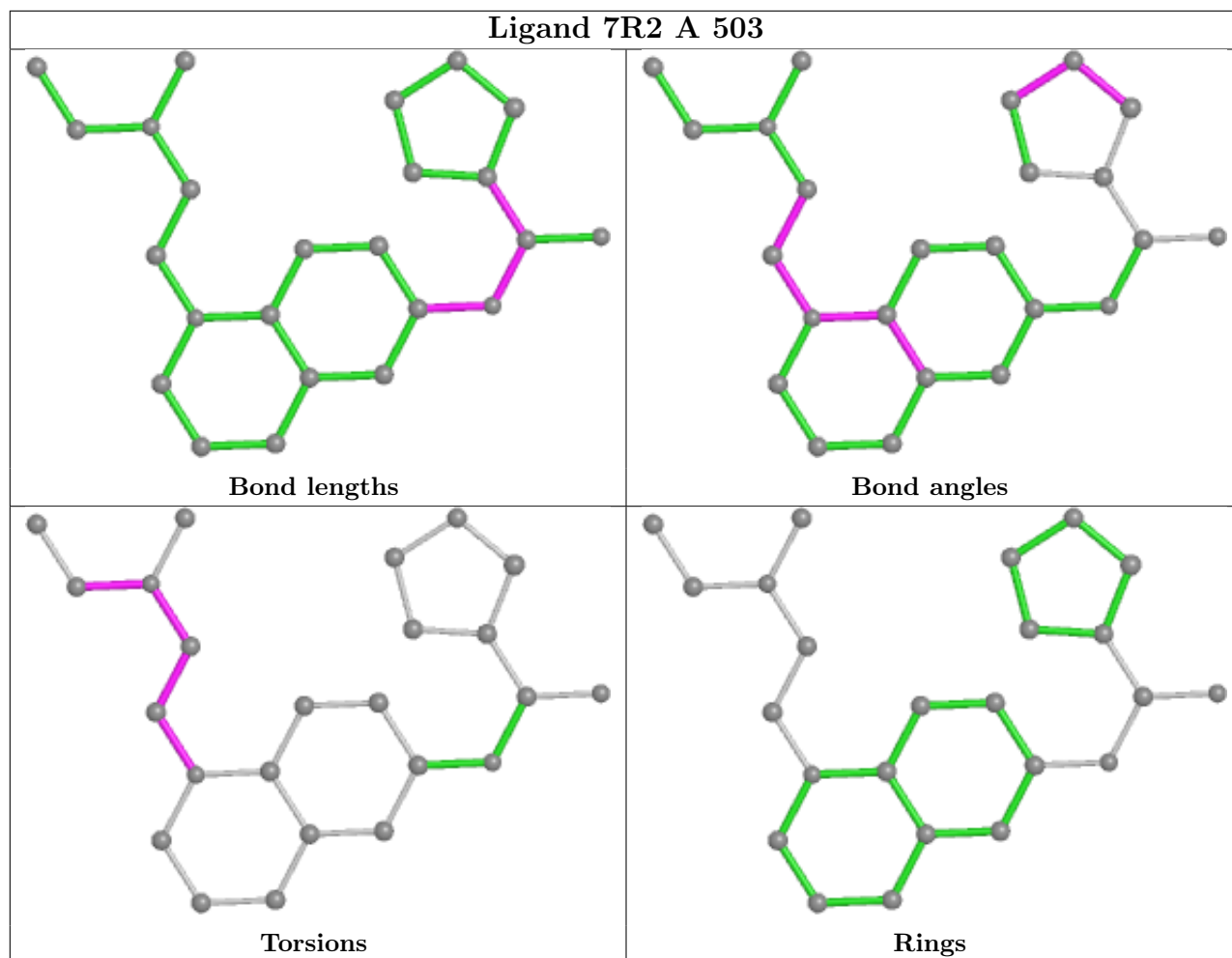
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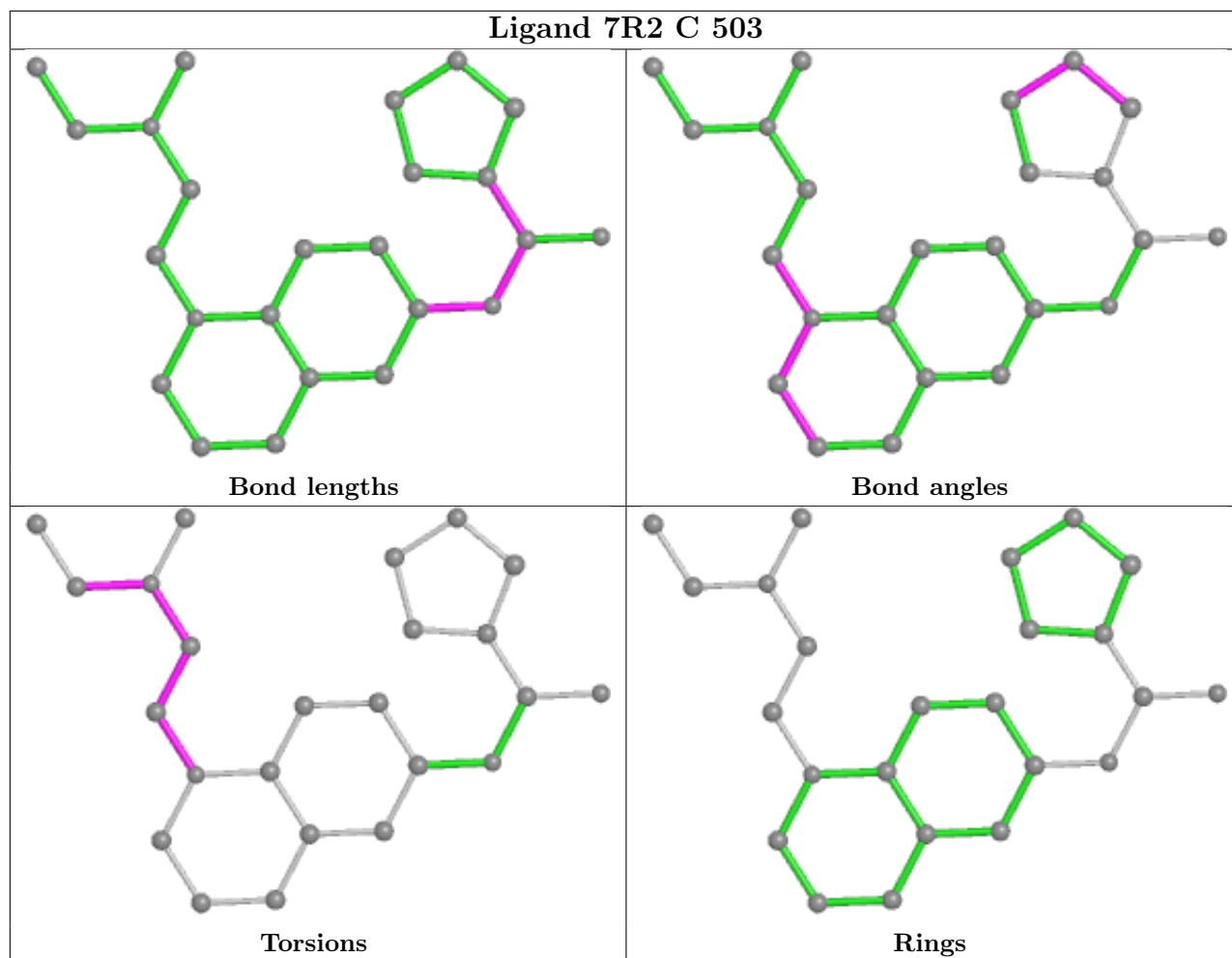
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	7	0
5	C	505	BTB	2	0
2	C	501	HEM	3	0
5	A	504	BTB	1	0
5	C	504	BTB	5	0
5	B	505	BTB	4	0
5	B	504	BTB	2	0
5	A	506	BTB	3	0

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.

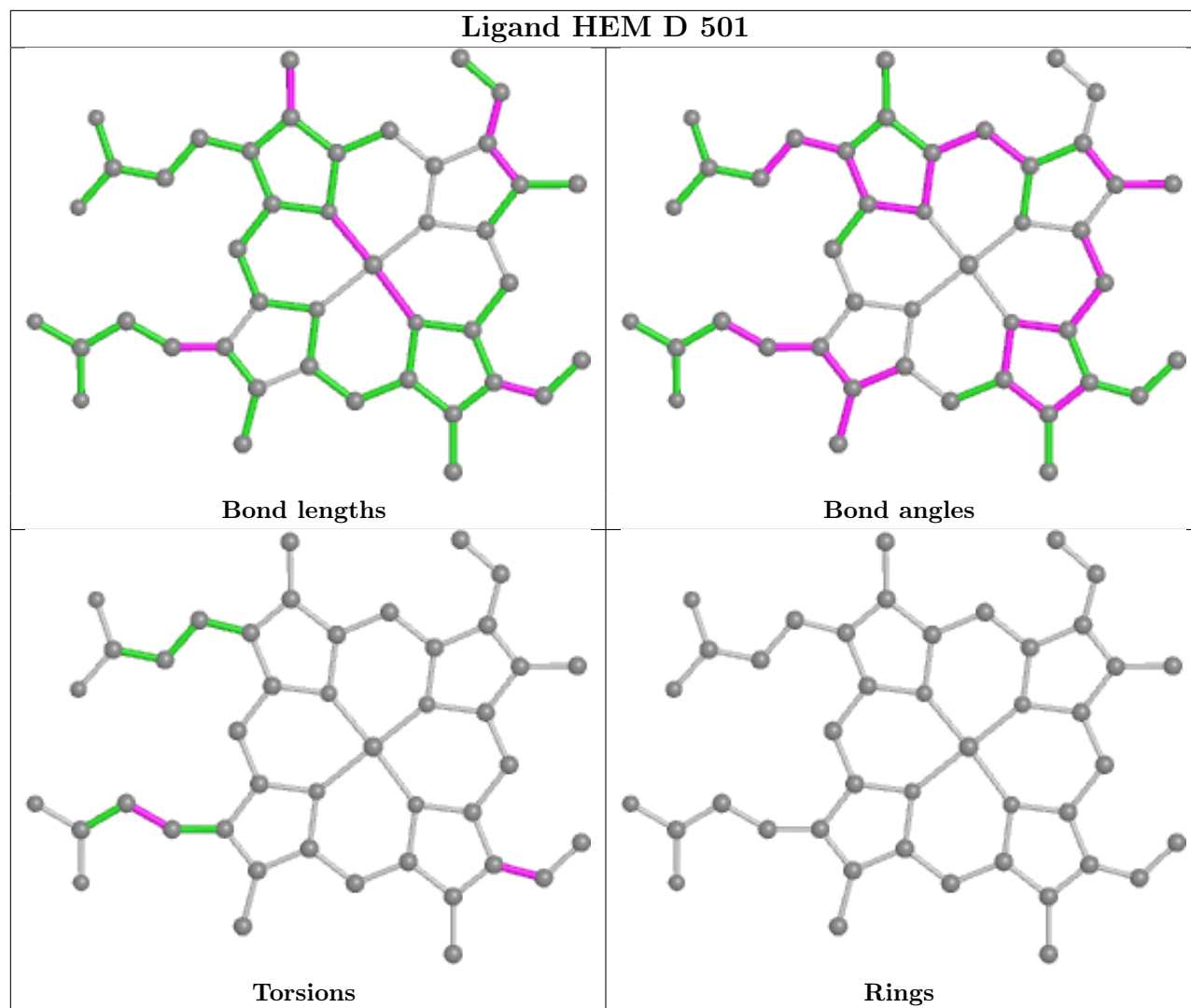


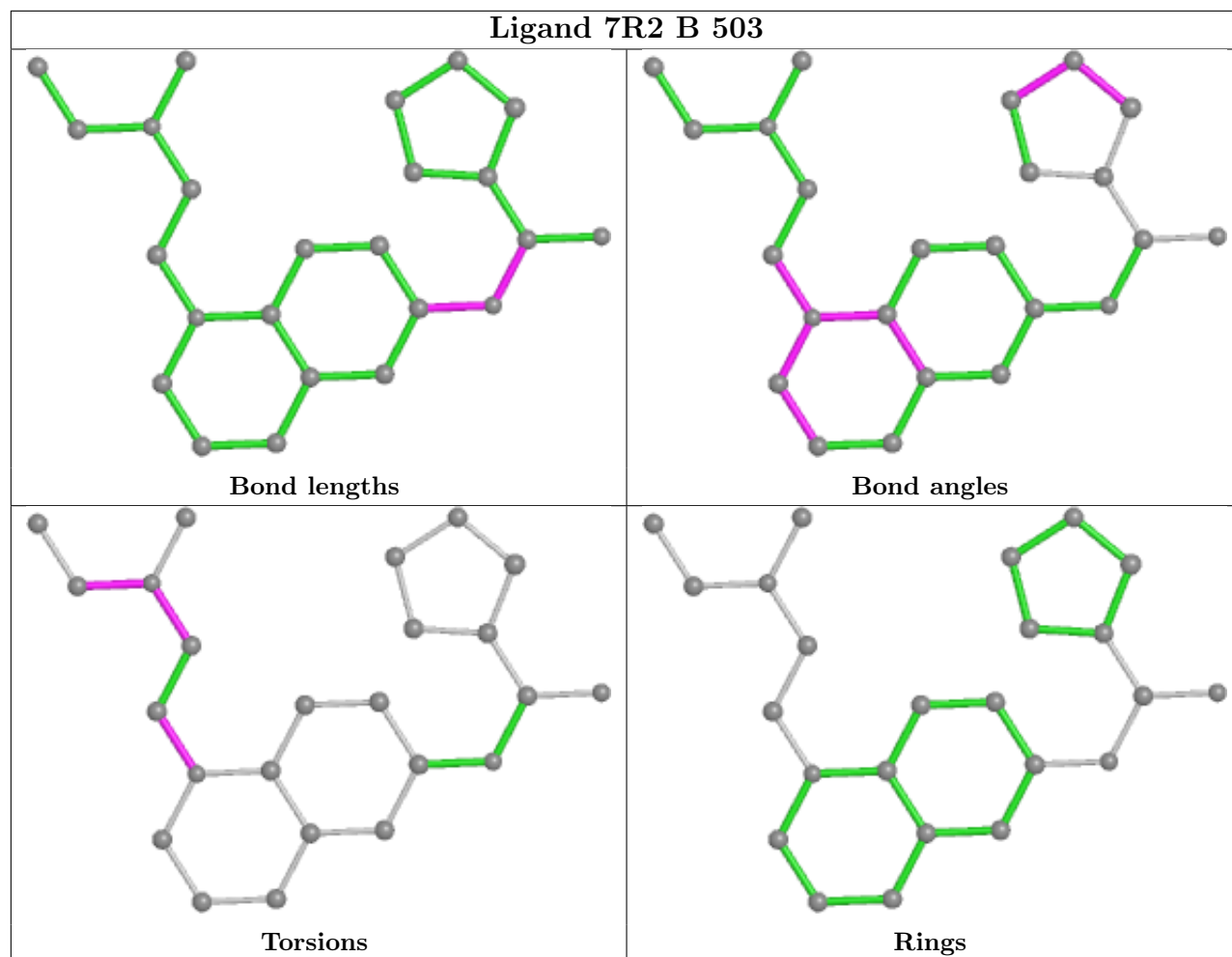


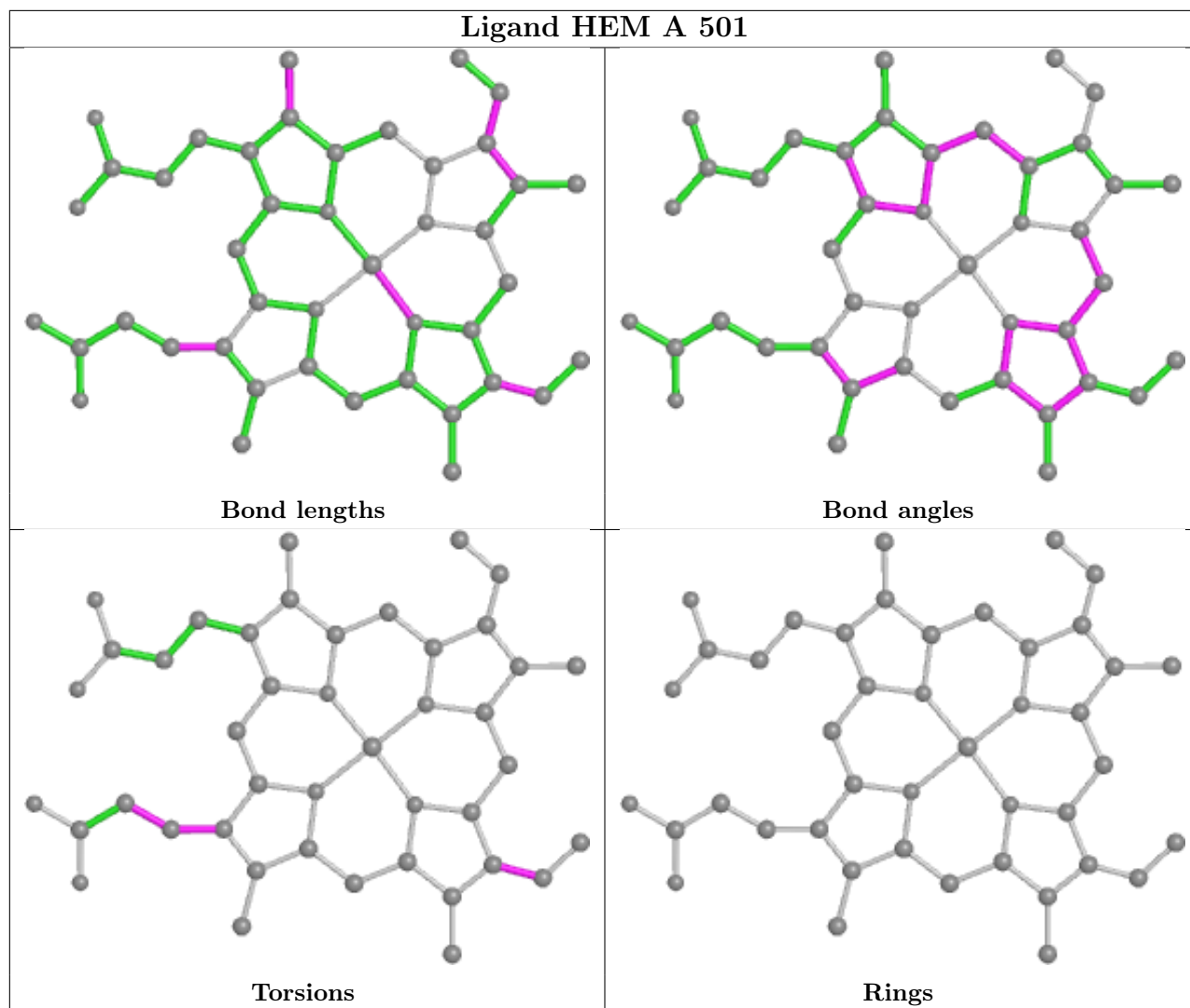


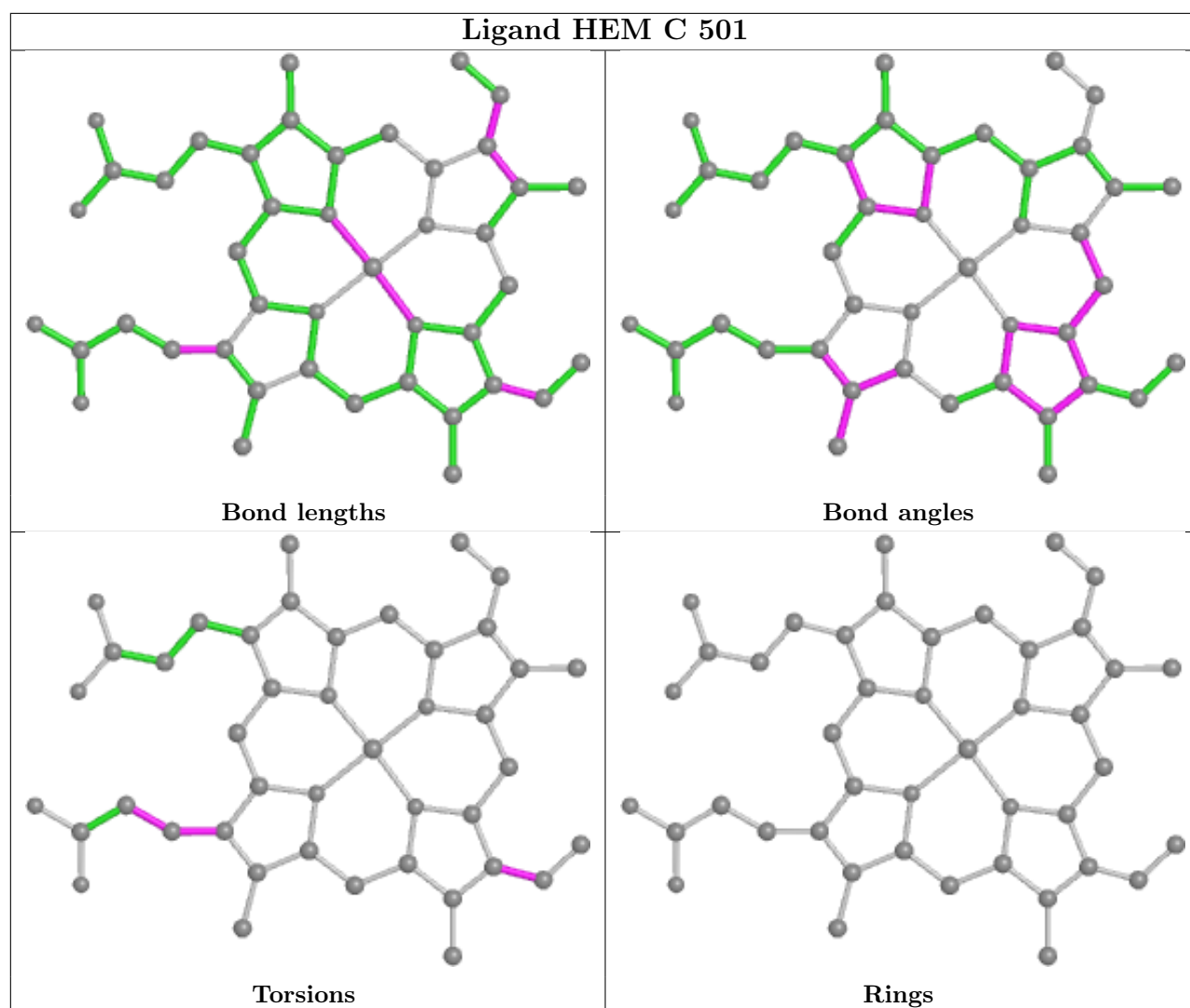












## 5.7 Other polymers [i](#)

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%)	0.70	43 (10%) <b>6</b> <b>9</b>	31, 69, 125, 149	0
1	B	402/440 (91%)	0.16	9 (2%) 62 70	27, 47, 88, 120	0
1	C	401/440 (91%)	0.39	19 (4%) 31 41	32, 62, 102, 125	0
1	D	402/440 (91%)	0.07	5 (1%) 79 84	28, 46, 75, 107	0
All	All	1606/1760 (91%)	0.33	76 (4%) 31 41	27, 55, 109, 149	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	6.8
1	A	480	TRP	6.6
1	A	244	TRP	6.3
1	A	204	ALA	6.0
1	D	89	GLN	5.9
1	A	293	LEU	5.1
1	B	259	GLY	5.1
1	A	259	GLY	5.0
1	C	238	ARG	5.0
1	B	257	GLN	4.7
1	A	346	LEU	4.3
1	C	130	PHE	4.2
1	A	163	TYR	4.0
1	A	89	GLN	3.9
1	C	480	TRP	3.8
1	A	202	ARG	3.7
1	B	141[A]	SER	3.7
1	A	280	THR	3.6
1	A	142	GLY	3.4
1	A	341	LEU	3.4
1	A	120	PRO	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	121	GLU	3.3
1	C	468	PHE	3.3
1	A	107	ARG	3.3
1	A	254	TYR	3.3
1	C	134	TYR	3.2
1	A	238	ARG	3.1
1	A	345	GLY	3.1
1	A	134	TYR	3.1
1	A	242	ARG	3.1
1	D	67	LYS	2.9
1	B	202	ARG	2.9
1	C	292	LEU	2.9
1	B	68	PHE	2.9
1	A	268	VAL	2.9
1	C	202	ARG	2.8
1	C	257	GLN	2.8
1	C	204	ALA	2.7
1	A	473	PHE	2.7
1	A	262	ARG	2.6
1	A	350	ALA	2.6
1	A	171	VAL	2.6
1	C	305	LEU	2.6
1	A	279	TRP	2.6
1	A	130	PHE	2.6
1	A	131	ILE	2.6
1	C	343	ILE	2.6
1	C	293	LEU	2.5
1	B	150	LEU	2.5
1	A	281	PRO	2.5
1	C	131	ILE	2.4
1	A	207	MET	2.4
1	C	144	GLN	2.4
1	A	106	PRO	2.4
1	C	140	ARG	2.4
1	C	236	PRO	2.4
1	A	468	PHE	2.4
1	B	255	ARG	2.4
1	D	468	PHE	2.3
1	C	244	TRP	2.3
1	A	140	ARG	2.3
1	A	257	GLN	2.3
1	A	205	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	GLN	2.2
1	A	211	ILE	2.2
1	A	285	ARG	2.2
1	A	129	ASP	2.2
1	A	289	LEU	2.1
1	D	202	ARG	2.1
1	A	231	PHE	2.1
1	C	299	PRO	2.1
1	A	141	SER	2.1
1	B	67	LYS	2.1
1	C	258	ASP	2.0
1	D	196	PHE	2.0
1	A	160	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	BTB	A	506	14/14	0.72	0.14	81,104,107,109	0
5	BTB	B	506	14/14	0.77	0.14	85,100,107,108	0
9	GD	A	510	1/1	0.81	0.09	158,158,158,158	0
4	7R2	A	503	24/24	0.83	0.23	67,84,92,94	0
5	BTB	C	506	14/14	0.85	0.13	79,100,104,105	0
4	7R2	C	503	24/24	0.85	0.17	47,76,85,87	0
5	BTB	D	504	14/14	0.86	0.17	57,74,96,101	0
5	BTB	B	505	14/14	0.87	0.19	48,63,78,79	0
7	GOL	C	508	6/6	0.88	0.17	45,59,63,65	0
9	GD	C	510	1/1	0.88	0.10	137,137,137,137	0

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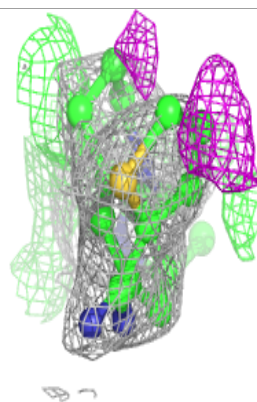
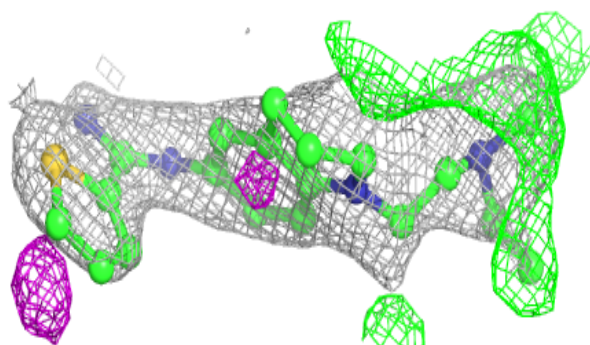
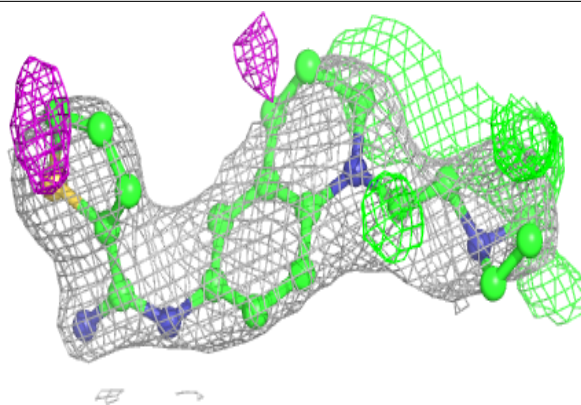
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BTB	D	505	14/14	0.89	0.19	60,70,84,87	0
5	BTB	C	504	14/14	0.90	0.19	51,79,87,93	0
5	BTB	C	505	14/14	0.90	0.23	50,70,79,80	0
4	7R2	B	503	24/24	0.93	0.11	38,59,79,85	0
3	H4B	C	502	17/17	0.93	0.15	40,58,66,67	0
7	GOL	A	508	6/6	0.93	0.16	56,76,89,92	0
5	BTB	A	505	14/14	0.93	0.20	64,71,79,81	0
3	H4B	A	502	17/17	0.93	0.14	56,62,79,82	0
5	BTB	B	504	14/14	0.93	0.12	45,62,83,85	0
4	7R2	D	503	24/24	0.94	0.12	34,60,77,81	0
5	BTB	A	504	14/14	0.94	0.16	61,93,107,114	0
3	H4B	D	502	17/17	0.95	0.11	34,53,66,67	0
3	H4B	B	502	17/17	0.96	0.12	38,49,64,66	0
8	CL	C	509	1/1	0.96	0.06	58,58,58,58	0
2	HEM	C	501	43/43	0.97	0.14	33,53,83,91	0
8	CL	D	506	1/1	0.97	0.08	45,45,45,45	0
2	HEM	A	501	43/43	0.97	0.15	47,65,96,99	0
8	CL	A	509	1/1	0.97	0.06	58,58,58,58	0
2	HEM	D	501	43/43	0.98	0.11	27,38,58,68	0
8	CL	B	507	1/1	0.98	0.07	52,52,52,52	0
2	HEM	B	501	43/43	0.98	0.12	27,37,76,89	0
9	GD	B	508	1/1	0.99	0.16	50,50,50,50	0
6	ZN	A	507	1/1	0.99	0.12	48,48,48,48	0
9	GD	D	507	1/1	0.99	0.15	52,52,52,52	0
6	ZN	C	507	1/1	1.00	0.12	43,43,43,43	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.

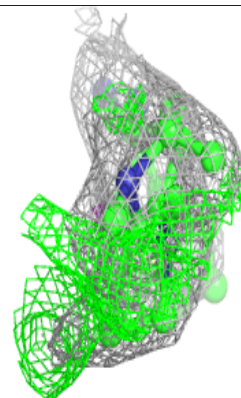
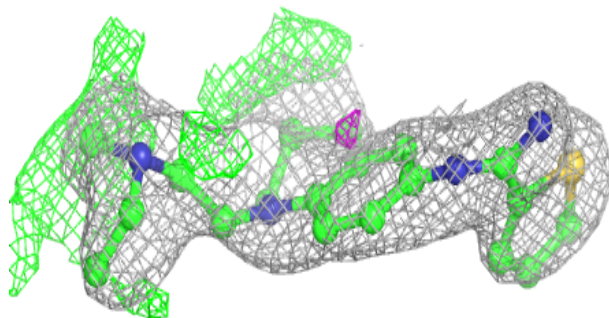
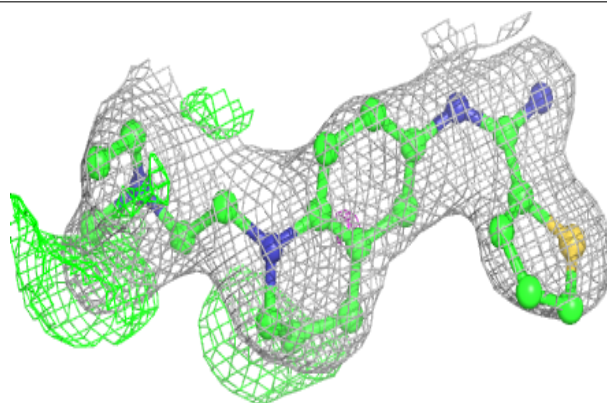


**Electron density around 7R2 A 503:**

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

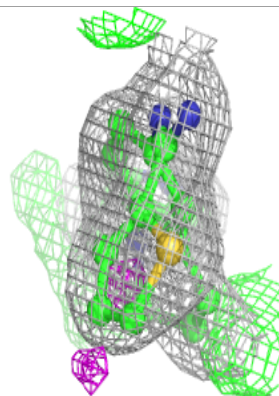
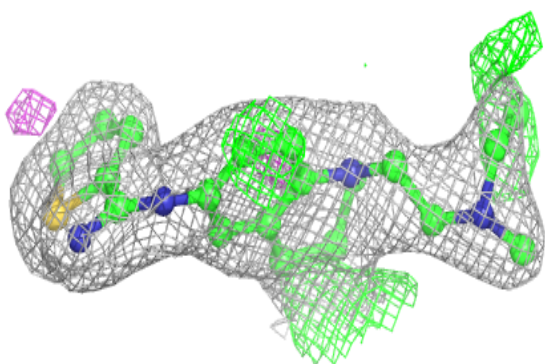
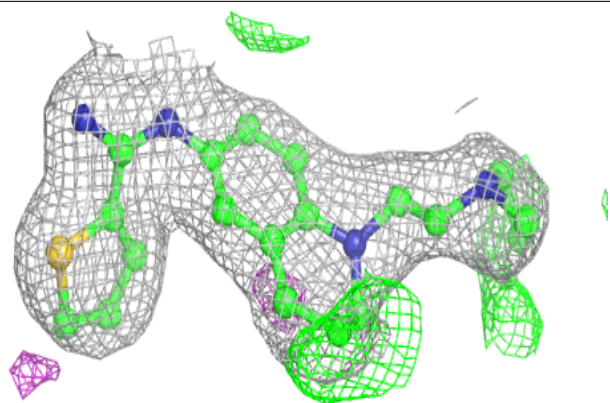
**Electron density around 7R2 C 503:**

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

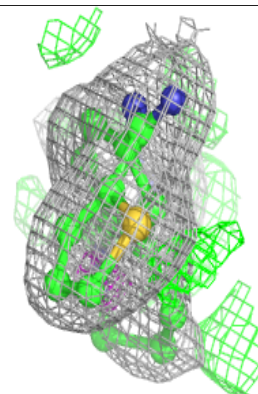
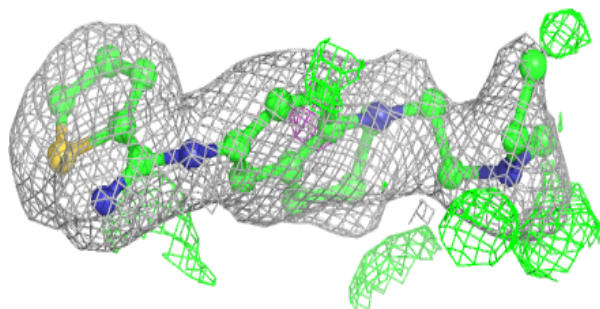
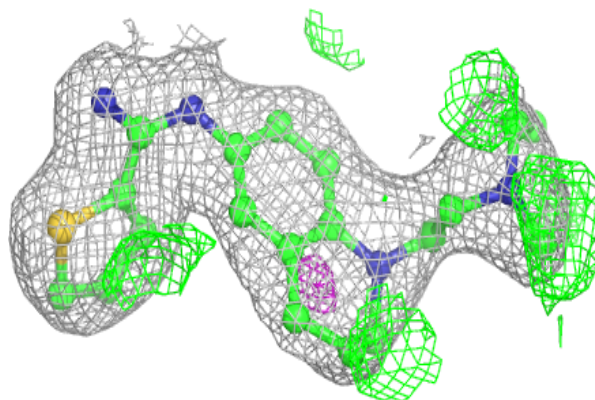


**Electron density around 7R2 B 503:**

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

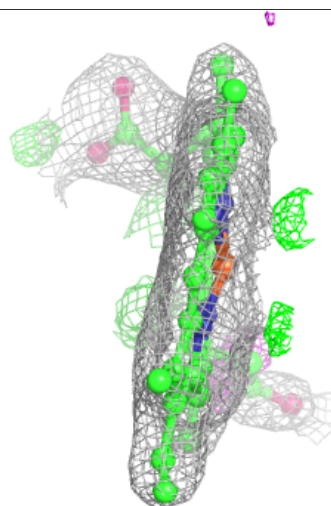
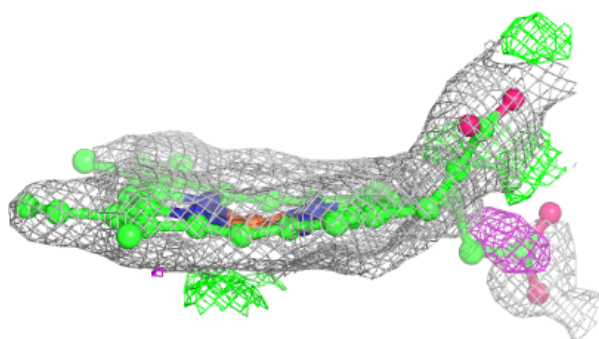
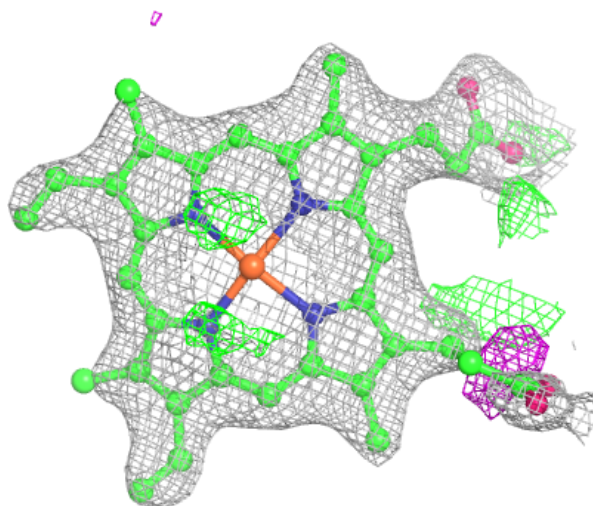
**Electron density around 7R2 D 503:**

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



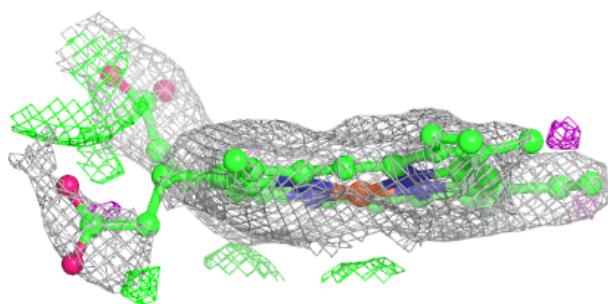
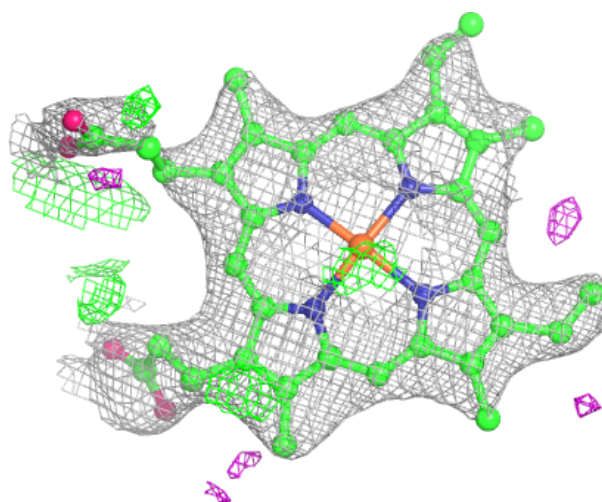
**Electron density around HEM C 501:**

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



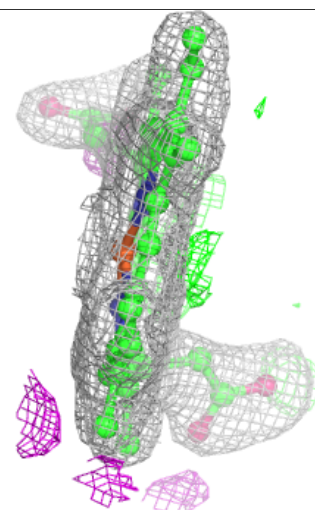
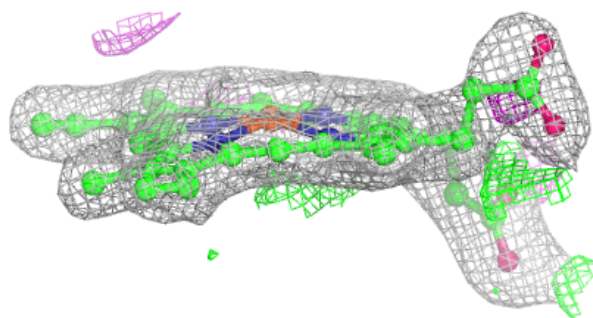
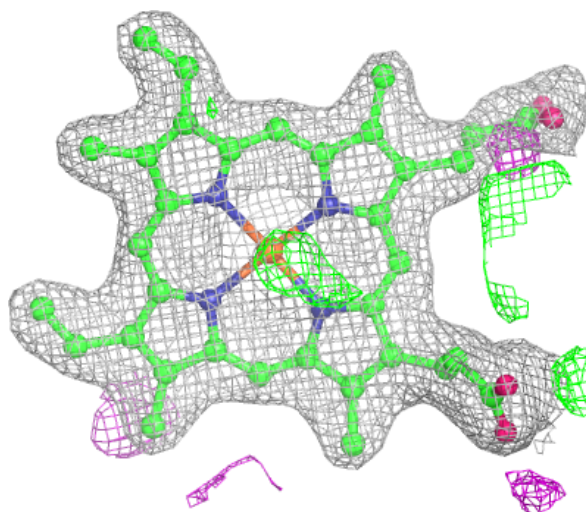
**Electron density around HEM A 501:**

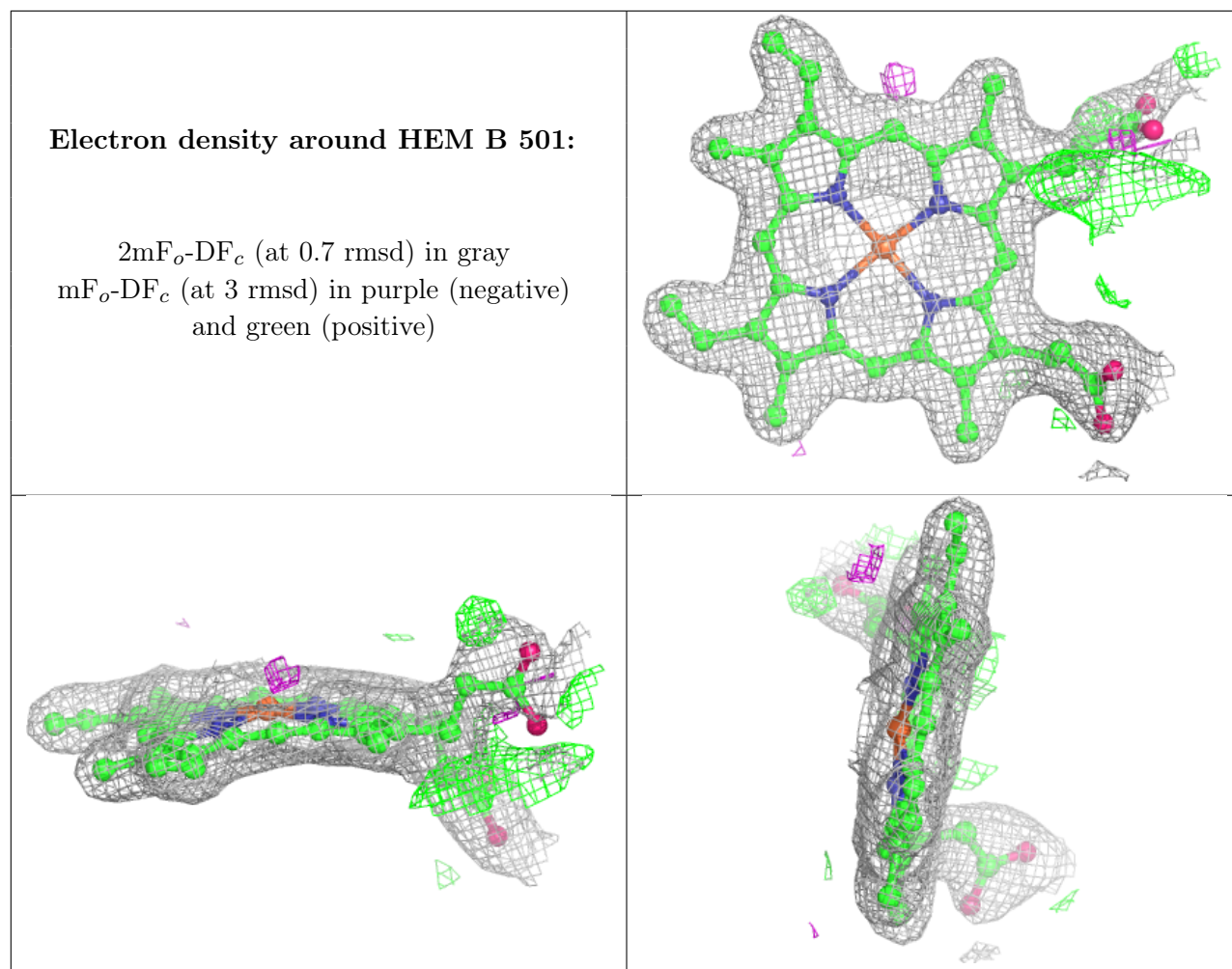
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM D 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.