



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:23 am BST

PDB ID : 2OT4  
Title : Structure of a hexameric multiheme c nitrite reductase from the extremophile bacterium *Thiobacillus nitratireducens*  
Authors : Polyakov, K.M.; Boyko, K.M.; Slutsky, A.; Tikhonova, T.V.; Antipov, A.N.; Zvyagilskaya, R.A.; Popov, A.N.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.  
Deposited on : 2007-02-07  
Resolution : 1.50 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 : 2.11  
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) : 2.11

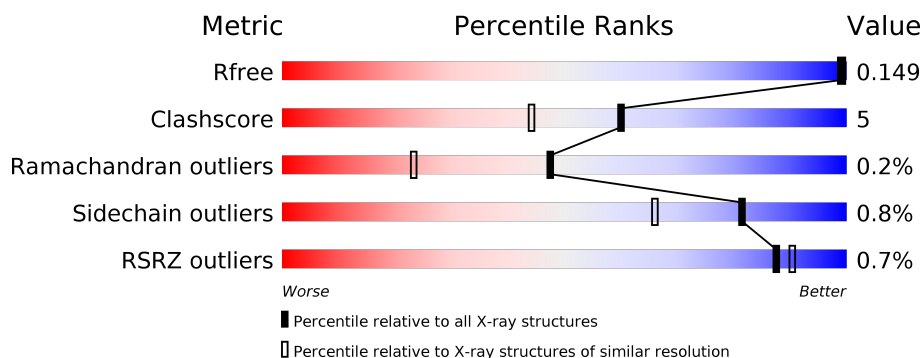
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	525	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7% ..</div> </div> </div>
1	B	525	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6% ..</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19040 atoms, of which 8559 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 Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	520	Total	C	H	N	O	S	1099	32	0
			8158	2605	3946	766	801	40			
1	B	520	Total	C	H	N	O	S	1095	27	0
			8146	2602	3939	764	802	39			

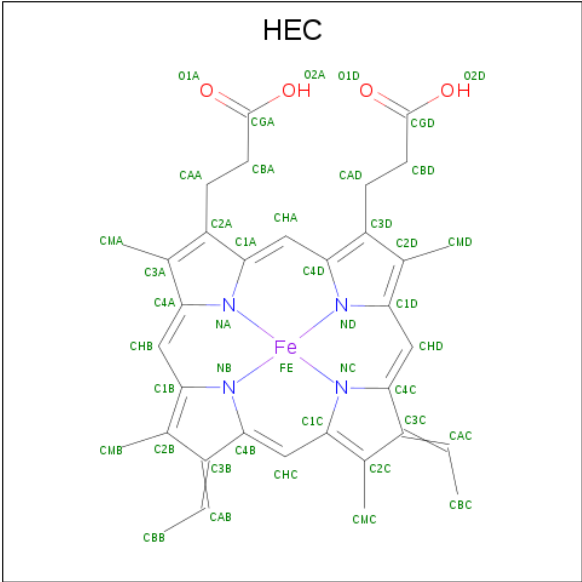
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	GLU	GLN	CONFLICT	UNP Q5F2I3
B	467	GLU	GLN	CONFLICT	UNP Q5F2I3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



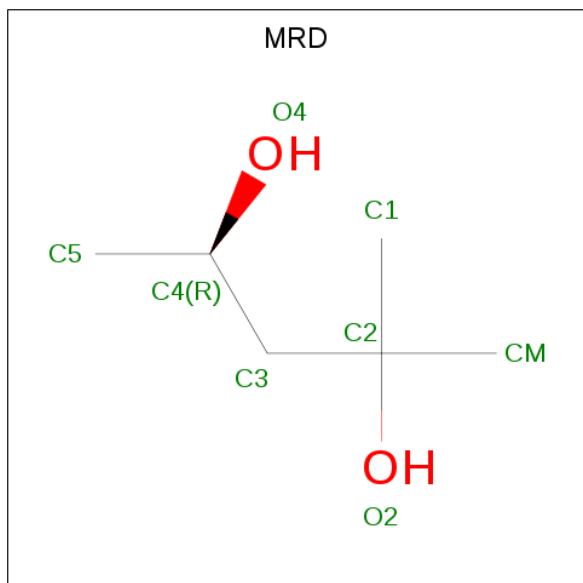
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	36	1
			150	68	2	64	8	8		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	A	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	36	1
			150	68	2	64	8	8		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



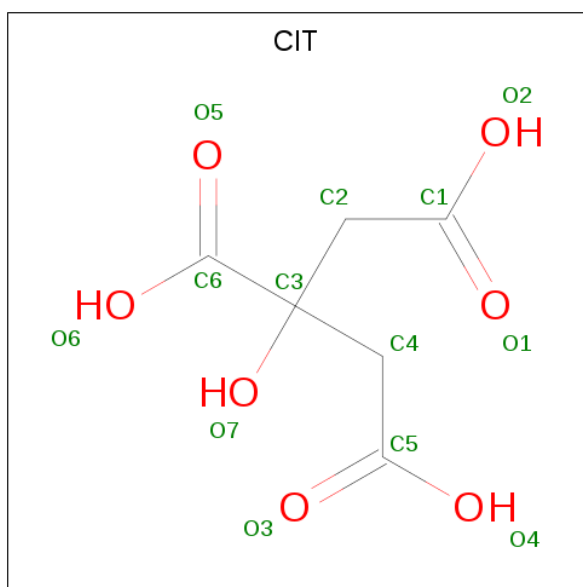
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	10	0
			22	6	14	2		
4	A	1	Total	C	H	O	10	0
			22	6	14	2		
4	B	1	Total	C	H	O	9	0
			21	6	13	2		
4	B	1	Total	C	H	O	10	0
			22	6	14	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	10	0
			22	6	14	2		
5	B	1	Total	C	H	O	10	0
			22	6	14	2		
5	B	1	Total	C	H	O	6	0
			18	6	10	2		

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	1	0
			18	6	5	7		

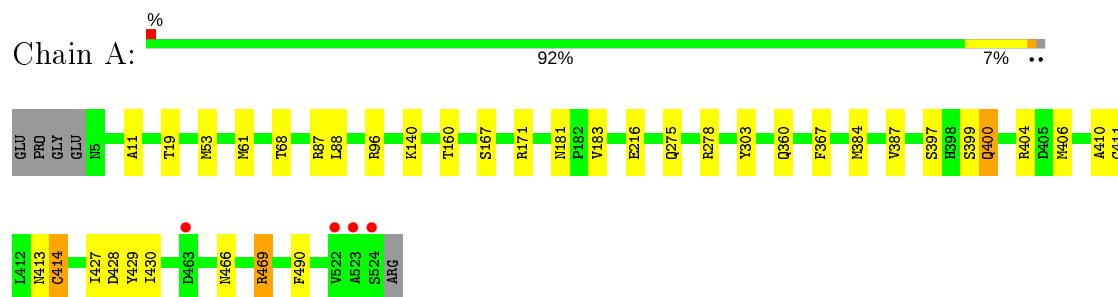
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	601	Total 601	O 601	0	0
7	B	616	Total 616	O 616	0	0

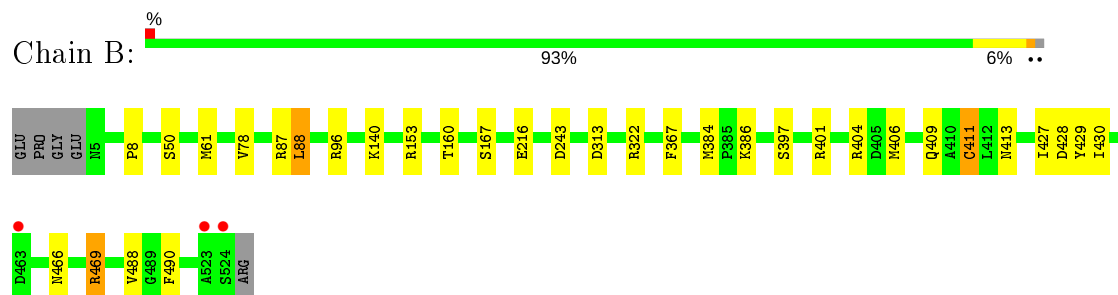
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: Eight-heme nitrite reductase



- Molecule 1: Eight-heme nitrite reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.92Å 193.92Å 193.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.04 – 1.50 23.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.04-1.50) 97.3 (23.87-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.126 , 0.141 0.136 , 0.149	Depositor DCC
$R_{free}$ test set	11295 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	19040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, CIT, CA, HEC

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	0.64	4/4477 (0.1%)	0.81	10/6068 (0.2%)
1	B	0.66	0/4435	0.82	7/6013 (0.1%)
All	All	0.65	4/8912 (0.0%)	0.81	17/12081 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411[A]	CYS	CB-SG	-5.72	1.72	1.81
1	A	411[B]	CYS	CB-SG	-5.72	1.72	1.81
1	A	414[A]	CYS	CB-SG	5.01	1.90	1.82
1	A	414[B]	CYS	CB-SG	5.01	1.90	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	401	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	404	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	404	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	414[A]	CYS	CA-CB-SG	6.21	125.19	114.00
1	A	414[B]	CYS	CA-CB-SG	6.21	125.19	114.00
1	B	243	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	469	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	53[A]	MET	CG-SD-CE	5.64	109.23	100.20
1	A	53[B]	MET	CG-SD-CE	5.64	109.23	100.20
1	B	404	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	469	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	411[A]	CYS	CB-CA-C	-5.16	100.08	110.40
1	A	411[B]	CYS	CB-CA-C	-5.16	100.08	110.40
1	A	387[A]	VAL	CB-CA-C	5.06	121.02	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387[B]	VAL	CB-CA-C	5.06	121.02	111.40
1	B	153	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	4212	3946	3857	27	1
1	B	4207	3939	3895	22	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	387	288	270	19	0
3	B	387	288	270	12	0
4	A	16	28	28	5	0
4	B	16	27	28	7	0
5	A	8	14	14	0	0
5	B	16	24	28	0	0
6	B	13	5	5	1	1
7	A	601	0	0	14	1
7	B	616	0	0	9	0
All	All	10481	8559	8395	82	4

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 5.

All (82) 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)
4:A:2005:MRD:H5C1	7:A:3345:HOH:O	1.32	1.24
4:A:2005:MRD:C5	7:A:3345:HOH:O	1.83	1.21
4:B:2004:MRD:H5C3	4:B:2004:MRD:H1C2	1.25	1.17
1:A:413[A]:ASN:CG	7:A:3263:HOH:O	1.93	1.07
1:A:410[B]:ALA:O	3:A:1008[B]:HEC:HMC2	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413[A]:ASN:OD1	7:A:3263:HOH:O	1.81	0.96
1:A:410[B]:ALA:O	3:A:1008[B]:HEC:CMC	2.15	0.94
4:B:2004:MRD:H5C3	4:B:2004:MRD:C1	2.01	0.89
4:B:2004:MRD:C5	4:B:2004:MRD:H1C2	2.03	0.87
3:A:1008[A]:HEC:HBC3	3:A:1008[A]:HEC:HMC1	1.57	0.85
4:B:2288:MRD:H5C2	4:B:2288:MRD:H1C2	1.58	0.85
3:B:1008[B]:HEC:HBB3	3:B:1008[B]:HEC:HMB1	1.61	0.82
3:A:1002:HEC:HMC1	3:A:1002:HEC:HBC3	1.62	0.80
3:A:1008[A]:HEC:HMC1	3:A:1008[A]:HEC:CBC	2.14	0.78
3:A:1008[B]:HEC:HBD2	3:A:1008[B]:HEC:HMD1	1.67	0.77
1:B:386:LYS:NZ	7:B:2672:HOH:O	2.13	0.77
3:B:1002:HEC:HBC3	3:B:1002:HEC:HMC1	1.68	0.76
3:A:1008[B]:HEC:HMC1	3:A:1008[B]:HEC:HBC3	1.71	0.72
6:B:2010:CIT:O3	7:B:2877:HOH:O	2.08	0.71
1:A:410[B]:ALA:O	3:A:1008[B]:HEC:HMC3	1.92	0.69
4:B:2288:MRD:C5	4:B:2288:MRD:H1C2	2.21	0.69
3:A:1008[B]:HEC:HBB3	3:A:1008[B]:HEC:HMB1	1.78	0.63
1:B:428:ASP:HB3	7:B:2881:HOH:O	1.98	0.62
3:B:1008[B]:HEC:HBC3	3:B:1008[B]:HEC:HMC1	1.82	0.61
1:A:68[B]:THR:HG23	7:A:3307:HOH:O	2.01	0.61
1:B:88[A]:LEU:HD13	7:B:2847:HOH:O	2.00	0.60
1:A:399[B]:SER:O	1:A:400[B]:GLN:C	2.40	0.60
1:A:384:MET:HB2	1:A:397:SER:O	2.01	0.60
3:A:1007:HEC:HMC1	3:A:1007:HEC:HBC3	1.84	0.59
1:A:181:ASN:HD22	1:A:183:VAL:H	1.50	0.59
1:A:171[B]:ARG:NH2	7:A:2967:HOH:O	0.72	0.57
3:A:1001:HEC:HBC3	3:A:1001:HEC:HMC1	1.88	0.56
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.04	0.56
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.03	0.56
3:A:1001:HEC:HMB1	3:A:1001:HEC:HBB3	1.87	0.55
1:B:413:ASN:ND2	7:B:2942:HOH:O	2.40	0.55
1:B:384:MET:HB2	1:B:397:SER:O	2.07	0.54
3:A:1004:HEC:HBB3	3:A:1004:HEC:HMB1	1.88	0.54
1:A:11:ALA:HB3	4:A:2005:MRD:H5C2	1.90	0.54
1:A:140:LYS:HG2	1:A:160[A]:THR:HG23	1.89	0.54
1:B:88[A]:LEU:CD1	7:B:2847:HOH:O	2.55	0.54
1:A:19:THR:HG22	7:A:2870:HOH:O	2.07	0.54
1:A:399[B]:SER:O	1:A:400[B]:GLN:O	2.27	0.53
1:B:427:ILE:HD11	3:B:1008[B]:HEC:HBB3	1.92	0.52
1:A:427:ILE:HD11	3:A:1008[B]:HEC:HBB3	1.91	0.52
3:A:1008[A]:HEC:HBD2	3:A:1008[A]:HEC:HMD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.93	0.51
1:B:140:LYS:HG2	1:B:160[A]:THR:HG23	1.92	0.51
1:A:68[B]:THR:CG2	7:A:3307:HOH:O	2.58	0.50
3:B:1008[A]:HEC:HMC1	3:B:1008[A]:HEC:CBC	2.40	0.50
1:A:413[A]:ASN:ND2	7:A:3263:HOH:O	2.34	0.50
1:B:167:SER:HB2	1:B:216[B]:GLU:HG3	1.94	0.49
1:A:303:TYR:OH	1:A:360[B]:GLN:NE2	2.45	0.48
3:B:1001:HEC:HMB1	3:B:1001:HEC:HBB3	1.94	0.48
3:A:1002:HEC:CBC	3:A:1002:HEC:HMC1	2.40	0.48
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.96	0.48
3:B:1004:HEC:HBB3	3:B:1004:HEC:HMB1	1.96	0.47
1:A:430:ILE:HG21	1:A:490:PHE:HA	1.97	0.47
4:A:2005:MRD:H5C2	7:A:3345:HOH:O	1.81	0.47
1:B:411[B]:CYS:HA	3:B:1008[B]:HEC:HHC	1.97	0.47
3:B:1007:HEC:HBC3	3:B:1007:HEC:HMC1	1.96	0.46
1:A:88[B]:LEU:HD21	7:A:2949:HOH:O	2.16	0.46
3:B:1003:HEC:HMC1	3:B:1003:HEC:HBC3	1.97	0.45
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.82	0.45
1:A:428:ASP:HB3	7:A:3337:HOH:O	2.16	0.44
4:A:2005:MRD:H1C1	1:B:8:PRO:HG3	1.99	0.43
1:B:413:ASN:HB2	7:B:2936:HOH:O	2.18	0.43
1:A:96[B]:ARG:NH2	7:A:3222:HOH:O	0.67	0.43
4:B:2288:MRD:C5	4:B:2288:MRD:C1	2.93	0.42
3:A:1008[A]:HEC:HBB3	3:A:1008[A]:HEC:HMB1	2.00	0.42
1:A:367:PHE:CZ	3:A:1007:HEC:HMC2	2.55	0.42
1:A:88[B]:LEU:CD2	7:A:2949:HOH:O	2.67	0.42
1:B:160[B]:THR:HG23	7:B:2457:HOH:O	2.19	0.41
1:B:367:PHE:CZ	3:B:1007:HEC:HMC2	2.55	0.41
1:A:167:SER:HB2	1:A:216[A]:GLU:HG2	2.02	0.41
1:B:409[B]:GLN:OE1	7:B:2675:HOH:O	2.22	0.41
1:B:313:ASP:C	4:B:2288:MRD:H5C3	2.41	0.41
1:B:96[B]:ARG:CZ	1:B:488:VAL:HG22	2.50	0.40
3:B:1008[A]:HEC:HBB3	3:B:1008[A]:HEC:HMB1	2.02	0.40
3:A:1003:HEC:HBC3	3:A:1003:HEC:HMC1	2.03	0.40

All (4) 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:A:87:ARG:HH11	1:A:429:TYR:HH[12_565]	1.31	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HH11	1:B:429:TYR:HH[6_456]	1.32	0.28
1:B:50:SER:OG	6:B:2010:CIT:O6[7_555]	2.12	0.08
7:A:3162:HOH:O	7:A:3164:HOH:O[12_565]	2.18	0.02

## 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	551/525 (105%)	523 (95%)	26 (5%)	2 (0%)	34	13
1	B	545/525 (104%)	521 (96%)	22 (4%)	2 (0%)	34	13
All	All	1096/1050 (104%)	1044 (95%)	48 (4%)	4 (0%)	47	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411[A]	CYS
1	B	411[B]	CYS
1	A	400[A]	GLN
1	A	400[B]	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	462/443 (104%)	453 (98%)	9 (2%)	57	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	459/443 (104%)	453 (99%)	6 (1%)	69	44
All	All	921/886 (104%)	906 (98%)	15 (2%)	81	36

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	MET
1	A	61[B]	MET
1	A	61[C]	MET
1	A	278[A]	ARG
1	A	278[B]	ARG
1	A	406[A]	MET
1	A	406[B]	MET
1	A	414[A]	CYS
1	A	414[B]	CYS
1	B	61[A]	MET
1	B	61[B]	MET
1	B	88[A]	LEU
1	B	88[B]	LEU
1	B	406[A]	MET
1	B	406[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	20	GLN
1	A	181	ASN
1	A	190	GLN
1	A	340	GLN
1	A	466	ASN
1	A	495	GLN
1	B	190	GLN
1	B	267	GLN
1	B	340	GLN
1	B	413	ASN
1	B	466	ASN
1	B	495	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	B	1006	1	26,50,50	1.81	6 (23%)	18,82,82	1.80	5 (27%)
4	MRD	B	2004	-	7,7,7	0.36	0	9,10,10	0.77	0
3	HEC	A	1001	1	26,50,50	2.14	6 (23%)	18,82,82	1.56	4 (22%)
4	MRD	B	2288	-	7,7,7	0.26	0	9,10,10	0.74	0
3	HEC	B	1008[A]	1	26,50,50	2.49	4 (15%)	18,82,82	2.07	5 (27%)
3	HEC	B	1008[B]	1	26,50,50	2.56	6 (23%)	18,82,82	1.87	4 (22%)
3	HEC	A	1003	1	26,50,50	2.01	3 (11%)	18,82,82	1.73	5 (27%)
4	MRD	A	2005	-	7,7,7	0.34	0	9,10,10	0.70	0
3	HEC	A	1004	1	26,50,50	2.15	3 (11%)	18,82,82	1.70	4 (22%)
6	CIT	B	2010	-	3,12,12	1.77	1 (33%)	3,17,17	2.76	2 (66%)
5	MPD	B	2002	-	7,7,7	0.31	0	9,10,10	0.81	0
3	HEC	A	1002	1	26,50,50	1.96	5 (19%)	18,82,82	1.56	4 (22%)
3	HEC	A	1006	1	26,50,50	1.96	5 (19%)	18,82,82	1.91	6 (33%)
3	HEC	A	1005	1	26,50,50	2.19	6 (23%)	18,82,82	1.91	7 (38%)
3	HEC	A	1008[B]	1	26,50,50	2.54	5 (19%)	18,82,82	1.73	5 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	A	1008[A]	1	26,50,50	2.60	3 (11%)	18,82,82	1.58	4 (22%)
3	HEC	B	1003	1	26,50,50	1.98	5 (19%)	18,82,82	1.85	5 (27%)
3	HEC	B	1001	1	26,50,50	1.97	4 (15%)	18,82,82	1.66	5 (27%)
5	MPD	B	2040	-	7,7,7	0.25	0	9,10,10	0.72	0
3	HEC	A	1007	1	26,50,50	2.29	3 (11%)	18,82,82	2.23	5 (27%)
3	HEC	B	1002	1	26,50,50	1.80	3 (11%)	18,82,82	1.82	6 (33%)
3	HEC	B	1007	1	26,50,50	2.24	4 (15%)	18,82,82	2.15	6 (33%)
3	HEC	B	1004	1	26,50,50	1.95	4 (15%)	18,82,82	1.76	4 (22%)
5	MPD	A	2001	-	7,7,7	0.28	0	9,10,10	1.01	1 (11%)
3	HEC	B	1005	1	26,50,50	1.95	3 (11%)	18,82,82	1.78	4 (22%)
4	MRD	A	2270	-	7,7,7	0.34	0	9,10,10	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	1006	1	-	0/6/54/54	-
4	MRD	B	2004	-	-	5/5/5/5	-
3	HEC	A	1001	1	-	0/6/54/54	-
4	MRD	B	2288	-	-	1/5/5/5	-
3	HEC	B	1008[A]	1	-	0/6/54/54	-
3	HEC	B	1008[B]	1	-	0/6/54/54	-
3	HEC	A	1003	1	-	0/6/54/54	-
4	MRD	A	2005	-	-	3/5/5/5	-
3	HEC	A	1004	1	-	0/6/54/54	-
6	CIT	B	2010	-	-	0/6/16/16	-
5	MPD	B	2002	-	-	0/5/5/5	-
3	HEC	A	1002	1	-	0/6/54/54	-
3	HEC	A	1006	1	-	0/6/54/54	-
3	HEC	A	1005	1	-	0/6/54/54	-
3	HEC	A	1008[B]	1	-	2/6/54/54	-
3	HEC	A	1008[A]	1	-	2/6/54/54	-
3	HEC	B	1003	1	-	0/6/54/54	-
3	HEC	B	1001	1	-	0/6/54/54	-
5	MPD	B	2040	-	-	1/5/5/5	-
3	HEC	A	1007	1	-	0/6/54/54	-
3	HEC	B	1002	1	-	0/6/54/54	-
3	HEC	B	1007	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	1004	1	-	0/6/54/54	-
5	MPD	A	2001	-	-	0/5/5/5	-
3	HEC	B	1005	1	-	0/6/54/54	-
4	MRD	A	2270	-	-	0/5/5/5	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	HEC	C3B-C2B	-8.16	1.32	1.40
3	B	1008[A]	HEC	C3B-C2B	-8.01	1.32	1.40
3	B	1008[B]	HEC	C3B-C2B	-7.71	1.32	1.40
3	A	1008[B]	HEC	C3B-C2B	-7.62	1.32	1.40
3	A	1008[A]	HEC	C3B-C2B	-7.54	1.32	1.40
3	A	1008[A]	HEC	C3C-C2C	-7.47	1.33	1.40
3	A	1005	HEC	C3B-C2B	-7.26	1.33	1.40
3	B	1007	HEC	C3B-C2B	-7.18	1.33	1.40
3	A	1004	HEC	C3C-C2C	-6.35	1.34	1.40
3	A	1004	HEC	C3B-C2B	-6.23	1.34	1.40
3	A	1001	HEC	C3B-C2B	-6.14	1.34	1.40
3	B	1007	HEC	C3C-C2C	-6.14	1.34	1.40
3	B	1001	HEC	C3C-C2C	-6.12	1.34	1.40
3	A	1003	HEC	C3C-C2C	-6.05	1.34	1.40
3	B	1008[A]	HEC	C3C-C2C	-5.98	1.34	1.40
3	B	1008[B]	HEC	C3C-C2C	-5.85	1.34	1.40
3	A	1002	HEC	C3C-C2C	-5.78	1.34	1.40
3	A	1008[B]	HEC	C3D-C2D	5.74	1.54	1.37
3	A	1001	HEC	C3C-C2C	-5.64	1.34	1.40
3	A	1008[B]	HEC	C3C-C2C	-5.57	1.34	1.40
3	B	1008[B]	HEC	C3D-C2D	5.55	1.54	1.37
3	A	1006	HEC	C3B-C2B	-5.41	1.35	1.40
3	B	1003	HEC	C3B-C2B	-5.40	1.35	1.40
3	B	1004	HEC	C3B-C2B	-5.25	1.35	1.40
3	A	1008[A]	HEC	C3D-C2D	5.09	1.52	1.37
3	B	1002	HEC	C3C-C2C	-5.05	1.35	1.40
3	B	1008[A]	HEC	C3D-C2D	4.93	1.52	1.37
3	B	1005	HEC	C3B-C2B	-4.80	1.35	1.40
3	B	1006	HEC	C3C-C2C	-4.80	1.35	1.40
3	B	1005	HEC	C3C-C2C	-4.75	1.35	1.40
3	A	1006	HEC	C3C-C2C	-4.69	1.35	1.40
3	A	1007	HEC	C3C-C2C	-4.62	1.35	1.40
3	B	1004	HEC	C3C-C2C	-4.60	1.35	1.40
3	B	1003	HEC	C3C-C2C	-4.58	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	HEC	C3B-C2B	-4.39	1.36	1.40
3	A	1005	HEC	C3C-C2C	-4.29	1.36	1.40
3	A	1003	HEC	C3B-C2B	-4.26	1.36	1.40
3	B	1006	HEC	C3B-C2B	-4.09	1.36	1.40
3	B	1001	HEC	C3B-C2B	-3.70	1.36	1.40
3	B	1001	HEC	C3D-C2D	3.69	1.48	1.37
3	A	1003	HEC	C3D-C2D	3.56	1.48	1.37
3	A	1006	HEC	C3D-C2D	3.43	1.47	1.37
3	B	1006	HEC	C3D-C2D	3.39	1.47	1.37
3	A	1005	HEC	C3D-C2D	3.39	1.47	1.37
3	A	1007	HEC	C3D-C2D	3.35	1.47	1.37
3	B	1003	HEC	C3D-C2D	3.31	1.47	1.37
3	A	1001	HEC	C3D-C2D	3.26	1.47	1.37
3	B	1005	HEC	C3D-C2D	3.25	1.47	1.37
3	B	1004	HEC	C3D-C2D	3.13	1.47	1.37
3	B	1002	HEC	C3D-C2D	3.08	1.46	1.37
3	A	1004	HEC	C3D-C2D	3.05	1.46	1.37
3	B	1007	HEC	C3D-C2D	2.96	1.46	1.37
3	A	1002	HEC	C3D-C2D	2.83	1.46	1.37
3	B	1002	HEC	C3B-C2B	-2.56	1.38	1.40
3	A	1005	HEC	C3C-C4C	2.54	1.47	1.43
3	A	1005	HEC	C3B-C4B	2.39	1.47	1.43
3	A	1005	HEC	C1D-ND	2.35	1.41	1.36
3	A	1008[B]	HEC	C4D-ND	2.32	1.40	1.36
3	B	1004	HEC	C4D-ND	2.29	1.40	1.36
3	B	1006	HEC	C3C-C4C	2.27	1.47	1.43
3	A	1002	HEC	C1B-NB	2.25	1.40	1.36
3	A	1001	HEC	C1D-ND	2.25	1.40	1.36
3	B	1003	HEC	C4D-CHA	-2.23	1.34	1.41
3	A	1008[B]	HEC	CAD-C3D	2.21	1.55	1.52
3	B	1003	HEC	C3C-C4C	2.20	1.47	1.43
3	B	1008[B]	HEC	C4D-ND	2.19	1.40	1.36
3	B	1006	HEC	C4D-ND	2.18	1.40	1.36
3	A	1006	HEC	C3C-C4C	2.15	1.47	1.43
3	A	1001	HEC	CBB-CAB	2.14	1.57	1.49
3	A	1001	HEC	C4D-ND	2.13	1.40	1.36
3	B	1008[B]	HEC	C1D-ND	2.08	1.40	1.36
3	B	1001	HEC	C4D-ND	2.08	1.40	1.36
3	A	1006	HEC	CBB-CAB	2.08	1.57	1.49
3	B	1007	HEC	C3B-C4B	2.05	1.46	1.43
6	B	2010	CIT	C2-C3	-2.04	1.52	1.54
3	B	1008[B]	HEC	C3C-C4C	2.02	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1006	HEC	C1D-CHD	-2.01	1.35	1.41
3	A	1002	HEC	CMB-C2B	2.00	1.56	1.51
3	B	1008[A]	HEC	C1D-CHD	-2.00	1.35	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1007	HEC	CMB-C2B-C1B	-6.24	118.88	128.46
3	B	1007	HEC	CMB-C2B-C1B	-5.22	120.44	128.46
3	B	1003	HEC	CMB-C2B-C1B	-4.59	121.41	128.46
3	A	1008[B]	HEC	CMC-C2C-C1C	-4.56	121.45	128.46
3	A	1005	HEC	CMB-C2B-C1B	-4.33	121.81	128.46
3	B	1008[B]	HEC	CMC-C2C-C1C	-4.24	121.95	128.46
3	B	1006	HEC	CMC-C2C-C1C	-4.19	122.02	128.46
3	B	1005	HEC	CMB-C2B-C1B	-4.18	122.04	128.46
3	A	1002	HEC	CMB-C2B-C1B	-4.05	122.25	128.46
3	B	1005	HEC	CMB-C2B-C3B	4.04	130.57	125.82
3	A	1004	HEC	CMB-C2B-C1B	-3.88	122.49	128.46
3	B	1002	HEC	CAA-CBA-CGA	-3.87	106.18	112.67
3	A	1007	HEC	CMB-C2B-C3B	3.83	130.32	125.82
3	B	1008[A]	HEC	C1D-C2D-C3D	-3.80	104.35	107.00
3	A	1003	HEC	CMB-C2B-C1B	-3.72	122.74	128.46
3	B	1008[A]	HEC	CMC-C2C-C1C	-3.68	122.81	128.46
3	B	1008[A]	HEC	CMC-C2C-C3C	3.62	130.07	125.82
3	A	1006	HEC	CMC-C2C-C1C	-3.58	122.95	128.46
3	B	1008[B]	HEC	CBD-CAD-C3D	-3.58	105.88	112.49
6	B	2010	CIT	C3-C4-C5	-3.57	109.27	114.98
3	B	1004	HEC	CMB-C2B-C1B	-3.52	123.05	128.46
3	B	1007	HEC	CBD-CAD-C3D	-3.48	106.07	112.49
3	B	1004	HEC	CMC-C2C-C1C	-3.45	123.17	128.46
3	B	1008[A]	HEC	CBD-CAD-C3D	-3.43	106.16	112.49
3	A	1007	HEC	CBD-CAD-C3D	-3.43	106.17	112.49
3	A	1008[A]	HEC	CBA-CAA-C2A	-3.42	106.17	112.48
3	A	1006	HEC	CMB-C2B-C1B	-3.42	123.21	128.46
3	A	1001	HEC	CMB-C2B-C1B	-3.42	123.21	128.46
3	A	1005	HEC	CMB-C2B-C3B	3.38	129.80	125.82
3	B	1007	HEC	CMB-C2B-C3B	3.32	129.73	125.82
3	B	1002	HEC	CMB-C2B-C1B	-3.28	123.43	128.46
3	B	1004	HEC	CMB-C2B-C3B	3.25	129.65	125.82
3	B	1006	HEC	CMB-C2B-C1B	-3.25	123.47	128.46
3	B	1008[A]	HEC	CBA-CAA-C2A	-3.18	106.62	112.48
3	B	1002	HEC	CMC-C2C-C1C	-3.17	123.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1005	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
3	B	1007	HEC	CMC-C2C-C1C	-3.16	123.61	128.46
3	A	1007	HEC	C1D-C2D-C3D	-3.13	104.82	107.00
6	B	2010	CIT	C3-C2-C1	-3.07	110.07	114.98
3	A	1008[A]	HEC	C1D-C2D-C3D	-3.04	104.88	107.00
3	A	1006	HEC	CMB-C2B-C3B	2.96	129.30	125.82
3	A	1004	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
3	A	1003	HEC	CMC-C2C-C1C	-2.94	123.95	128.46
3	B	1005	HEC	CMC-C2C-C1C	-2.93	123.96	128.46
3	B	1001	HEC	CMC-C2C-C1C	-2.92	123.97	128.46
3	B	1003	HEC	CMB-C2B-C3B	2.90	129.23	125.82
3	A	1004	HEC	CMB-C2B-C3B	2.87	129.19	125.82
3	B	1007	HEC	C1D-C2D-C3D	-2.86	105.00	107.00
3	A	1006	HEC	CMC-C2C-C3C	2.86	129.18	125.82
3	B	1001	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
3	A	1004	HEC	CMC-C2C-C1C	-2.80	124.16	128.46
3	B	1008[B]	HEC	CMC-C2C-C3C	-2.80	122.53	125.82
3	A	1002	HEC	CMB-C2B-C3B	2.80	129.11	125.82
3	A	1001	HEC	CAD-CBD-CGD	-2.77	108.03	112.67
3	A	1001	HEC	CMC-C2C-C1C	-2.68	124.34	128.46
5	A	2001	MPD	CM-C2-C1	-2.66	105.02	110.57
3	A	1002	HEC	CAA-CBA-CGA	-2.63	108.25	112.67
3	B	1001	HEC	CBD-CAD-C3D	-2.62	107.65	112.49
3	B	1008[B]	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
3	B	1003	HEC	C1D-C2D-C3D	-2.56	105.21	107.00
3	B	1006	HEC	CMA-C3A-C2A	2.56	129.76	124.94
3	A	1005	HEC	CMC-C2C-C3C	2.55	128.82	125.82
3	B	1006	HEC	CMC-C2C-C3C	2.55	128.82	125.82
3	B	1005	HEC	CMA-C3A-C2A	2.55	129.74	124.94
3	B	1003	HEC	CMC-C2C-C1C	-2.54	124.56	128.46
3	A	1003	HEC	CBA-CAA-C2A	-2.54	107.80	112.48
3	B	1004	HEC	C1D-C2D-C3D	-2.52	105.24	107.00
3	A	1003	HEC	CMC-C2C-C3C	2.49	128.75	125.82
3	B	1002	HEC	CAD-CBD-CGD	2.49	116.84	112.67
3	B	1003	HEC	CBA-CAA-C2A	-2.47	107.93	112.48
3	A	1008[B]	HEC	CBA-CAA-C2A	-2.46	107.95	112.48
3	A	1006	HEC	CMA-C3A-C2A	2.44	129.55	124.94
3	A	1008[B]	HEC	CMD-C2D-C1D	-2.40	124.77	128.46
3	B	1002	HEC	CMC-C2C-C3C	2.36	128.59	125.82
3	B	1002	HEC	CMB-C2B-C3B	2.35	128.59	125.82
3	A	1006	HEC	CBD-CAD-C3D	-2.28	108.28	112.49
3	B	1007	HEC	CMA-C3A-C2A	2.27	129.21	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1008[A]	HEC	C4B-C3B-C2B	2.25	108.78	106.35
3	B	1001	HEC	C3C-C4C-NC	-2.22	106.75	110.94
3	A	1005	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
3	B	1006	HEC	CBD-CAD-C3D	-2.15	108.53	112.49
3	A	1001	HEC	CMC-C2C-C3C	2.14	128.34	125.82
3	A	1008[A]	HEC	CMD-C2D-C3D	2.14	128.97	124.94
3	A	1005	HEC	CAD-CBD-CGD	-2.11	109.14	112.67
3	A	1003	HEC	CMA-C3A-C2A	2.10	128.90	124.94
3	B	1001	HEC	C4C-C3C-C2C	2.10	108.62	106.35
3	A	1002	HEC	CAD-CBD-CGD	2.09	116.17	112.67
3	A	1007	HEC	CBA-CAA-C2A	-2.07	108.67	112.48
3	A	1005	HEC	CMA-C3A-C2A	2.05	128.81	124.94
3	A	1008[B]	HEC	CMD-C2D-C3D	2.05	128.81	124.94
3	A	1008[B]	HEC	CMB-C2B-C1B	-2.02	125.36	128.46

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2004	MRD	C1-C2-C3-C4
4	B	2004	MRD	O2-C2-C3-C4
4	B	2004	MRD	C2-C3-C4-O4
4	B	2004	MRD	C2-C3-C4-C5
4	A	2005	MRD	C1-C2-C3-C4
4	A	2005	MRD	O2-C2-C3-C4
3	A	1008[B]	HEC	C2D-C3D-CAD-CBD
3	A	1008[B]	HEC	C4D-C3D-CAD-CBD
3	A	1008[A]	HEC	C2D-C3D-CAD-CBD
3	A	1008[A]	HEC	C4D-C3D-CAD-CBD
4	B	2004	MRD	CM-C2-C3-C4
4	B	2288	MRD	C2-C3-C4-C5
4	A	2005	MRD	C2-C3-C4-C5
5	B	2040	MPD	C2-C3-C4-O4

There are no ring outliers.

18 monomers are involved in 45 short contacts:

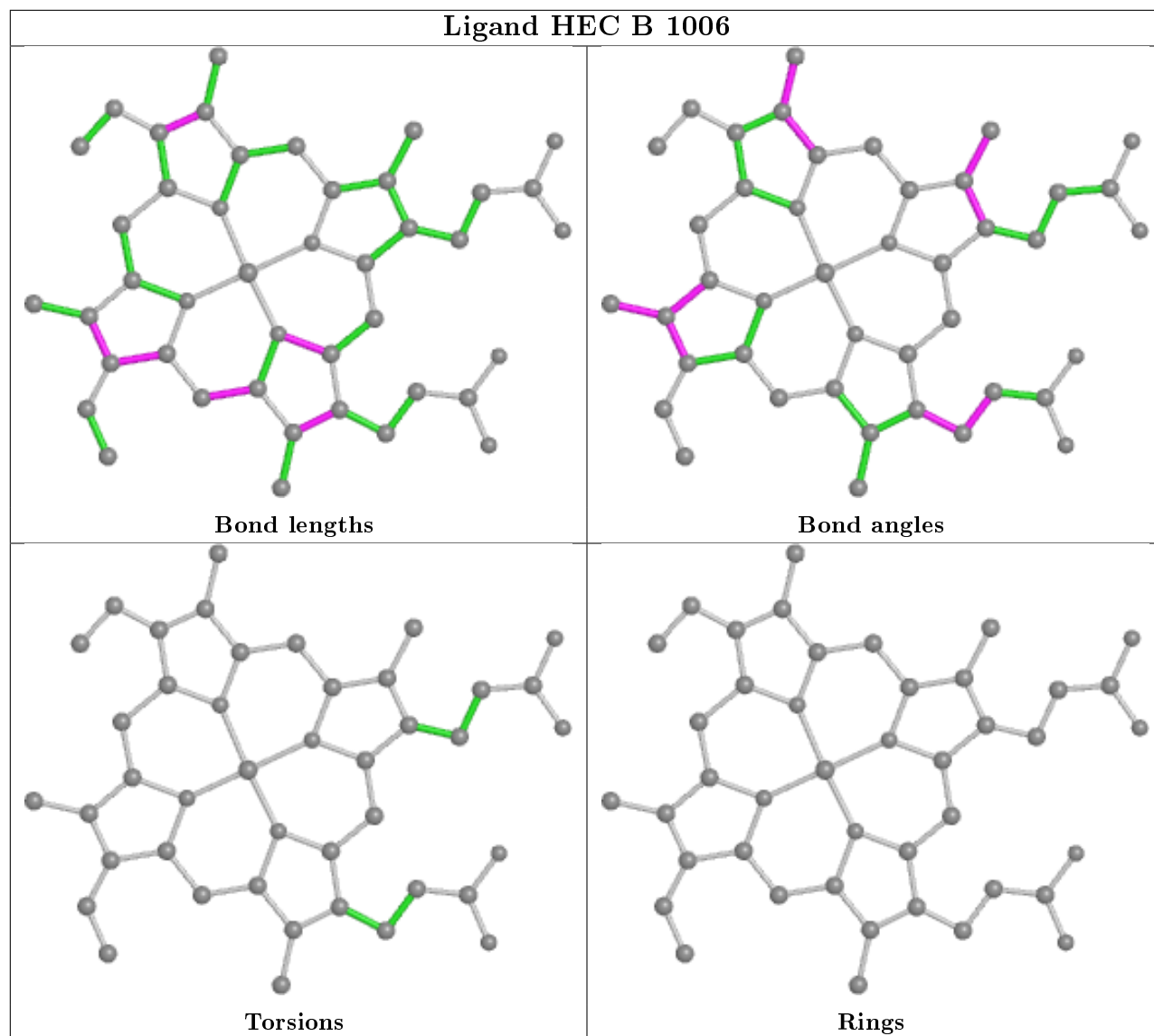
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2004	MRD	3	0
3	A	1001	HEC	2	0
4	B	2288	MRD	4	0

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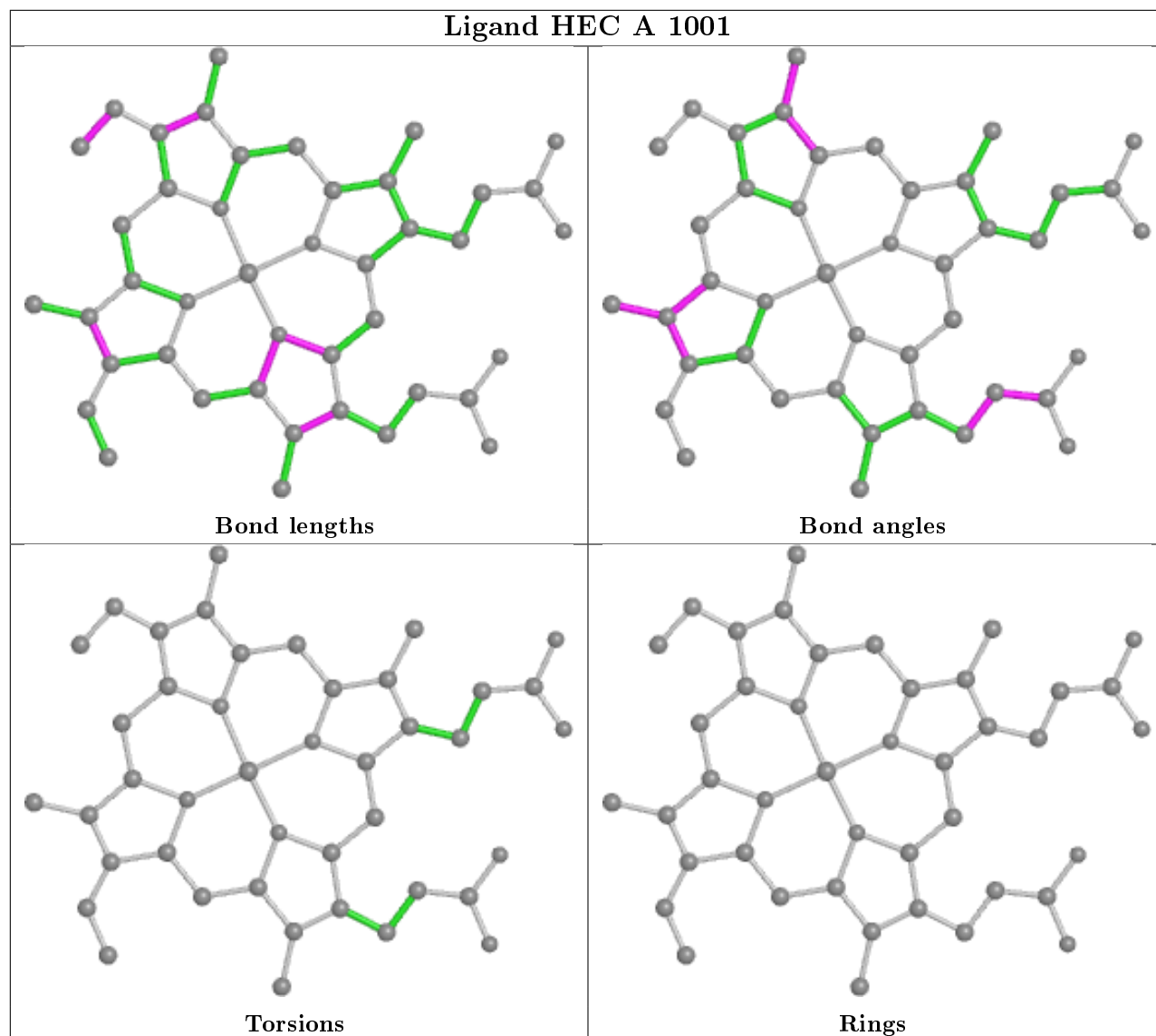
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1008[A]	HEC	2	0
3	B	1008[B]	HEC	4	0
3	A	1003	HEC	1	0
4	A	2005	MRD	5	0
3	A	1004	HEC	1	0
6	B	2010	CIT	1	1
3	A	1002	HEC	2	0
3	A	1008[B]	HEC	7	0
3	A	1008[A]	HEC	4	0
3	B	1003	HEC	1	0
3	B	1001	HEC	1	0
3	A	1007	HEC	2	0
3	B	1002	HEC	1	0
3	B	1007	HEC	2	0
3	B	1004	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

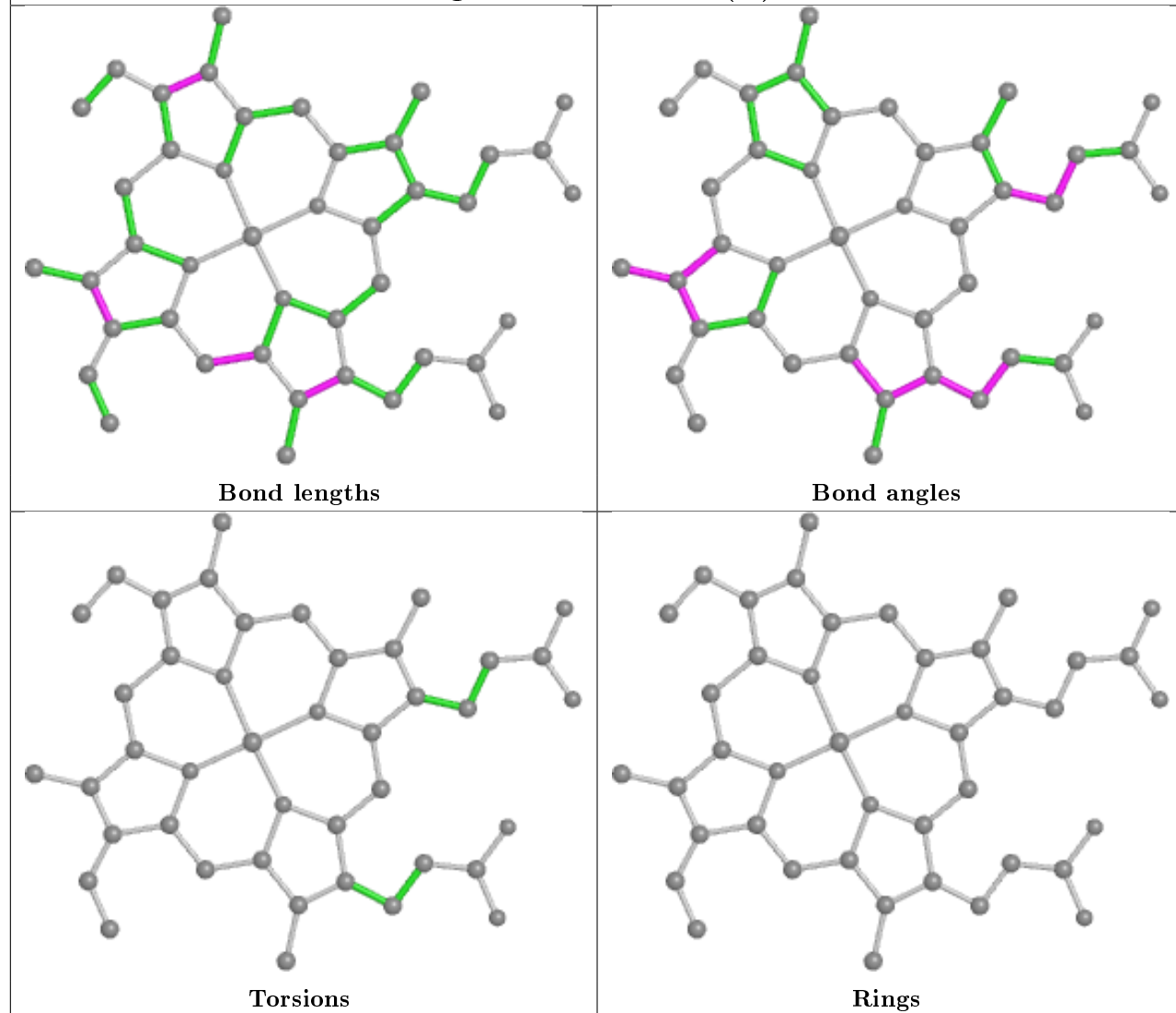




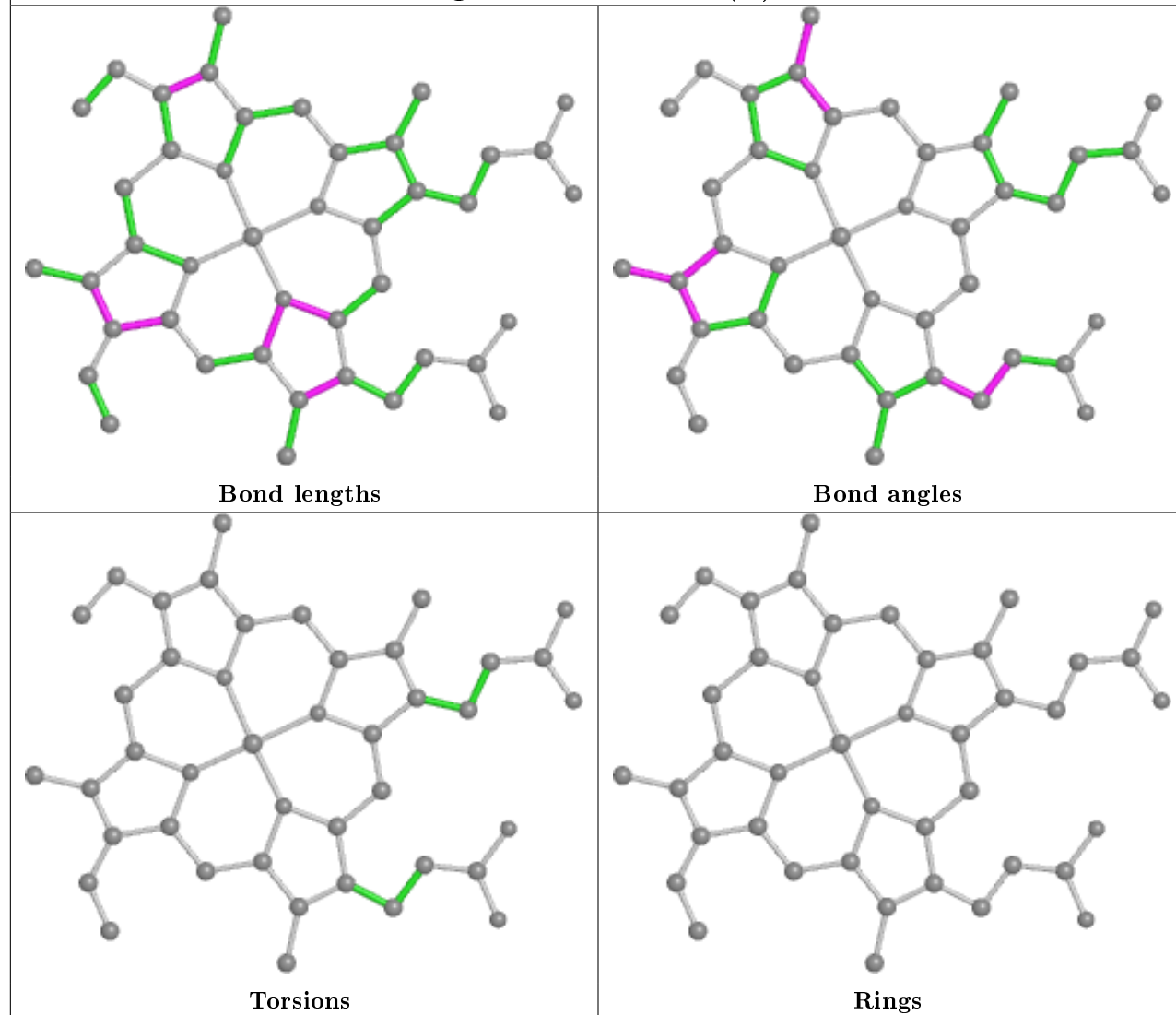
## Ligand HEC A 1001

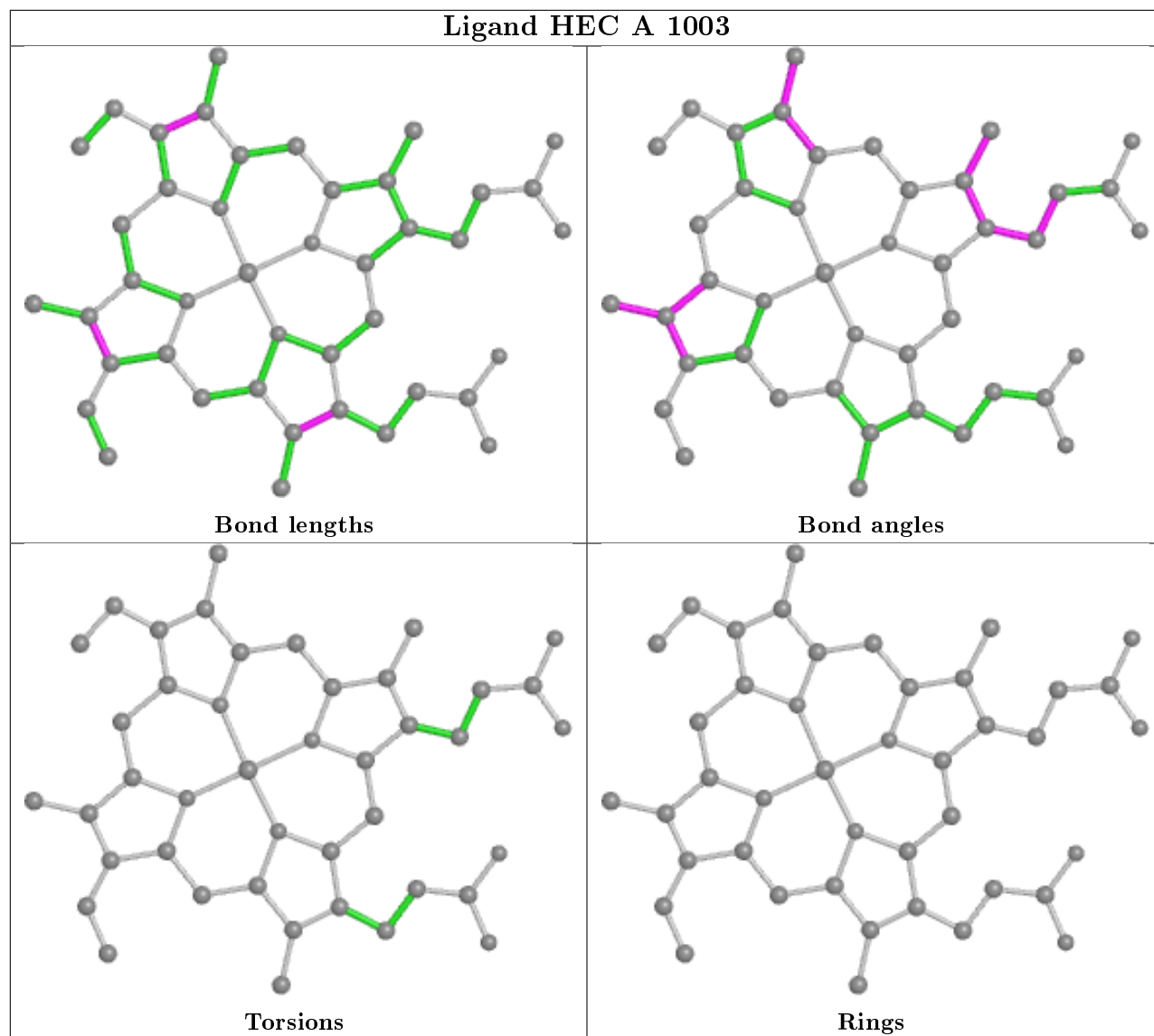


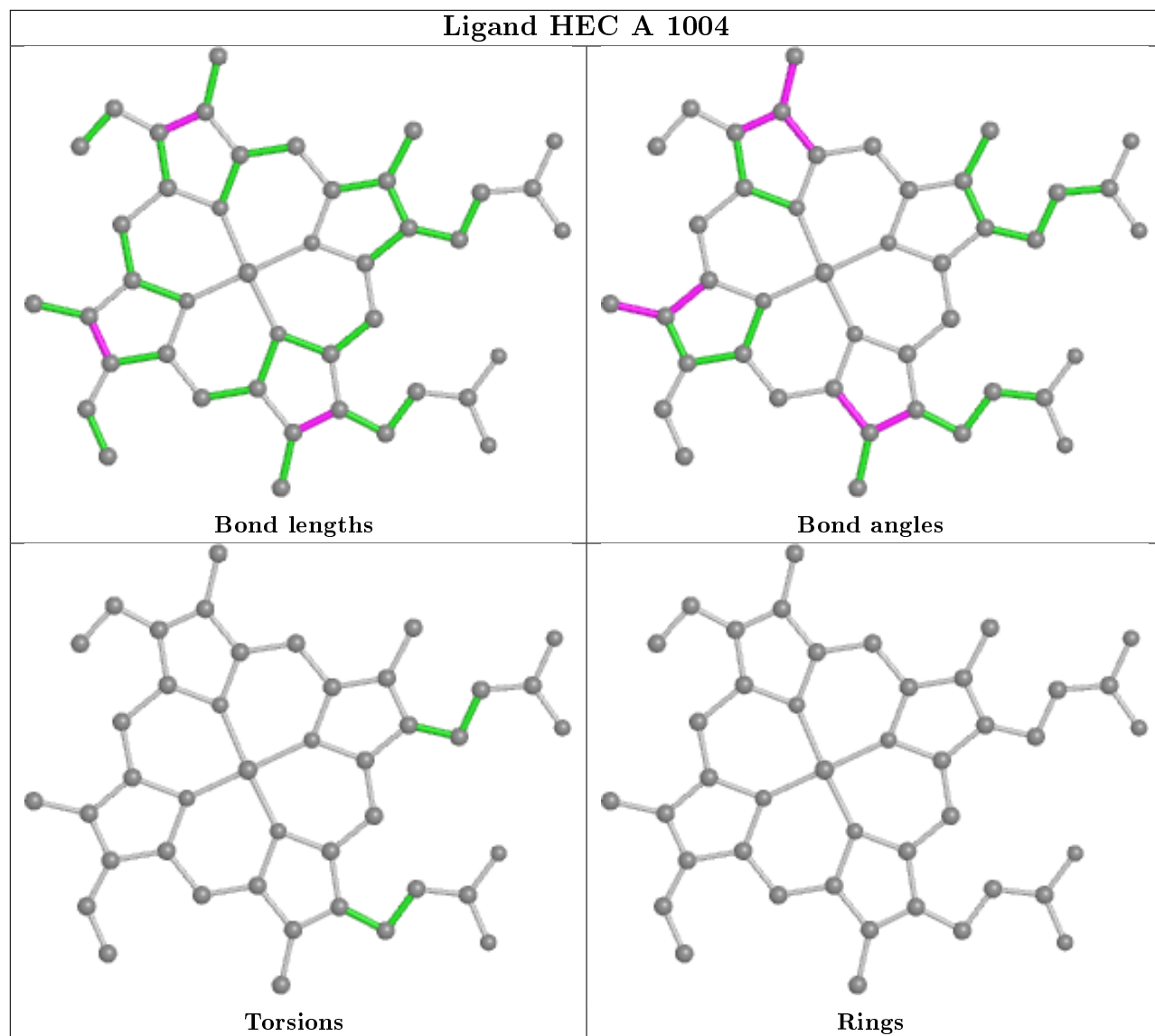
## Ligand HEC B 1008 (A)

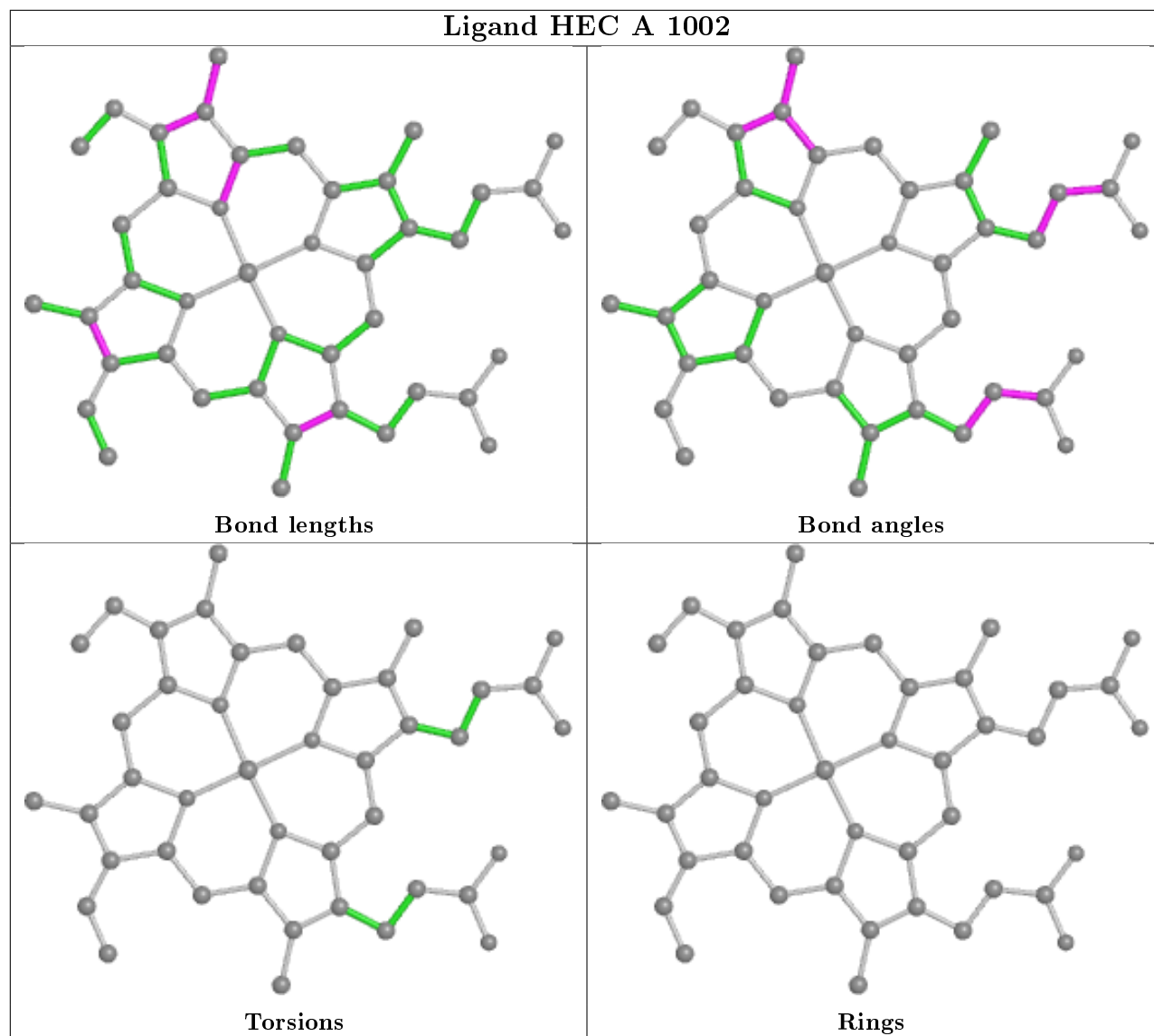


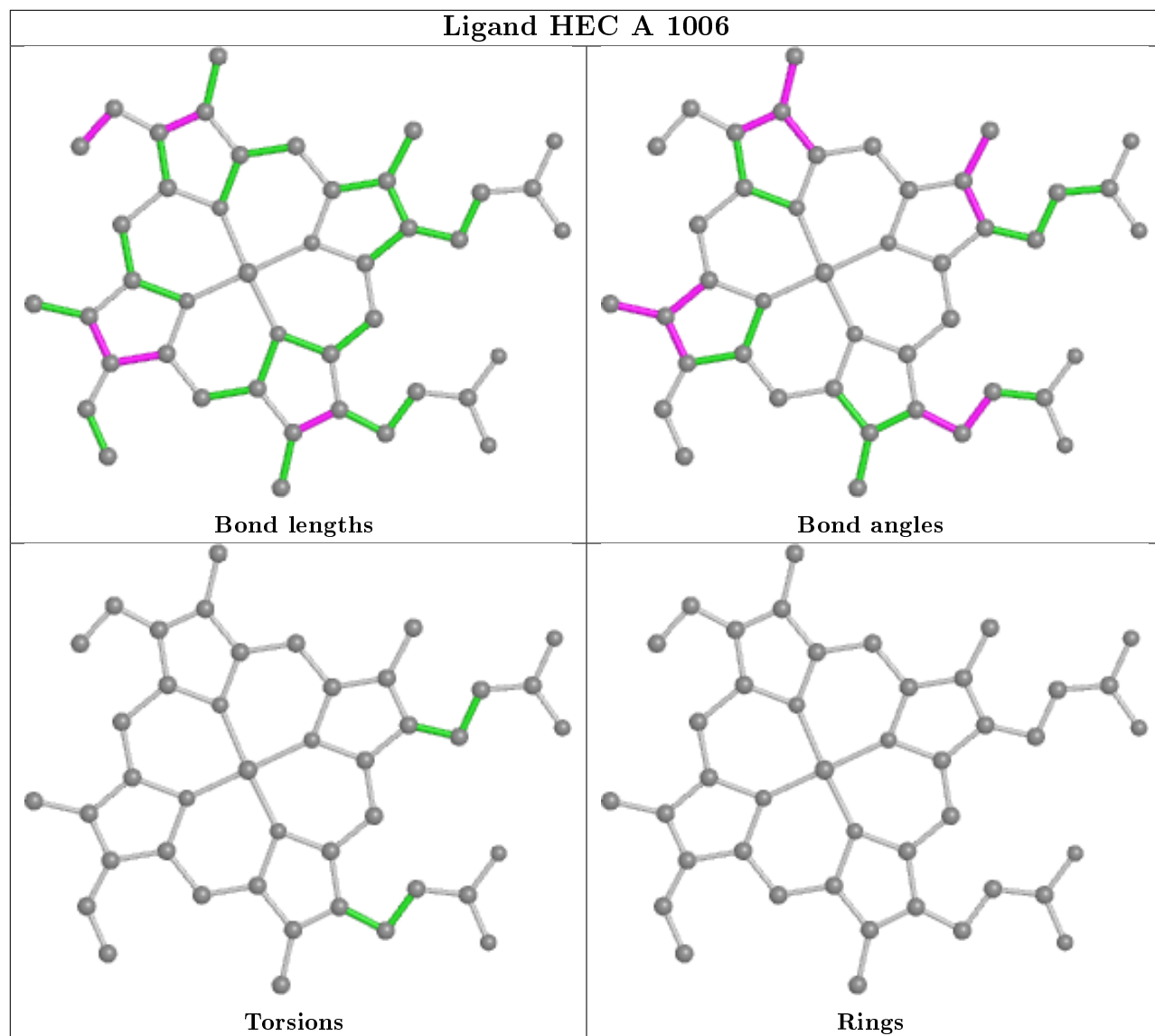
## Ligand HEC B 1008 (B)



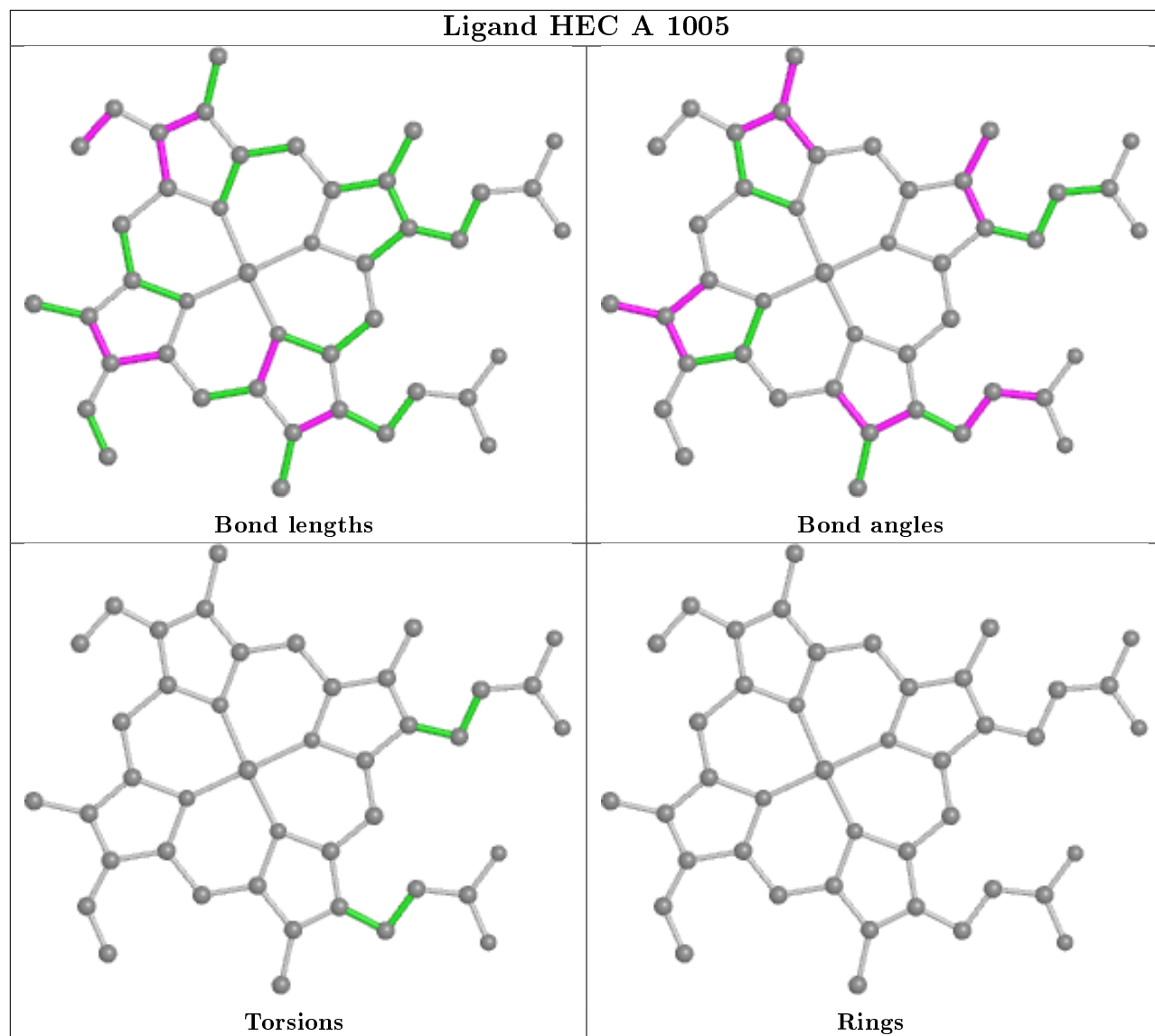




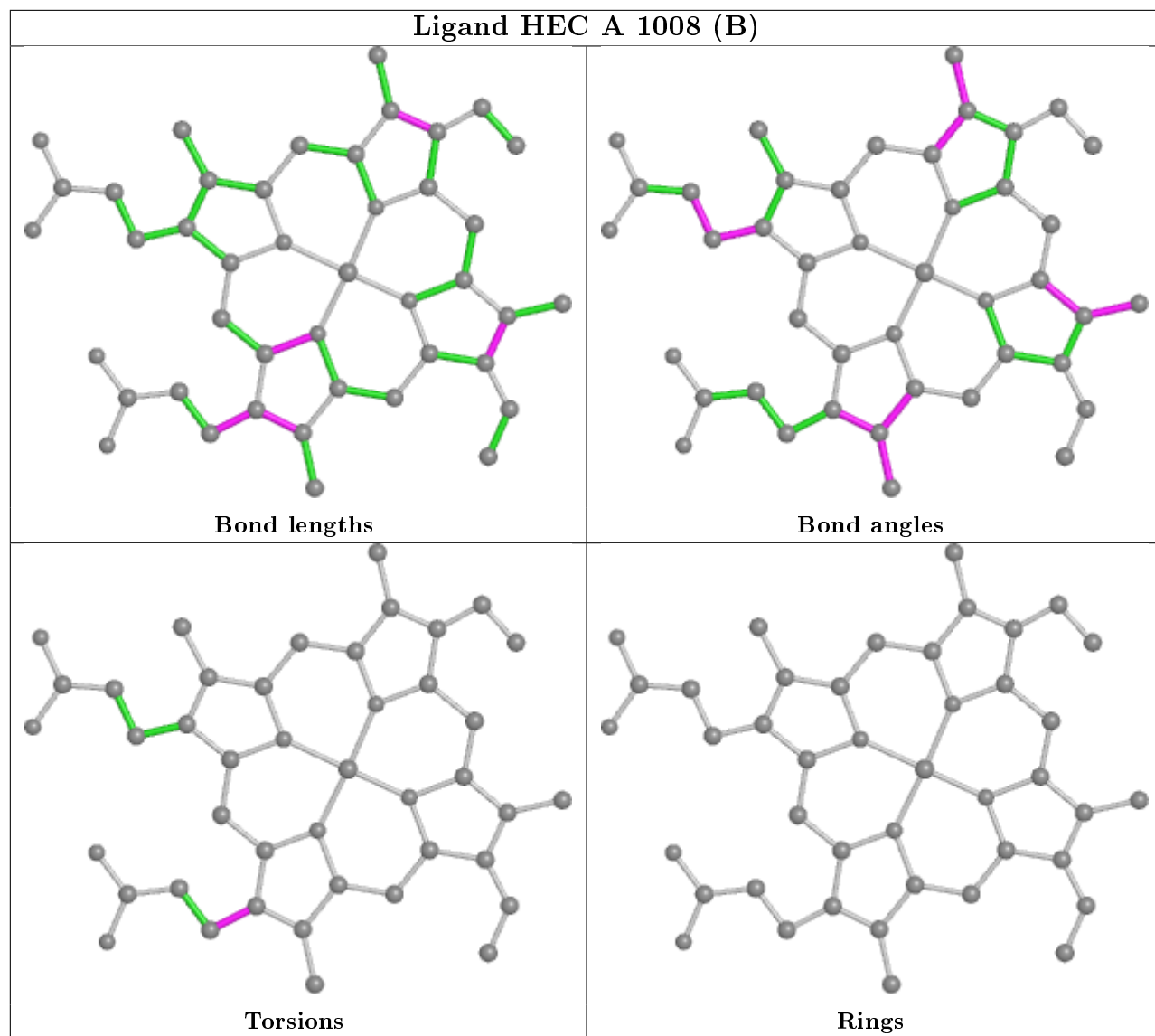




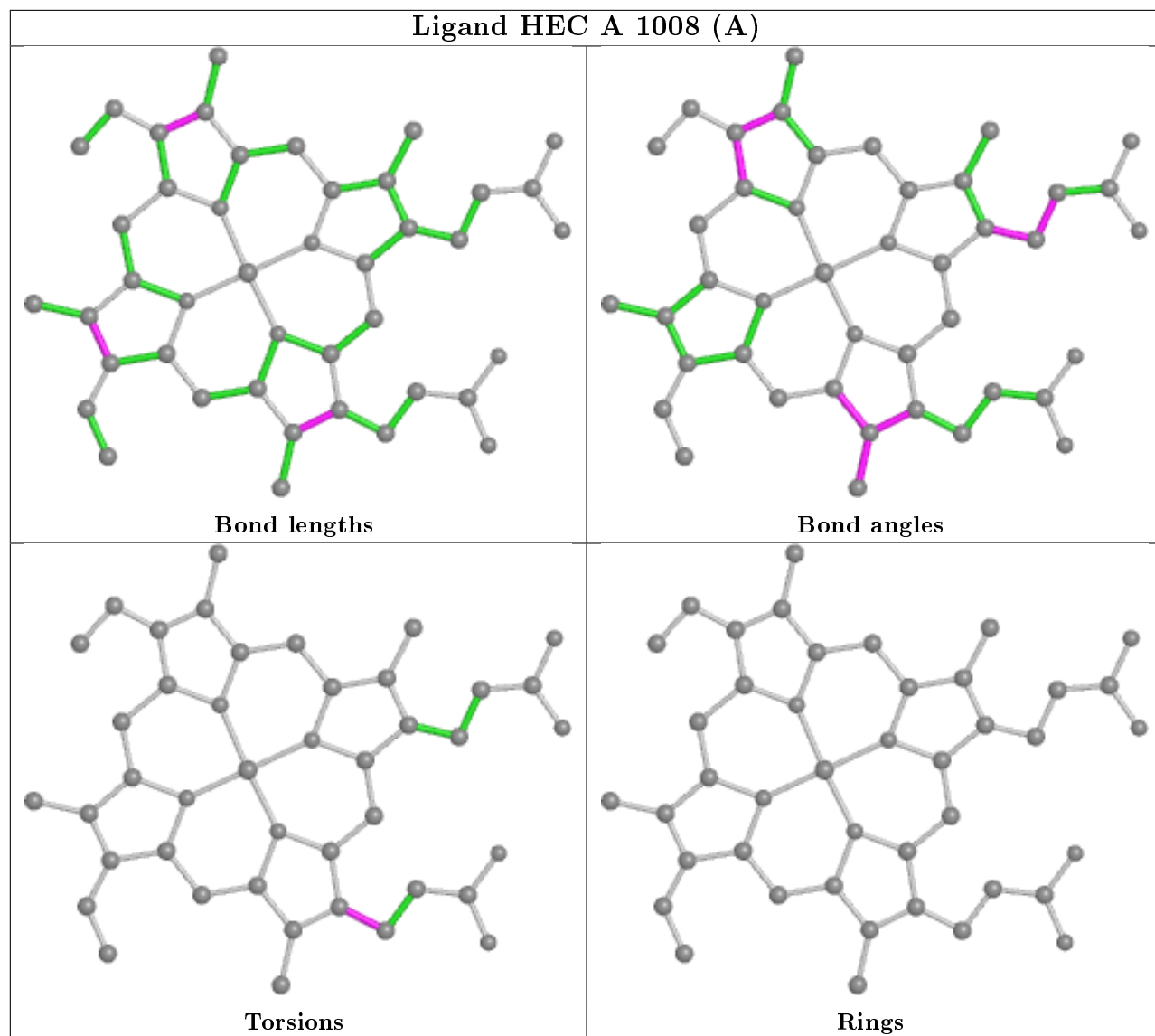
## Ligand HEC A 1005



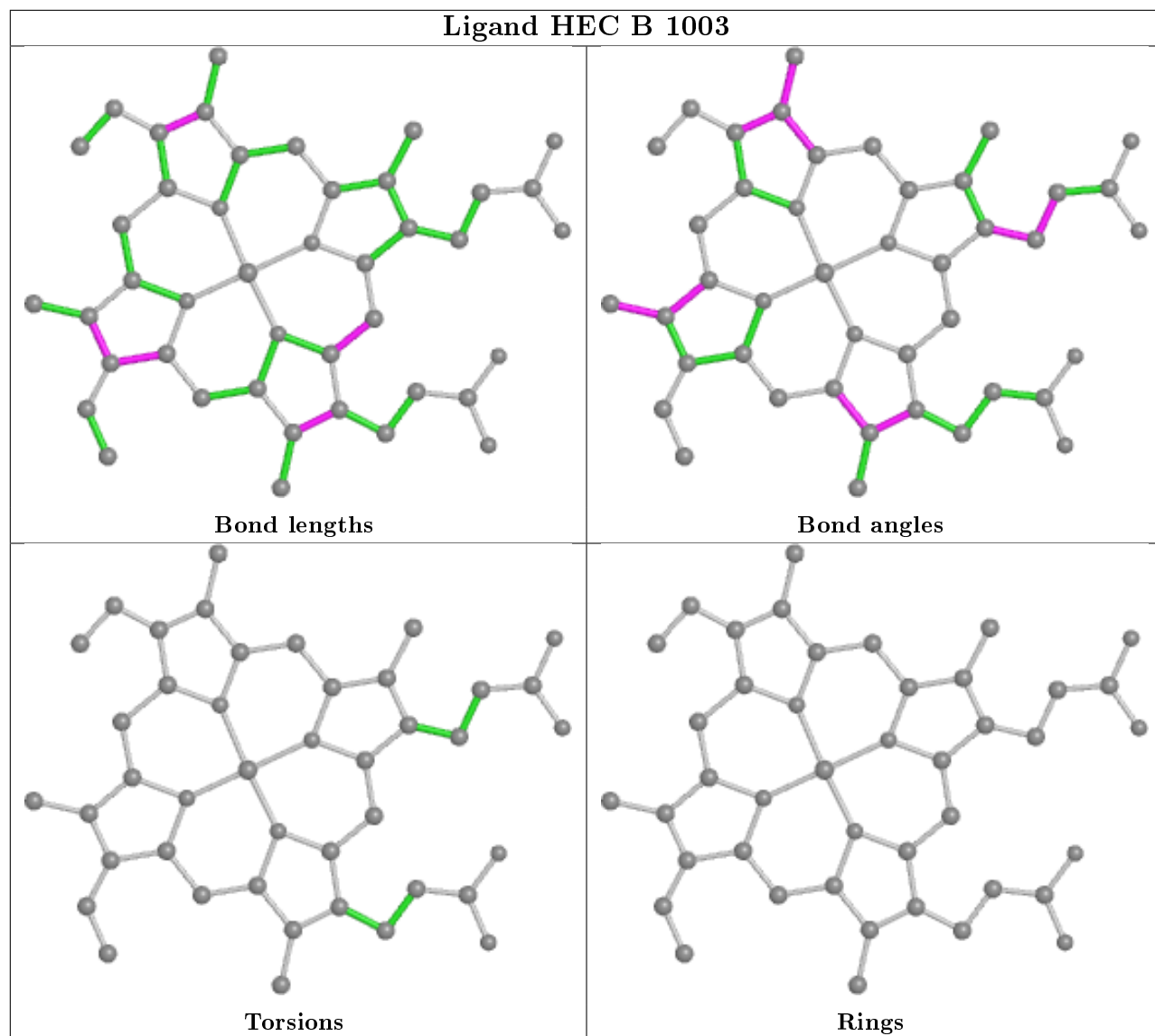




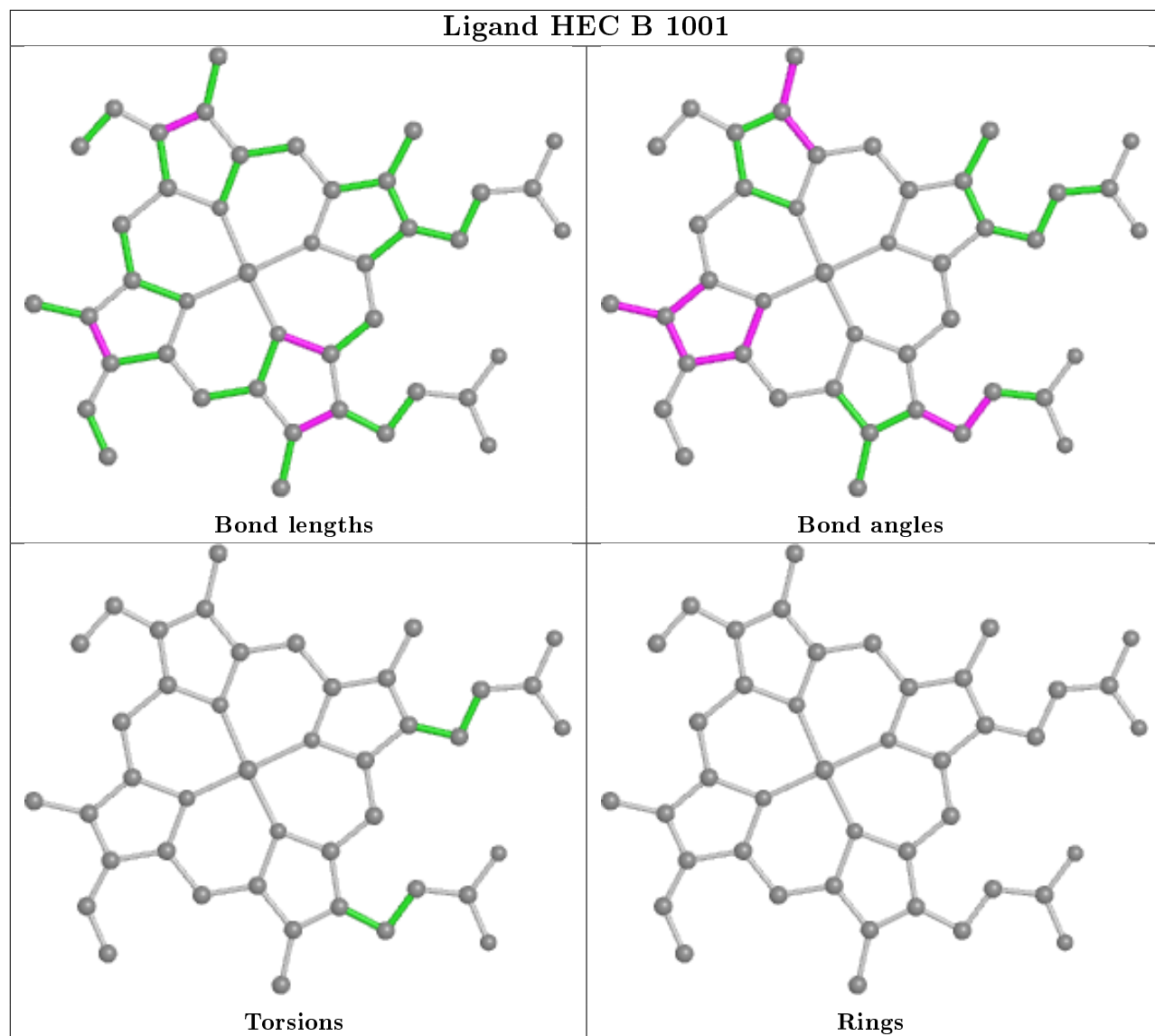
## Ligand HEC A 1008 (A)



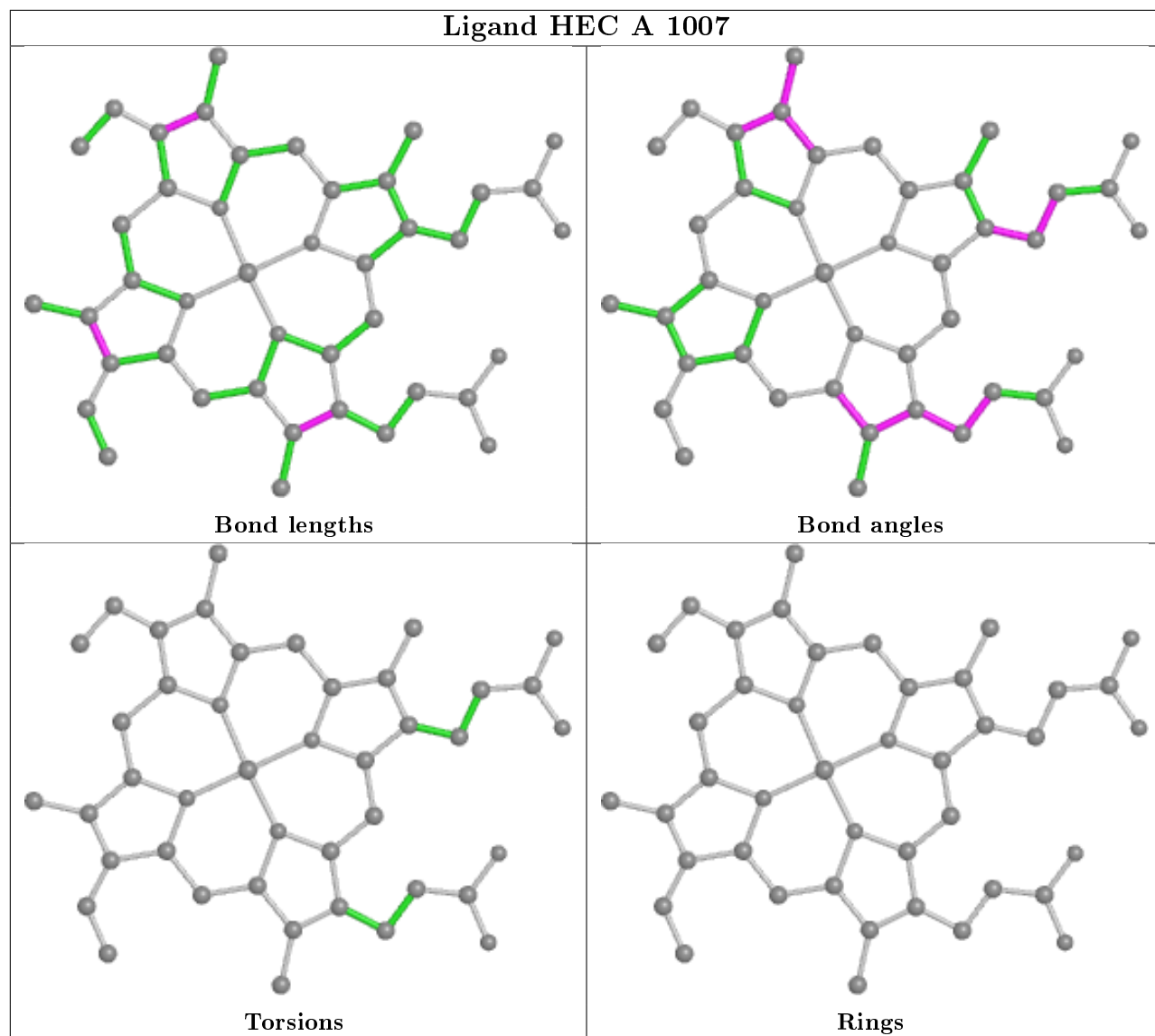
## Ligand HEC B 1003



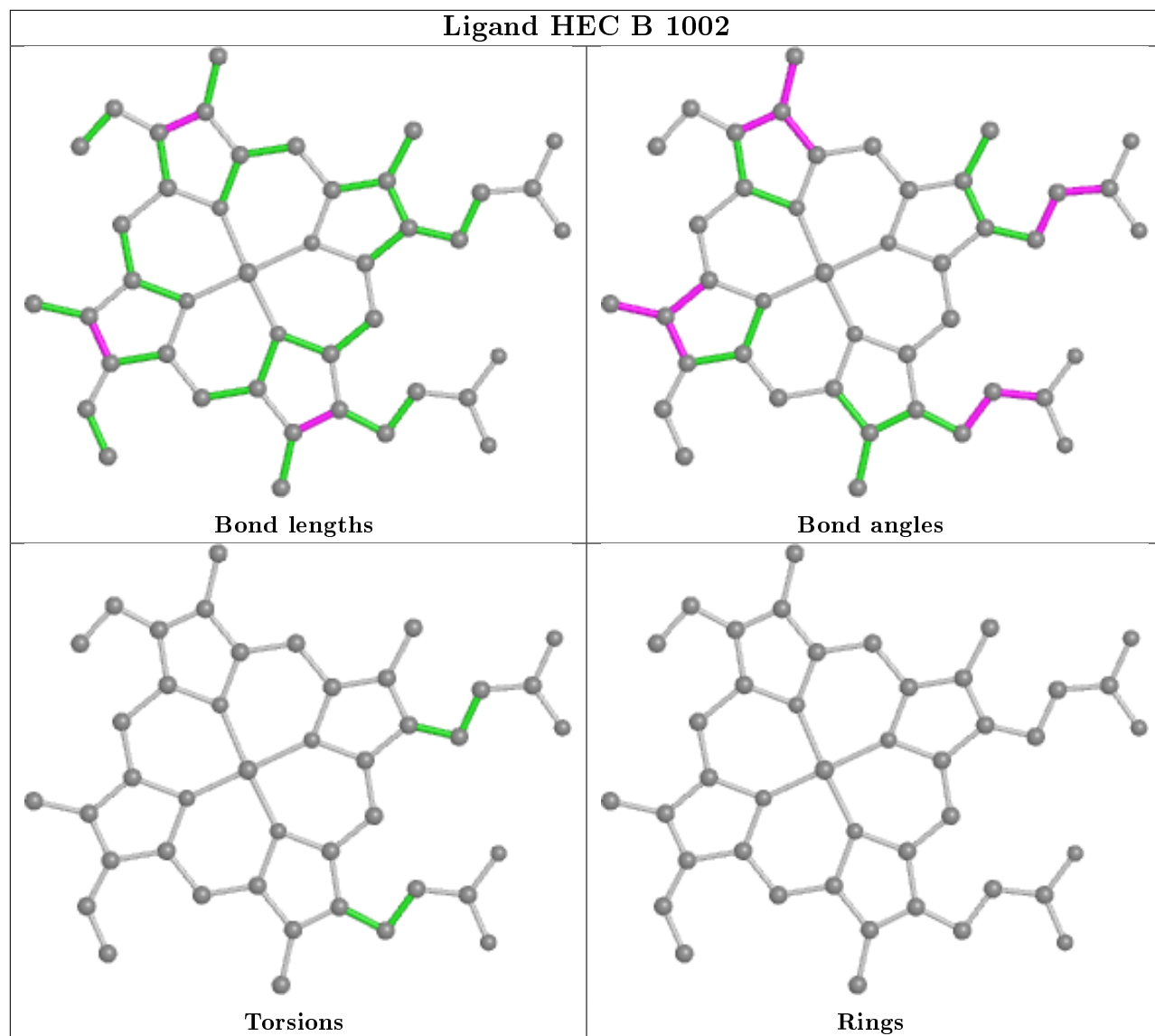
## Ligand HEC B 1001



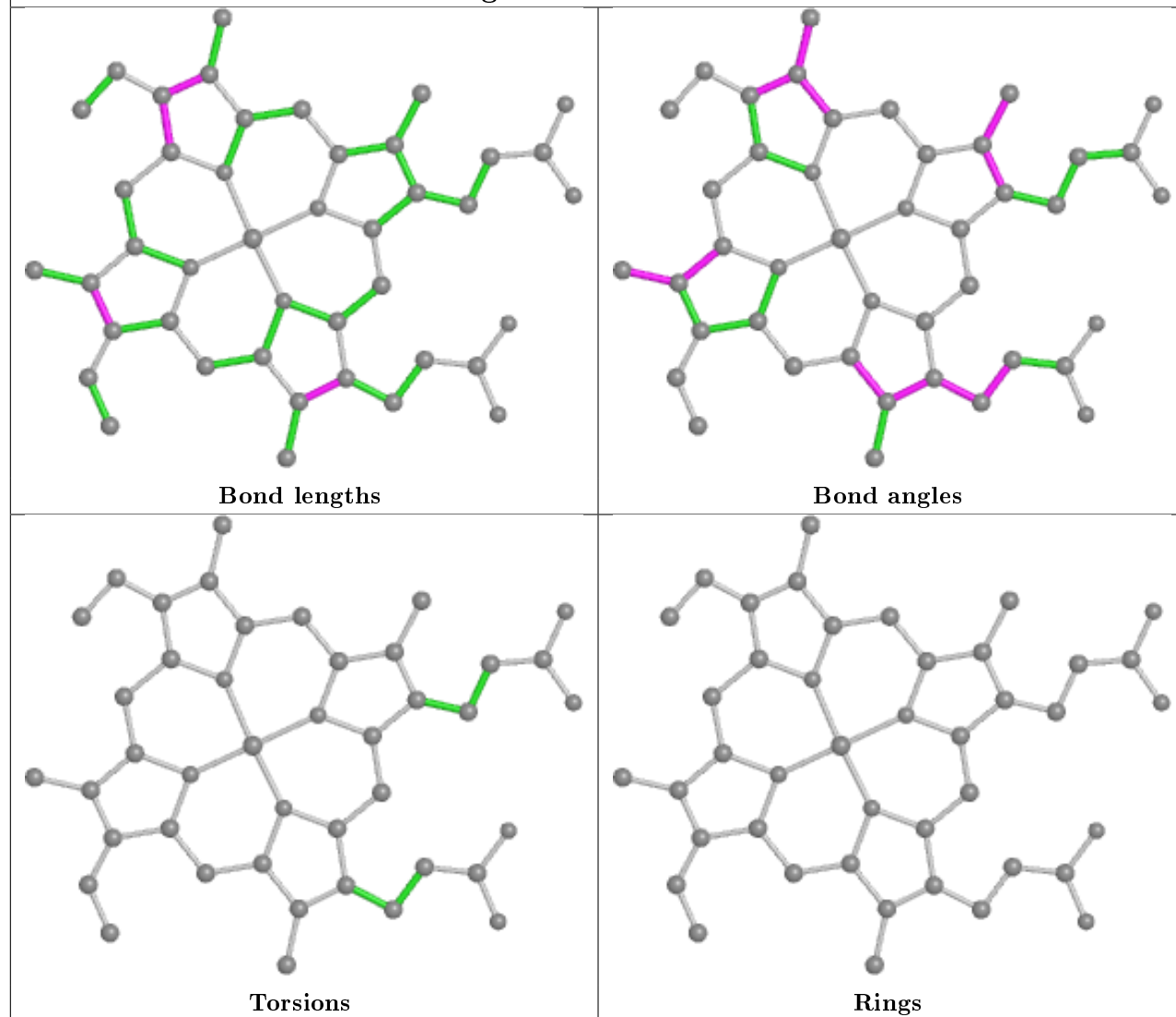
## Ligand HEC A 1007

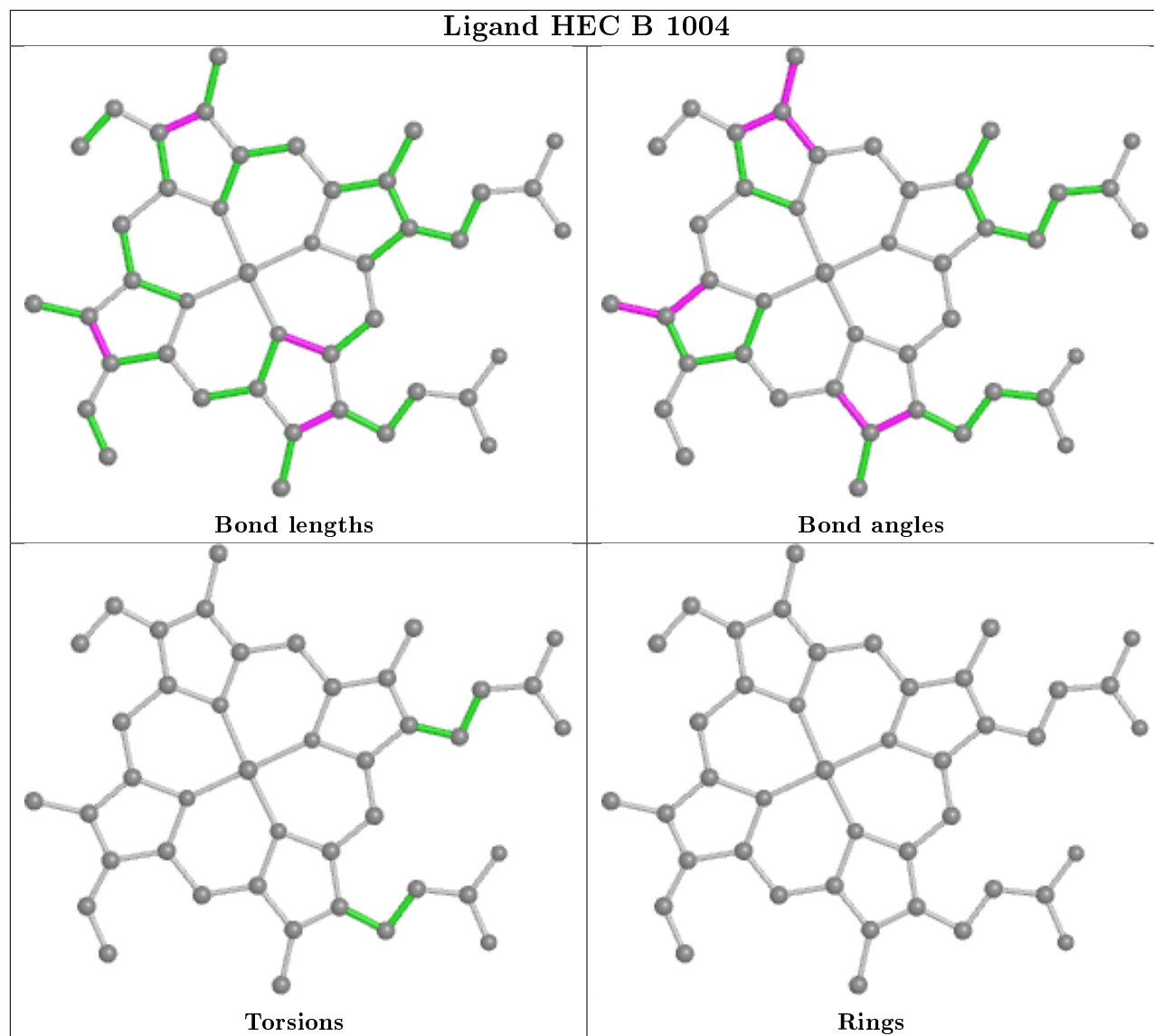


## Ligand HEC B 1002

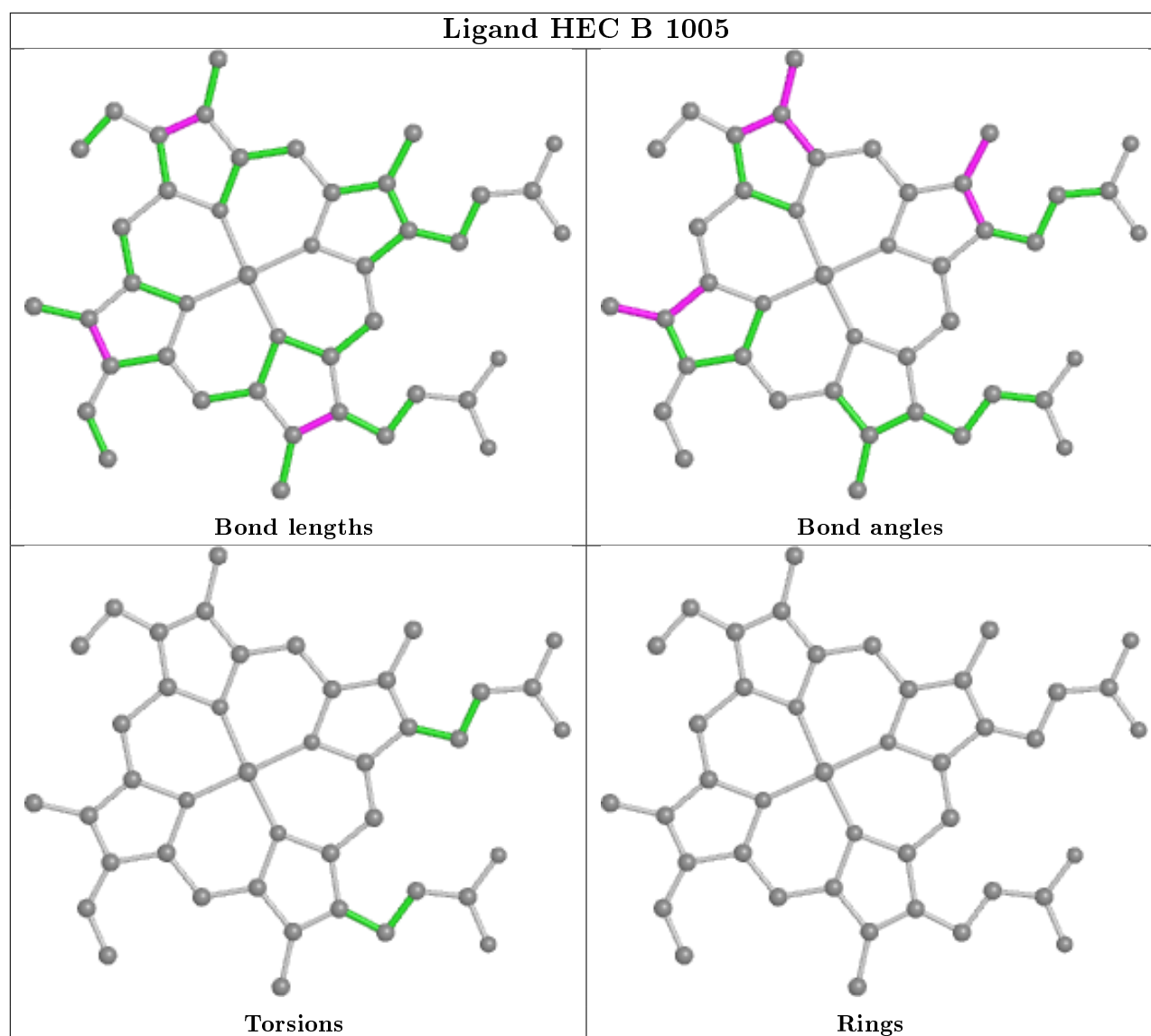


## Ligand HEC B 1007









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	520/525 (99%)	-0.66	4 (0%)	86 89	11, 17, 25, 44	1 (0%)
1	B	520/525 (99%)	-0.65	3 (0%)	89 91	10, 15, 25, 43	0
All	All	1040/1050 (99%)	-0.65	7 (0%)	87 90	10, 16, 25, 44	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	3.5
1	B	524	SER	3.1
1	A	463	ASP	3.0
1	A	522	VAL	2.8
1	A	524	SER	2.8
1	B	523	ALA	2.3
1	B	463[A]	ASP	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

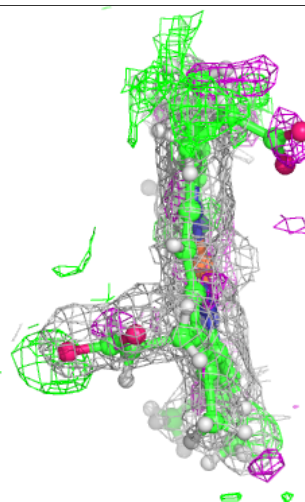
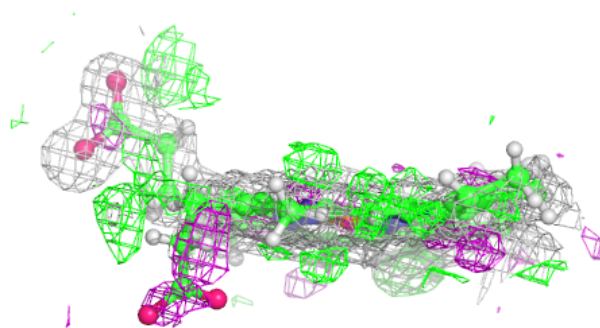
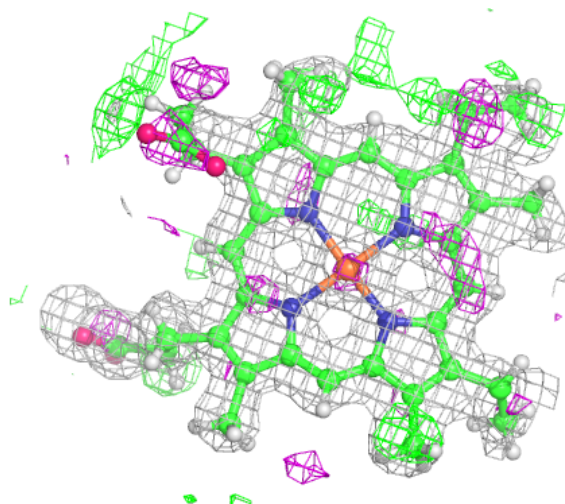
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	B	2040	8/8	0.64	0.27	29,33,36,36	18
4	MRD	B	2288	8/8	0.70	0.25	28,31,35,35	22
4	MRD	A	2005	8/8	0.78	0.33	24,26,30,32	22
4	MRD	A	2270	8/8	0.82	0.20	22,24,26,26	22
4	MRD	B	2004	8/8	0.84	0.36	21,26,31,31	21
5	MPD	A	2001	8/8	0.93	0.10	17,20,21,21	10
6	CIT	B	2010	13/13	0.93	0.15	23,28,31,31	18
5	MPD	B	2002	8/8	0.94	0.08	16,19,22,22	10
3	HEC	A	1008[A]	43/43	0.95	0.15	12,17,29,37	75
3	HEC	A	1008[B]	43/43	0.95	0.15	20,23,34,40	75
3	HEC	B	1008[A]	43/43	0.96	0.14	10,15,26,34	75
3	HEC	B	1008[B]	43/43	0.96	0.14	19,22,32,38	75
3	HEC	B	1003	43/43	0.98	0.08	11,13,21,33	18
3	HEC	A	1003	43/43	0.98	0.07	11,13,22,33	18
3	HEC	A	1004	43/43	0.99	0.05	11,13,16,16	18
3	HEC	A	1001	43/43	0.99	0.05	12,15,19,23	18
3	HEC	B	1006	43/43	0.99	0.06	9,11,12,13	18
3	HEC	B	1001	43/43	0.99	0.06	14,17,20,22	18
3	HEC	A	1005	43/43	0.99	0.06	11,13,18,26	18
3	HEC	A	1007	43/43	0.99	0.07	11,13,15,18	18
3	HEC	B	1002	43/43	0.99	0.09	11,14,17,17	18
3	HEC	B	1007	43/43	0.99	0.07	10,12,13,17	18
3	HEC	B	1004	43/43	0.99	0.06	10,11,14,15	18
3	HEC	A	1002	43/43	0.99	0.07	12,14,15,17	18
3	HEC	B	1005	43/43	0.99	0.06	10,12,18,26	18
3	HEC	A	1006	43/43	0.99	0.06	10,12,13,13	18
2	CA	A	2744	1/1	1.00	0.04	18,18,18,18	0
2	CA	B	2333	1/1	1.00	0.05	17,17,17,17	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.

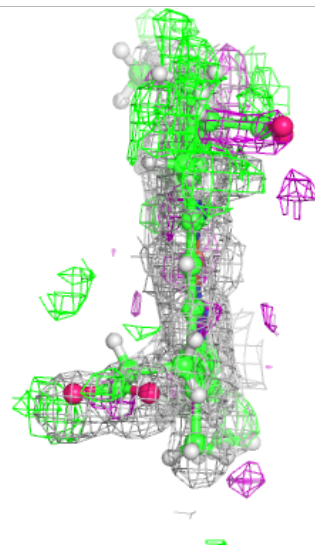
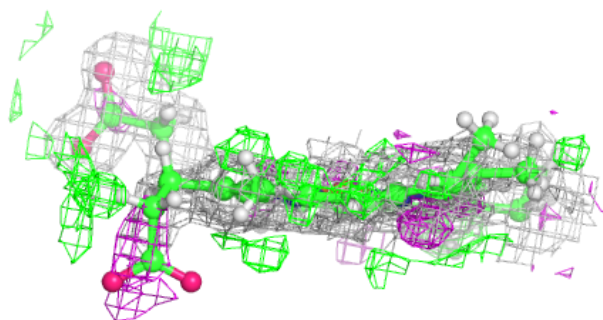
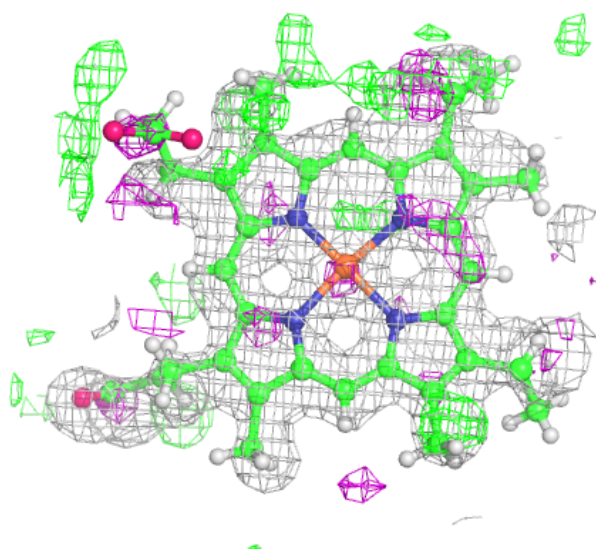
**Electron density around HEC A 1008 (A):**

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



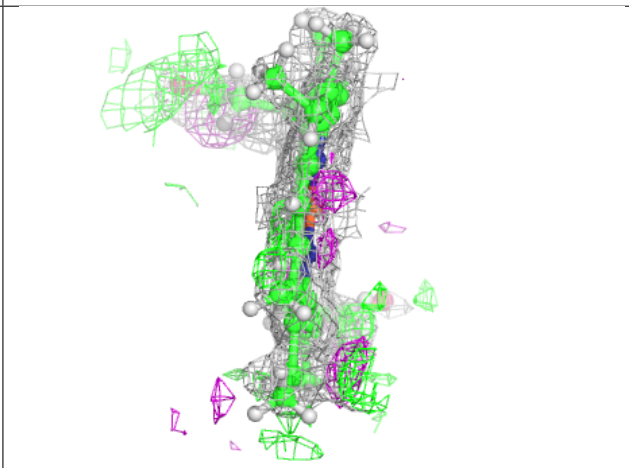
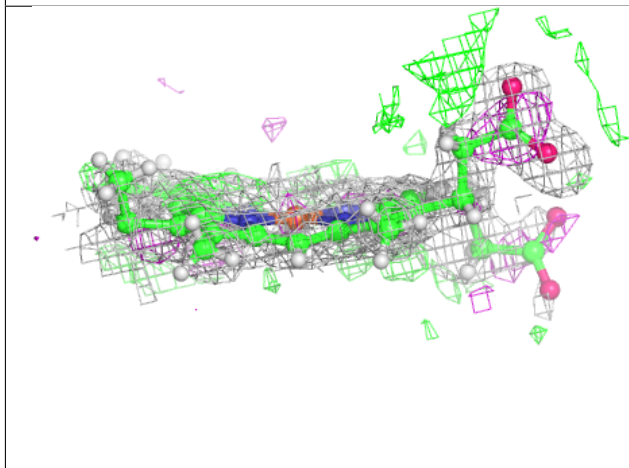
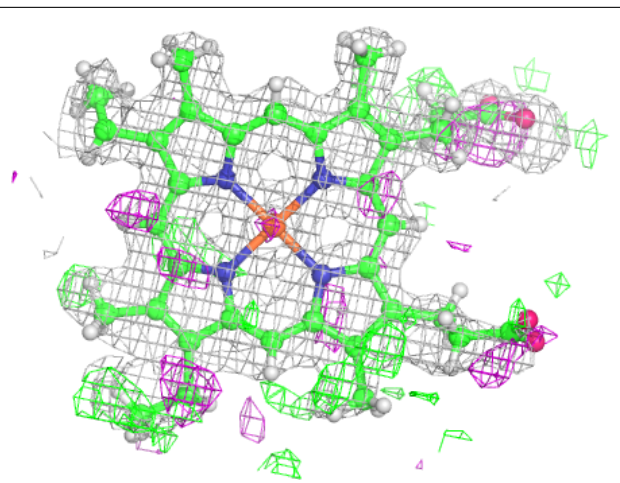
**Electron density around HEC A 1008 (B):**

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



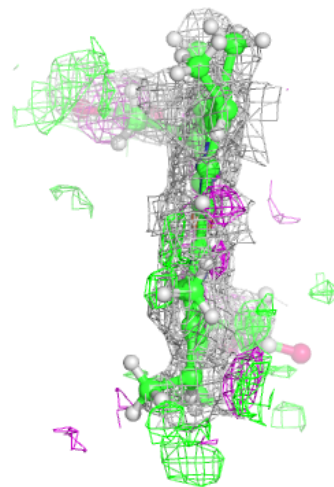
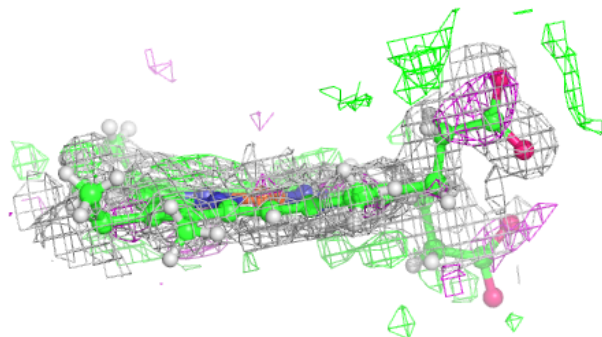
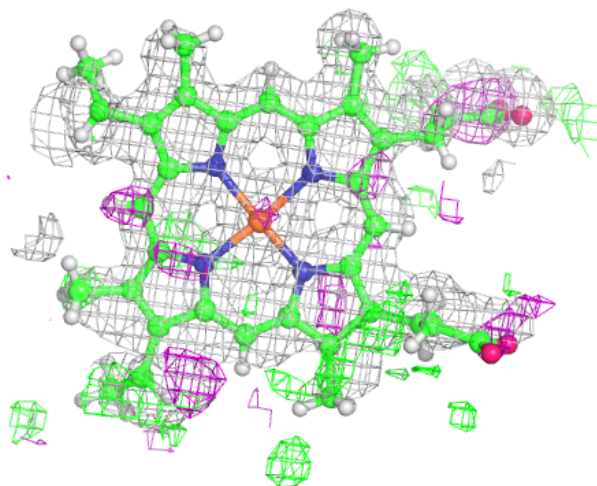
**Electron density around HEC B 1008 (A):**

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



**Electron density around HEC B 1008 (B):**

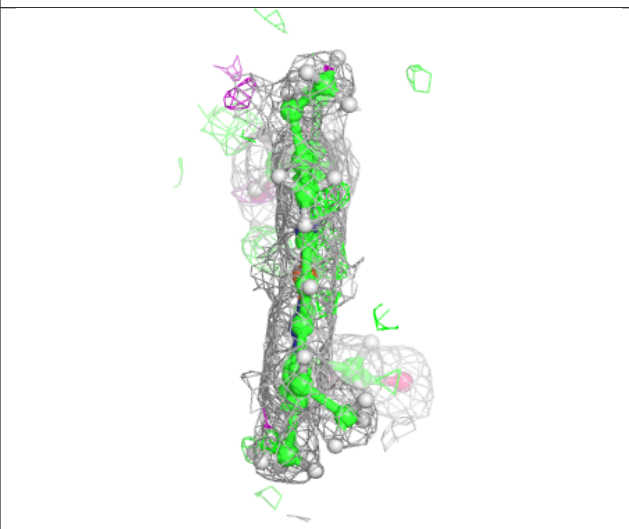
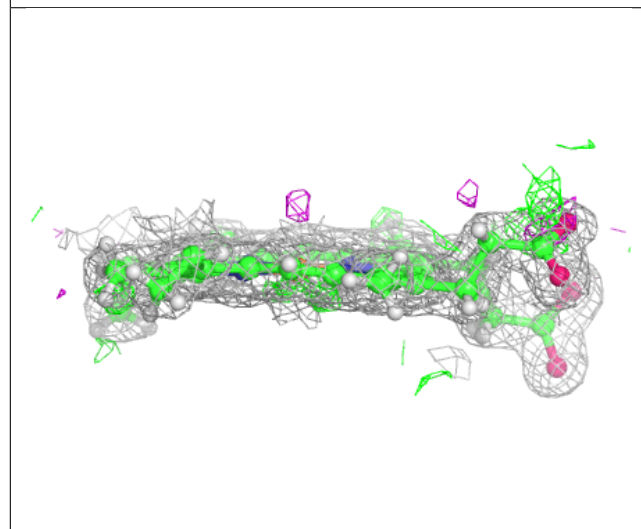
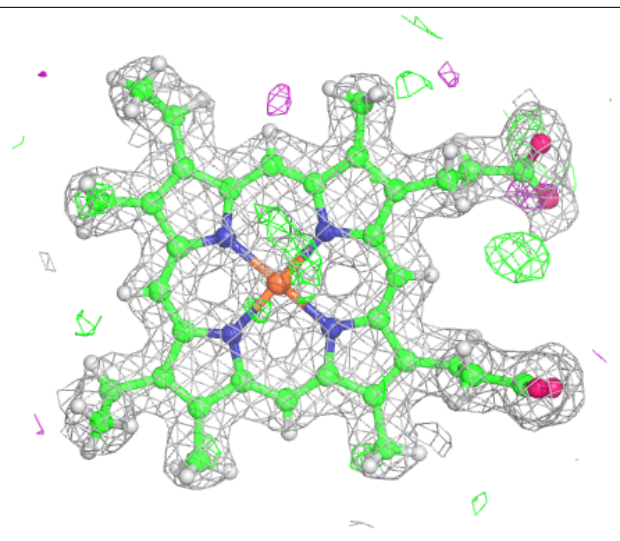
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and green (positive)





**Electron density around HEC B 1003:**

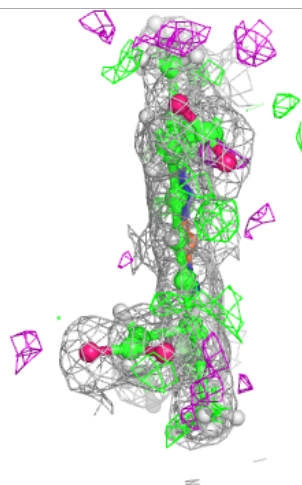
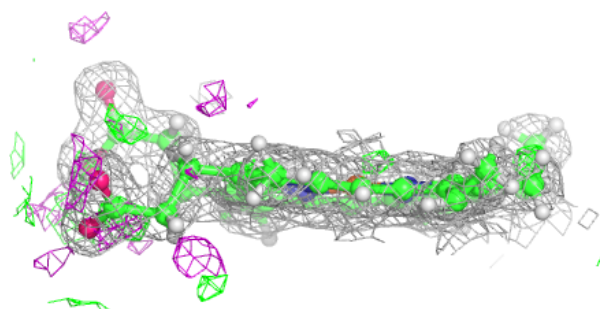
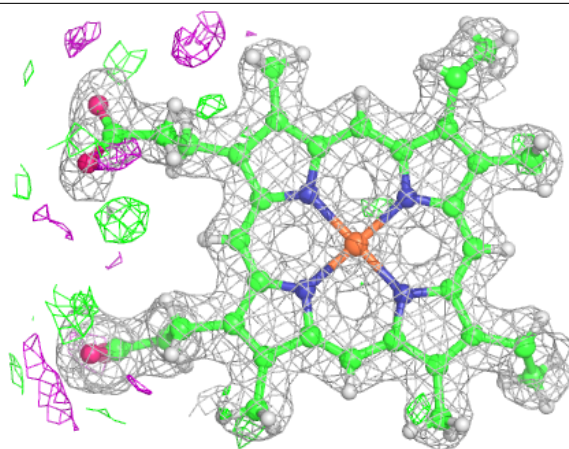
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





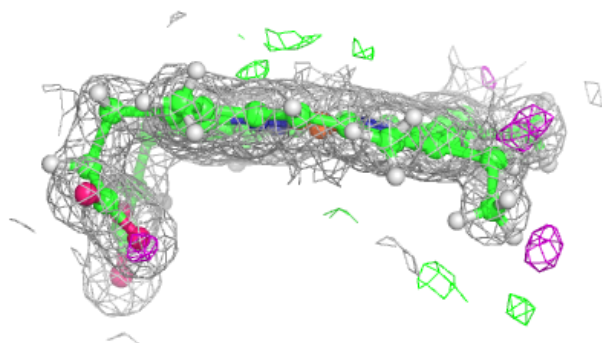
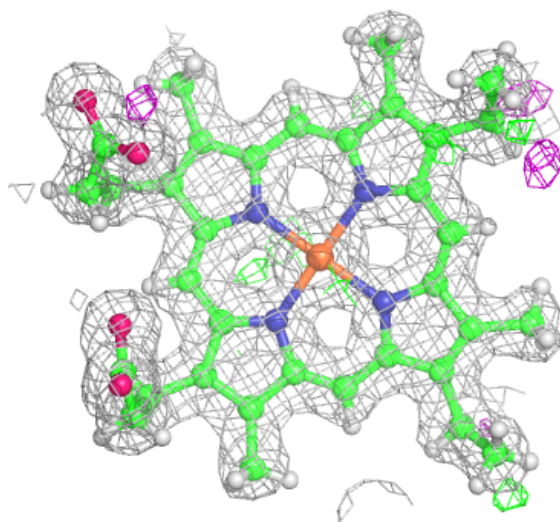
**Electron density around HEC A 1003:**

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



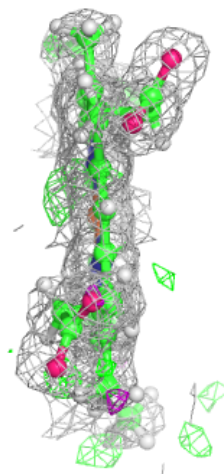
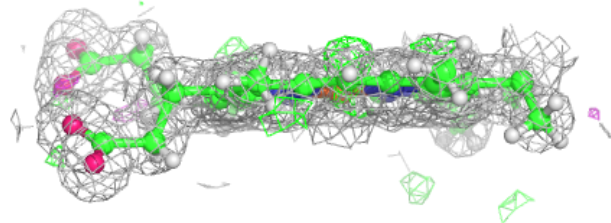
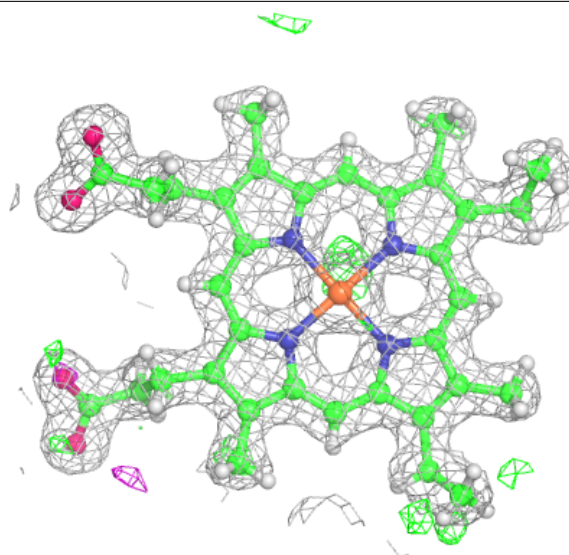
**Electron density around HEC A 1004:**

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and green (positive)



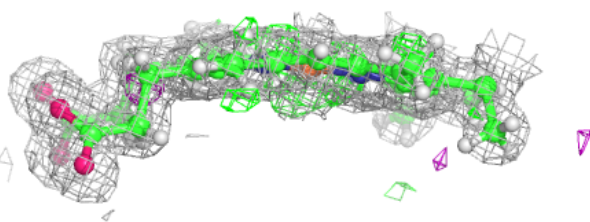
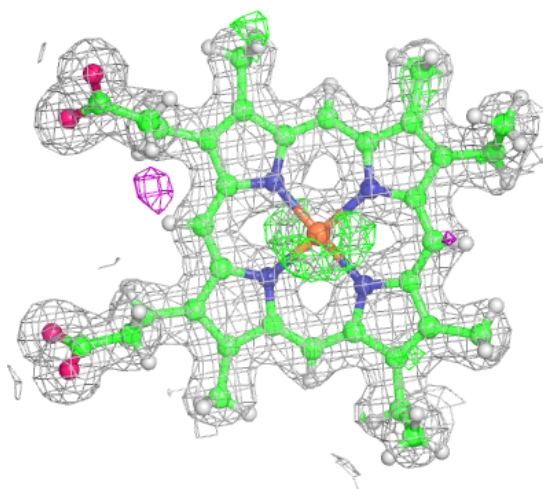
**Electron density around HEC A 1001:**

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and green (positive)



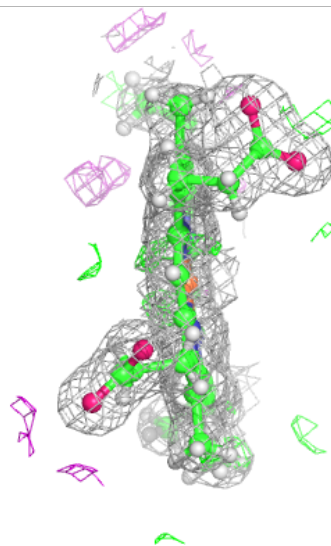
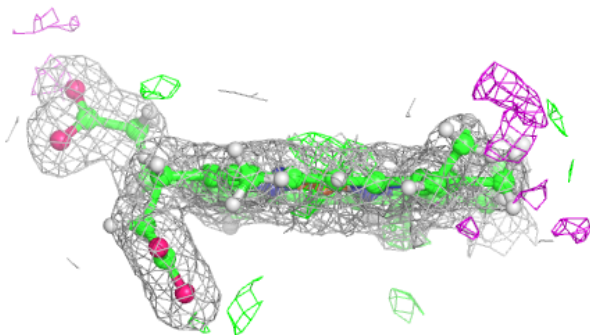
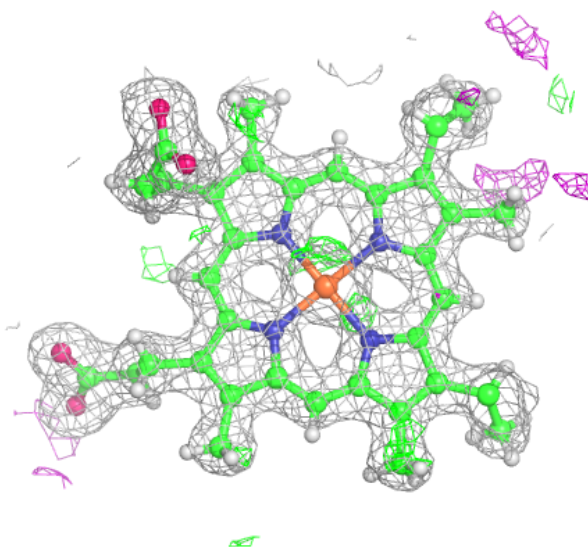
**Electron density around HEC B 1006:**

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



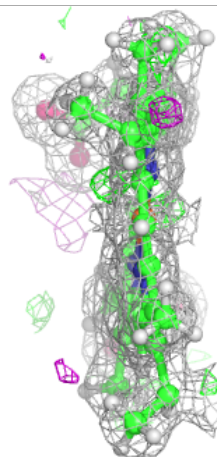
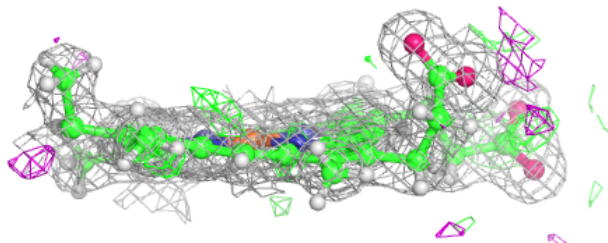
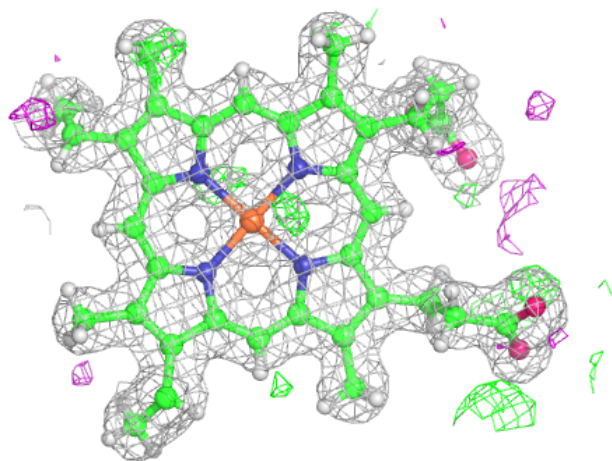
**Electron density around HEC B 1001:**

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



**Electron density around HEC A 1005:**

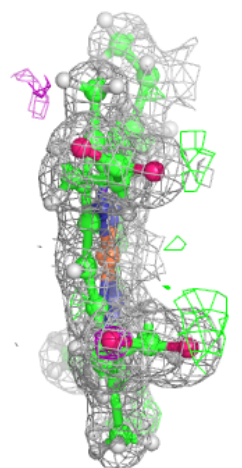
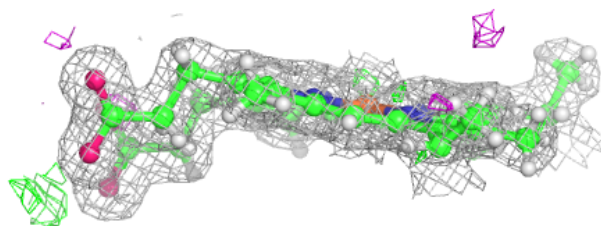
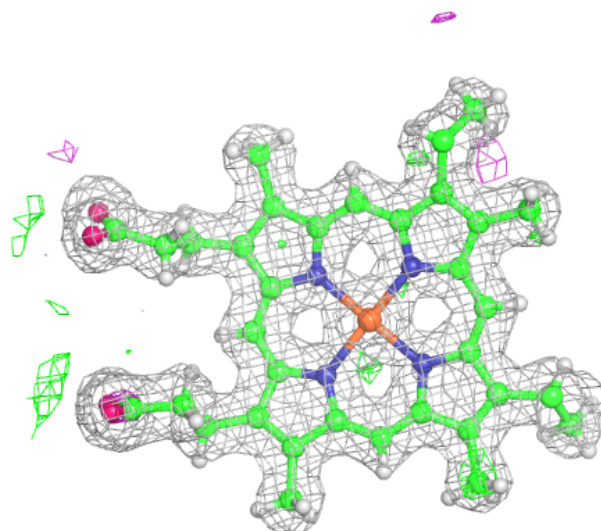
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





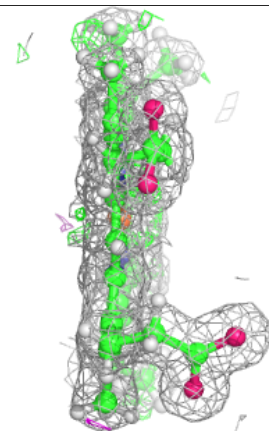
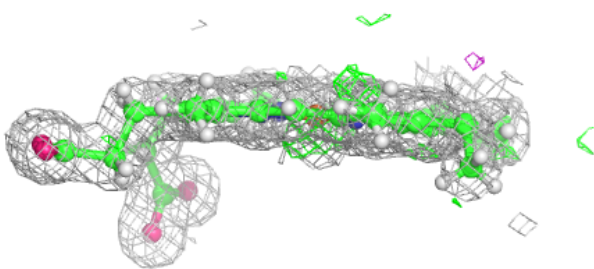
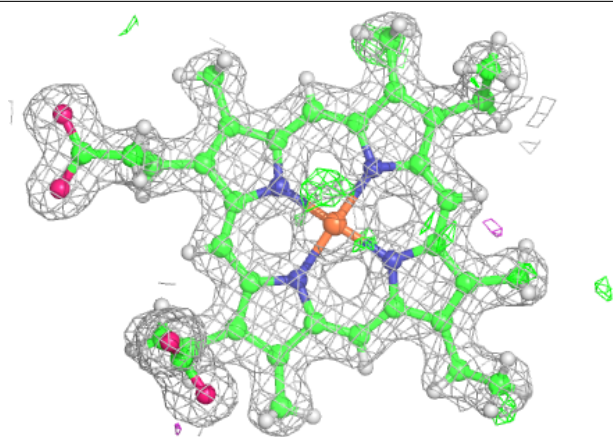
**Electron density around HEC A 1007:**

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



**Electron density around HEC B 1002:**

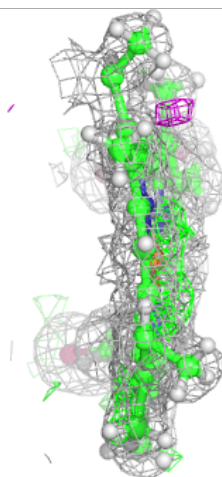
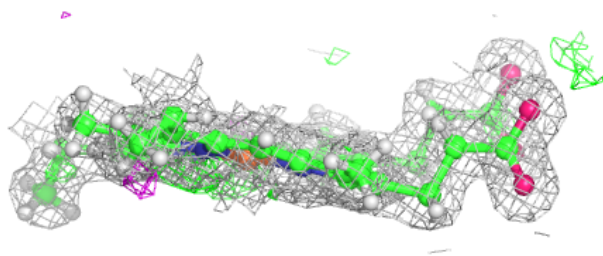
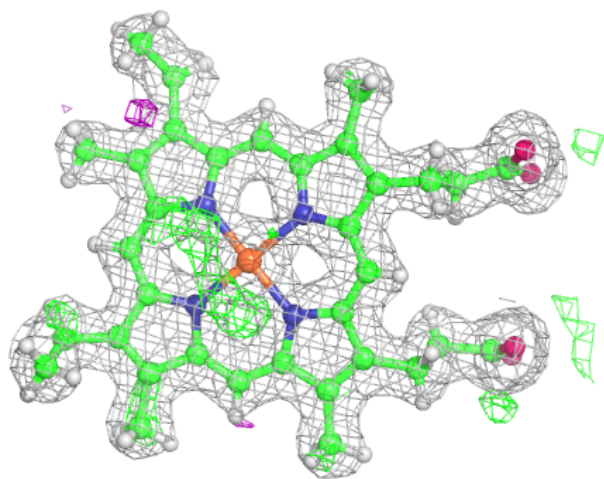
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





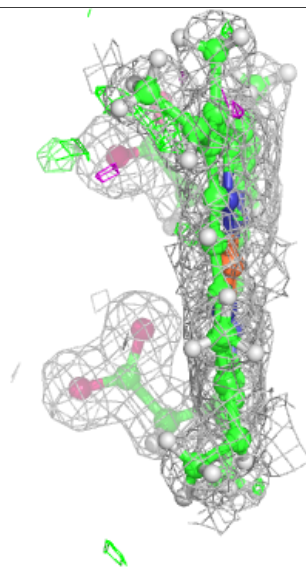
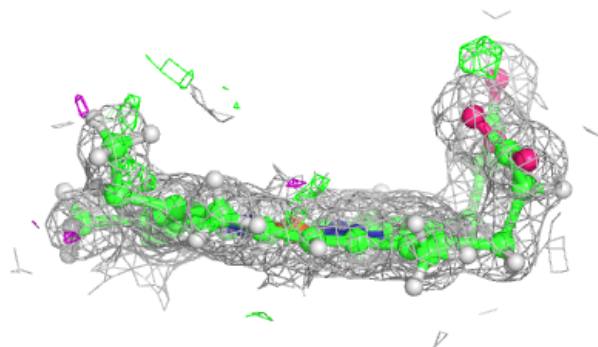
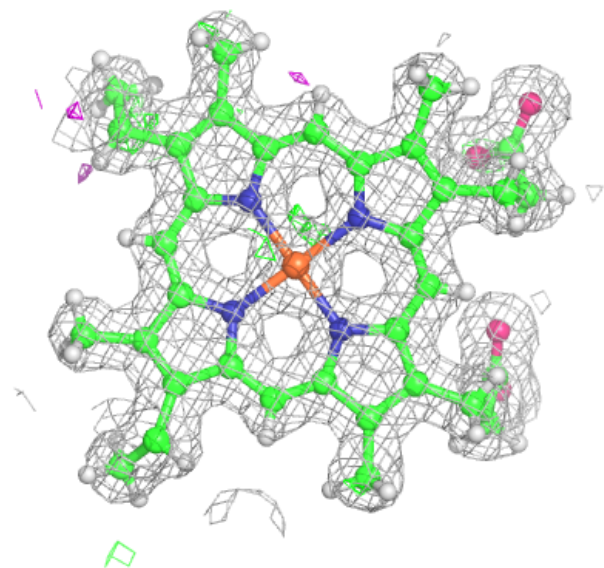
**Electron density around HEC B 1007:**

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



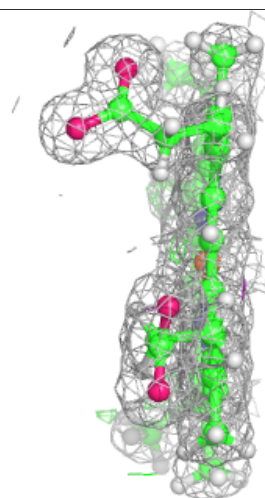
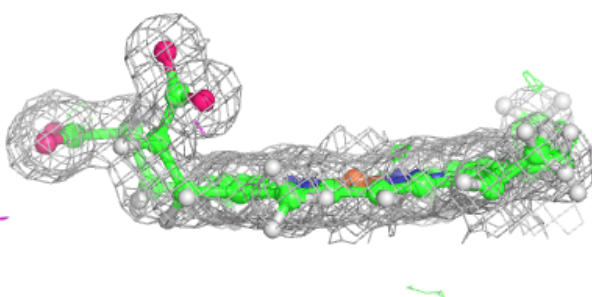
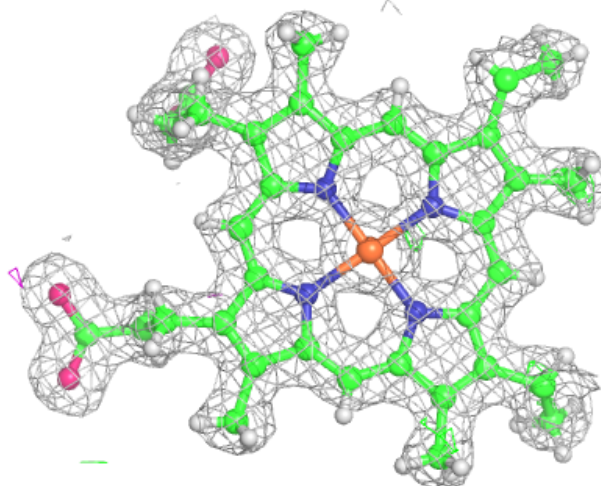
**Electron density around HEC B 1004:**

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



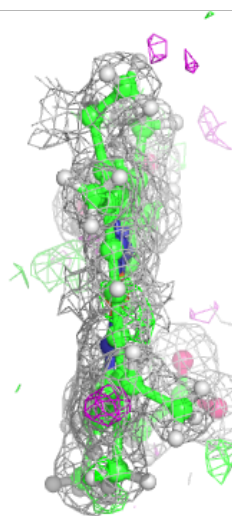
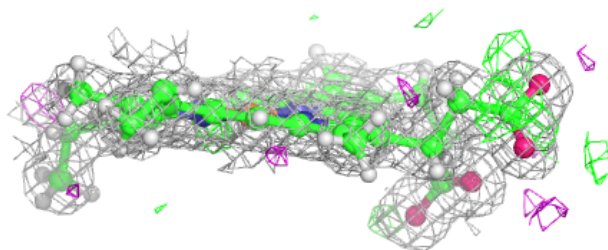
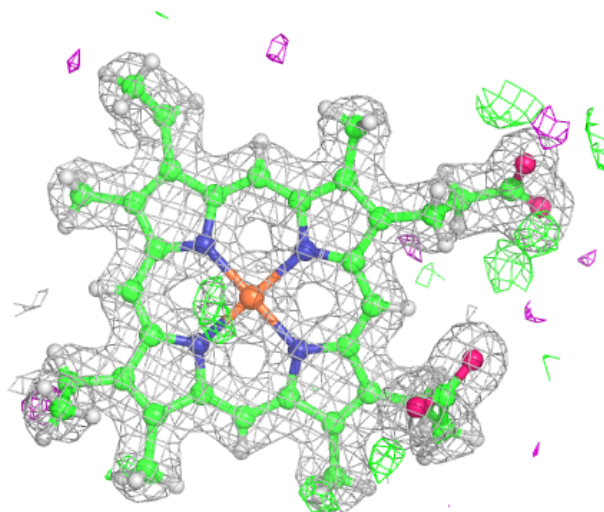
**Electron density around HEC A 1002:**

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



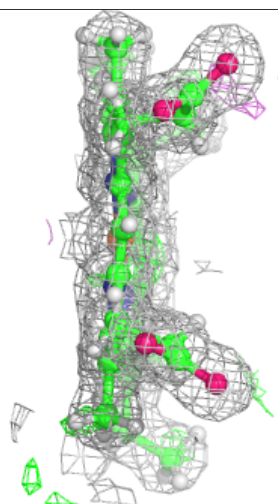
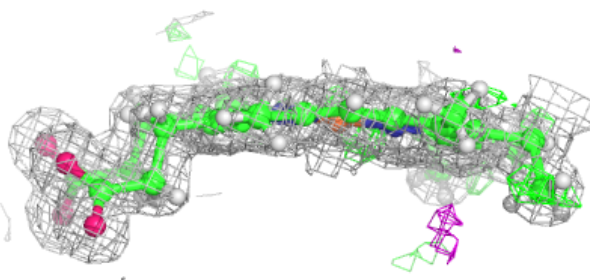
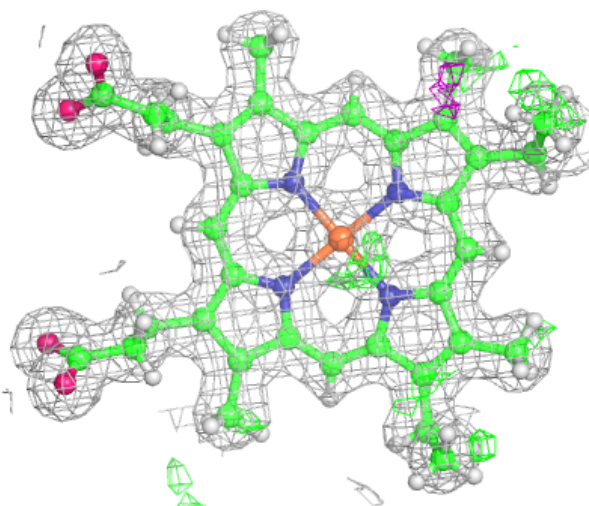
**Electron density around HEC B 1005:**

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



**Electron density around HEC A 1006:**

$2mF_o-DF_c$  (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.