



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:09 pm BST

PDB ID : 3MMO  
Title : Structure of the Thioalkalivibrio nitratireducens cytochrome c nitrite reductase in complex with cyanide  
Authors : Trofimov, A.A.; Polyakov, K.M.; Boyko, K.M.; Tikhonova, T.V.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.  
Deposited on : 2010-04-20  
Resolution : 1.55 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

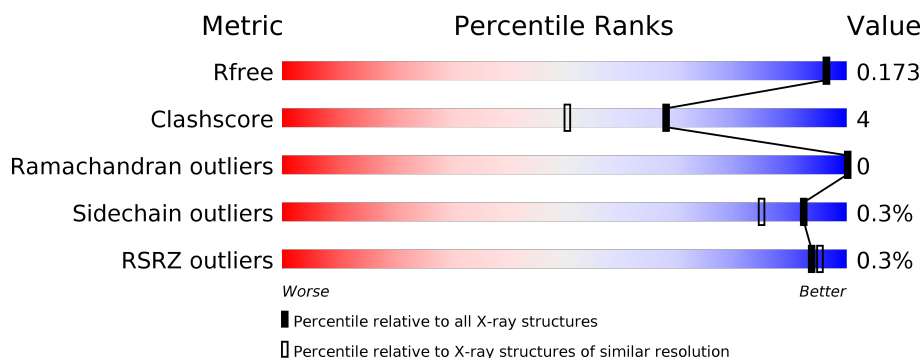
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	 93% 5% •
1	B	525	 93% 6% •

## 2 Entry composition i

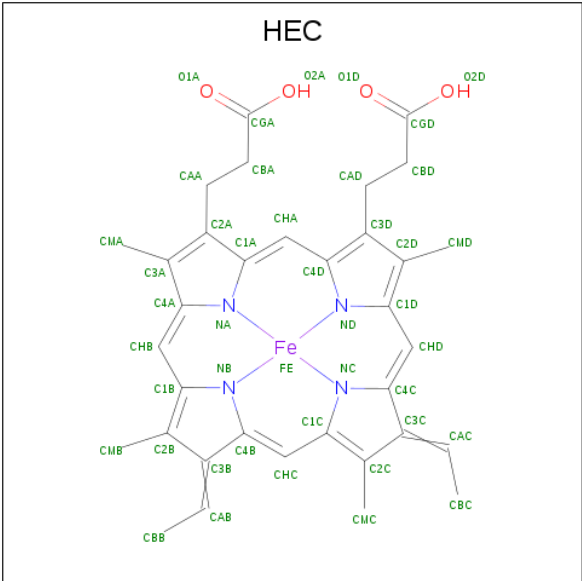
There are 9 unique types of molecules in this entry. The entry contains 16063 atoms, of which 5701 are hydrogens and 0 are deuteriums.

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	518	Total	C	H	N	O	S	0	20	0
			6896	2583	2735	752	788	38			
1	B	518	Total	C	H	N	O	S	0	17	0
			6903	2578	2746	756	786	37			

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



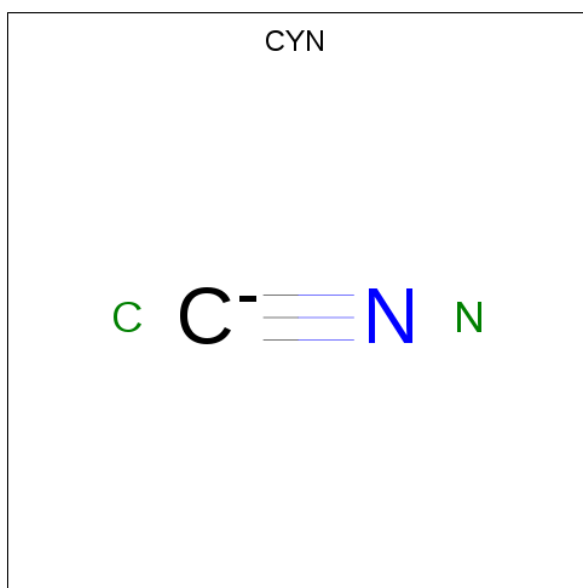
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	1
			55	34	1	12	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	1
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).

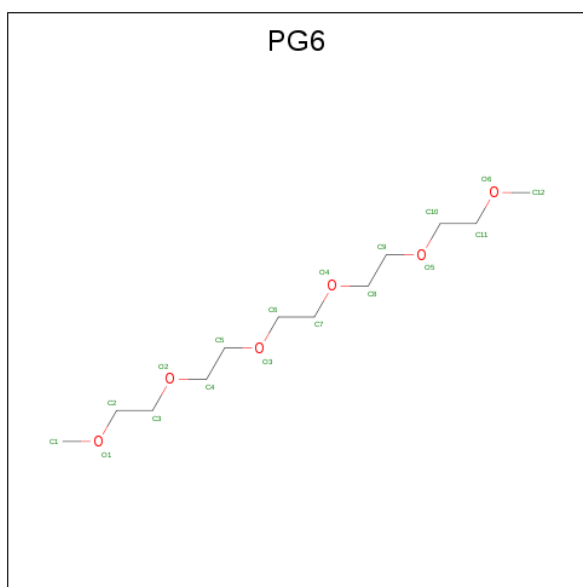


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			2	1	1		
3	B	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



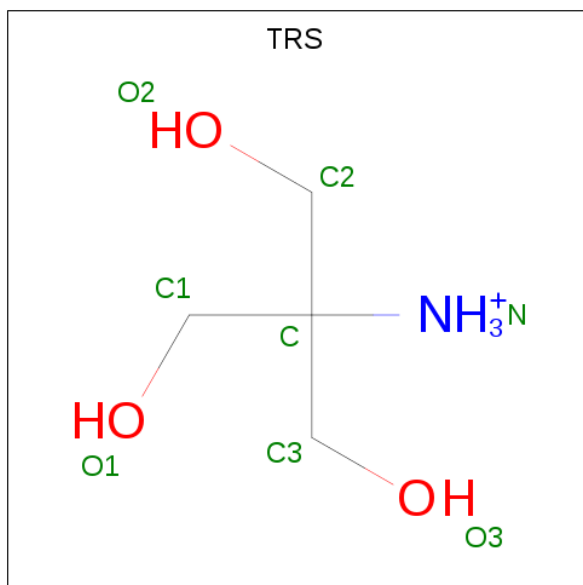
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			5	4	1		
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			8	5	3		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			5	3	2		
6	B	1	Total	C	O	0	0
			7	5	2		
6	B	1	Total	C	O	0	0
			11	7	4		
6	B	1	Total	C	O	0	0
			5	3	2		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			5	3	2		
6	B	1	Total	C	O	0	0
			5	3	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Na	0	0
			3	3		
8	A	3	Total	Na	0	0
			3	3		

- Molecule 9 is water.

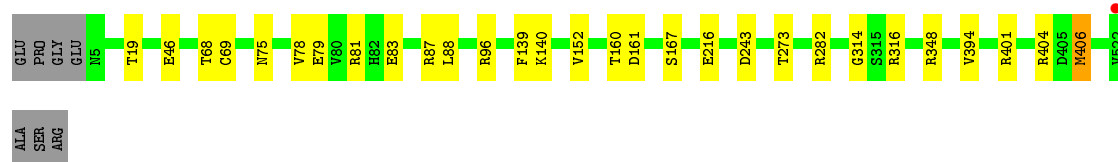
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	597	Total	O	0	0
			597	597		
9	B	621	Total	O	0	0
			621	621		

### 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 ( $RSRZ > 2$ ). 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.

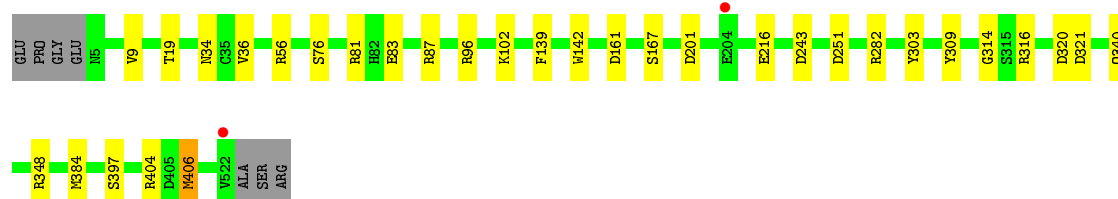
- Molecule 1: Eight-heme nitrite reductase

Chain A: 



- Molecule 1: Eight-heme nitrite reductase

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.56Å 194.56Å 194.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 1.55 11.97 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (11.98-1.55) 99.9 (11.97-1.55)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.148 , 0.162 0.159 , 0.173	Depositor DCC
$R_{free}$ test set	17636 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: NA, CA, PG6, PG4, HEC, TRS, CYN

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	0.74	1/4386 (0.0%)	0.82	9/5946 (0.2%)
1	B	0.78	3/4361 (0.1%)	0.87	15/5910 (0.3%)
All	All	0.76	4/8747 (0.0%)	0.84	24/11856 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76[A]	SER	CB-OG	-5.20	1.35	1.42
1	B	76[B]	SER	CB-OG	-5.20	1.35	1.42
1	A	83	GLU	CD-OE1	5.08	1.31	1.25
1	B	83	GLU	CD-OE1	5.04	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	404	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	87	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	96	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	81	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	56	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	282	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	404	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	251	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	161	ASP	CB-CG-OD1	5.84	123.55	118.30
1	B	320	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	87	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	401	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	243	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	404	ARG	NE-CZ-NH2	-5.52	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	303	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
1	B	201	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	81	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	161	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	96	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	161	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	87	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	243	ASP	CB-CG-OD1	5.03	122.82	118.30

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	4161	2735	3869	21	0
1	B	4157	2746	3863	22	0
2	A	344	110	212	7	0
2	B	344	110	212	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	18	0	20	2	0
5	B	5	0	4	0	0
6	A	33	0	34	5	0
6	B	60	0	64	20	0
7	A	8	0	12	0	0
8	A	3	0	0	1	0
8	B	3	0	0	1	0
9	A	597	0	0	13	0
9	B	621	0	0	9	0
All	All	10362	5701	8290	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) 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)
6:B:530:PG4:C4	9:B:658:HOH:O	1.69	1.28
1:B:316:ARG:HG3	6:B:538:PG4:O1	1.64	0.96
1:B:348[B]:ARG:HH21	6:B:532:PG4:H71	1.27	0.96
1:A:316[A]:ARG:HG3	9:A:665:HOH:O	1.73	0.88
6:B:533:PG4:H52	6:B:533:PG4:H11	1.59	0.85
1:A:273[A]:THR:HG23	9:A:983:HOH:O	1.82	0.79
1:B:316:ARG:CG	6:B:538:PG4:O1	2.31	0.78
8:B:540:NA:NA	9:B:1167:HOH:O	1.55	0.78
1:B:314:GLY:HA3	6:B:532:PG4:H72	1.66	0.77
8:A:537:NA:NA	9:A:1089:HOH:O	1.58	0.75
1:A:316[A]:ARG:HH11	1:A:316[A]:ARG:HG2	1.52	0.75
1:A:19[A]:THR:HG23	9:A:588:HOH:O	1.87	0.74
2:A:1008:HEC:HMC1	2:A:1008:HEC:HBC3	1.70	0.74
5:A:533:PG6:C2	9:A:947:HOH:O	2.34	0.73
1:B:406[B]:MET:SD	9:B:1074:HOH:O	2.46	0.73
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.71	0.71
5:A:533:PG6:H21	9:A:947:HOH:O	1.89	0.71
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.73	0.71
2:B:1002:HEC:HBC3	2:B:1002:HEC:HMC1	1.74	0.70
1:B:348[B]:ARG:NH2	6:B:532:PG4:H71	2.05	0.70
1:B:348[A]:ARG:HH21	6:B:532:PG4:H71	1.56	0.69
6:B:533:PG4:H31	9:B:1143:HOH:O	1.93	0.67
1:A:406[B]:MET:SD	9:A:989:HOH:O	2.53	0.66
1:B:9:VAL:HG13	1:B:36[B]:VAL:CG1	2.27	0.64
1:B:340:GLN:HE21	6:B:537:PG4:C3	2.10	0.64
1:A:19[B]:THR:HG22	9:A:1115:HOH:O	1.97	0.64
1:B:309:TYR:CZ	6:B:538:PG4:H11	2.33	0.63
1:B:316:ARG:NE	6:B:538:PG4:O1	2.34	0.60
1:B:348[B]:ARG:HH21	6:B:532:PG4:C7	2.07	0.59
1:B:348[B]:ARG:HD3	9:B:663:HOH:O	2.02	0.59
1:B:348[A]:ARG:HH21	6:B:532:PG4:C7	2.16	0.58
1:A:88[B]:LEU:CD1	9:A:726:HOH:O	2.52	0.56
1:B:316:ARG:HG3	6:B:538:PG4:HO1	1.70	0.56
1:A:316[A]:ARG:HG2	1:A:316[A]:ARG:NH1	2.21	0.55
1:B:384:MET:HB2	1:B:397:SER:O	2.07	0.55
1:A:348[A]:ARG:HH21	6:A:532:PG4:C7	2.20	0.54
1:A:348[B]:ARG:NH1	6:A:532:PG4:O2	2.41	0.54
2:A:1001:HEC:HMB1	2:A:1001:HEC:HBB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HB2	6:A:530:PG4:H22	1.91	0.53
2:A:1004:HEC:HBB3	2:A:1004:HEC:HMB1	1.92	0.50
2:B:1004:HEC:HBB3	2:B:1004:HEC:HMB1	1.94	0.49
6:B:530:PG4:C3	9:B:963:HOH:O	2.60	0.49
1:A:167:SER:HB2	1:A:216[A]:GLU:HG2	1.95	0.49
1:A:88[B]:LEU:HD13	9:A:726:HOH:O	2.11	0.49
1:A:88[B]:LEU:HD11	9:A:726:HOH:O	2.13	0.48
1:A:68[B]:THR:HG23	1:A:69:CYS:SG	2.55	0.47
1:B:102[A]:LYS:NZ	9:B:1095:HOH:O	2.47	0.47
6:B:530:PG4:H31	9:B:963:HOH:O	2.14	0.47
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.97	0.46
1:B:167:SER:HB2	1:B:216[B]:GLU:HG3	1.98	0.46
6:B:537:PG4:H21	9:B:919:HOH:O	2.15	0.46
2:B:1003:HEC:HMC1	2:B:1003:HEC:HBC3	1.97	0.45
1:B:142:TRP:CD2	6:B:530:PG4:H21	2.52	0.45
6:A:532:PG4:C4	6:A:532:PG4:O4	2.66	0.43
1:A:314:GLY:HA3	6:A:532:PG4:H61	2.00	0.43
2:A:1003:HEC:HBC3	2:A:1003:HEC:HMC1	2.00	0.43
1:A:78[B]:VAL:HG23	1:A:152:VAL:HG21	2.00	0.43
2:A:1001:HEC:HMC1	2:A:1001:HEC:HBC3	2.00	0.42
1:A:46[A]:GLU:HG3	9:A:993:HOH:O	2.19	0.42
1:A:75:ASN:O	1:A:79[A]:GLU:HG3	2.19	0.42
1:A:394[B]:VAL:HG12	9:A:1120:HOH:O	2.19	0.42
1:B:139:PHE:HB2	6:B:530:PG4:H22	2.01	0.42
2:A:1002:HEC:CBC	2:A:1002:HEC:HMC1	2.47	0.41
1:B:34:ASN:OD1	1:B:36[B]:VAL:HG22	2.20	0.41
1:A:140:LYS:HG2	1:A:160:THR:HG23	2.01	0.41

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	537/525 (102%)	514 (96%)	23 (4%)	0	100	100
1	B	533/525 (102%)	512 (96%)	21 (4%)	0	100	100
All	All	1070/1050 (102%)	1026 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/443 (102%)	452 (100%)	2 (0%)	91	82
1	B	453/443 (102%)	449 (99%)	4 (1%)	78	61
All	All	907/886 (102%)	901 (99%)	6 (1%)	92	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406[A]	MET
1	A	406[B]	MET
1	B	19[A]	THR
1	B	19[B]	THR
1	B	406[A]	MET
1	B	406[B]	MET

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

Mol	Chain	Res	Type
1	B	340	GLN
1	B	409	GLN
1	B	413	ASN

### 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 47 ligands modelled in this entry, 10 are monoatomic - leaving 37 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	B	1001	1	26,50,50	2.15	9 (34%)	18,82,82	1.98	6 (33%)
7	TRS	A	536	-	7,7,7	0.35	0	9,9,9	0.12	0
2	HEC	B	1004	1,3	26,50,50	2.13	6 (23%)	18,82,82	1.59	2 (11%)
2	HEC	B	1008	1	26,50,50	2.73	5 (19%)	18,82,82	1.99	4 (22%)
2	HEC	A	1005	1	26,50,50	1.97	4 (15%)	18,82,82	2.05	5 (27%)
5	PG6	A	529	-	6,6,17	0.57	0	5,5,16	0.22	0
2	HEC	A	1001	1	26,50,50	2.41	8 (30%)	18,82,82	1.91	5 (27%)
2	HEC	A	1003	1	26,50,50	2.36	5 (19%)	18,82,82	1.55	3 (16%)
6	PG4	B	538	-	3,3,12	0.34	0	2,2,11	0.59	0
6	PG4	A	535	-	7,7,12	0.49	0	6,6,11	0.37	0
6	PG4	B	534	-	4,4,12	0.50	0	3,3,11	0.21	0
6	PG4	A	534	-	5,5,12	0.49	0	4,4,11	0.24	0
2	HEC	A	1004	1,3	26,50,50	2.25	8 (30%)	18,82,82	2.06	5 (27%)
6	PG4	B	539	-	4,4,12	0.56	0	3,3,11	0.26	0
6	PG4	B	535	-	6,6,12	0.34	0	5,5,11	0.41	0
2	HEC	A	1006	1,4	26,50,50	2.28	6 (23%)	18,82,82	1.67	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PG4	A	532	-	7,7,12	0.45	0	6,6,11	0.60	0
2	HEC	A	1008	1	26,50,50	2.60	7 (26%)	18,82,82	1.77	3 (16%)
3	CYN	A	526	2	0,1,1	0.00	-	-	-	-
6	PG4	B	533	-	10,10,12	0.57	0	9,9,11	0.39	0
2	HEC	B	1005	1	26,50,50	2.10	3 (11%)	18,82,82	2.04	6 (33%)
6	PG4	A	531	-	4,4,12	0.63	0	3,3,11	0.22	0
6	PG4	A	530	-	5,5,12	0.70	0	4,4,11	0.60	0
6	PG4	B	531	-	4,4,12	0.43	0	3,3,11	0.43	0
6	PG4	B	532	-	6,6,12	0.64	0	5,5,11	0.72	0
5	PG6	A	533	-	10,10,17	0.49	0	9,9,16	0.39	0
2	HEC	B	1002	1	26,50,50	2.21	7 (26%)	18,82,82	2.19	7 (38%)
6	PG4	B	530	-	5,5,12	0.80	0	4,4,11	1.20	0
2	HEC	B	1003	1	26,50,50	2.48	6 (23%)	18,82,82	1.81	4 (22%)
3	CYN	B	526	2	0,1,1	0.00	-	-	-	-
2	HEC	A	1002	1	26,50,50	2.22	9 (34%)	18,82,82	1.82	4 (22%)
2	HEC	B	1006	1,4	26,50,50	2.14	7 (26%)	18,82,82	1.76	6 (33%)
6	PG4	B	537	-	4,4,12	0.40	0	3,3,11	0.47	0
6	PG4	B	536	-	4,4,12	0.40	0	3,3,11	0.46	0
5	PG6	B	529	-	4,4,17	0.53	0	3,3,16	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1001	1	-	0/6/54/54	-
7	TRS	A	536	-	-	9/9/9/9	-
2	HEC	B	1004	1,3	-	0/6/54/54	-
2	HEC	B	1008	1	-	0/6/54/54	-
2	HEC	A	1005	1	-	0/6/54/54	-
5	PG6	A	529	-	-	2/4/4/15	-
2	HEC	A	1001	1	-	0/6/54/54	-
2	HEC	A	1003	1	-	0/6/54/54	-
6	PG4	B	538	-	-	1/1/1/10	-
6	PG4	A	535	-	-	4/5/5/10	-
6	PG4	B	534	-	-	1/2/2/10	-
6	PG4	A	534	-	-	2/3/3/10	-
2	HEC	A	1004	1,3	-	0/6/54/54	-
6	PG4	B	539	-	-	2/2/2/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	B	535	-	-	2/4/4/10	-
2	HEC	A	1006	1,4	-	0/6/54/54	-
6	PG4	A	532	-	-	3/5/5/10	-
2	HEC	A	1008	1	-	0/6/54/54	-
6	PG4	B	537	-	-	2/2/2/10	-
6	PG4	B	533	-	-	5/8/8/10	-
2	HEC	B	1005	1	-	0/6/54/54	-
6	PG4	A	531	-	-	2/2/2/10	-
6	PG4	A	530	-	-	0/3/3/10	-
6	PG4	B	531	-	-	2/2/2/10	-
6	PG4	B	532	-	-	1/4/4/10	-
5	PG6	A	533	-	-	4/8/8/15	-
2	HEC	B	1002	1	-	0/6/54/54	-
6	PG4	B	530	-	-	1/3/3/10	-
2	HEC	B	1003	1	-	0/6/54/54	-
2	HEC	A	1002	1	-	0/6/54/54	-
2	HEC	B	1006	1,4	-	0/6/54/54	-
6	PG4	B	536	-	-	2/2/2/10	-
5	PG6	B	529	-	-	0/2/2/15	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1008	HEC	C3B-C2B	-9.28	1.31	1.40
2	A	1008	HEC	C3C-C2C	-8.03	1.32	1.40
2	B	1003	HEC	C3C-C2C	-7.72	1.32	1.40
2	A	1003	HEC	C3C-C2C	-7.43	1.33	1.40
2	B	1008	HEC	C3C-C2C	-7.13	1.33	1.40
2	B	1004	HEC	C3C-C2C	-6.81	1.33	1.40
2	A	1004	HEC	C3C-C2C	-6.72	1.33	1.40
2	A	1008	HEC	C3B-C2B	-6.63	1.33	1.40
2	A	1001	HEC	C3C-C2C	-6.58	1.33	1.40
2	B	1003	HEC	C3B-C2B	-6.52	1.33	1.40
2	B	1006	HEC	C3C-C2C	-6.49	1.34	1.40
2	A	1006	HEC	C3B-C2B	-6.37	1.34	1.40
2	B	1005	HEC	C3B-C2B	-6.22	1.34	1.40
2	A	1003	HEC	C3B-C2B	-6.17	1.34	1.40
2	B	1005	HEC	C3C-C2C	-5.94	1.34	1.40
2	A	1005	HEC	C3B-C2B	-5.85	1.34	1.40
2	A	1002	HEC	C3B-C2B	-5.82	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	HEC	C3C-C2C	-5.71	1.34	1.40
2	B	1002	HEC	C3C-C2C	-5.45	1.35	1.40
2	A	1001	HEC	C3B-C2B	-5.42	1.35	1.40
2	B	1001	HEC	C3C-C2C	-5.27	1.35	1.40
2	A	1005	HEC	C3C-C2C	-5.09	1.35	1.40
2	B	1002	HEC	C3B-C2B	-4.85	1.35	1.40
2	A	1004	HEC	C3B-C2B	-4.63	1.35	1.40
2	B	1001	HEC	C3B-C2B	-4.38	1.36	1.40
2	B	1006	HEC	C3B-C2B	-4.36	1.36	1.40
2	A	1002	HEC	C3C-C2C	-4.34	1.36	1.40
2	A	1008	HEC	C3D-C2D	4.04	1.49	1.37
2	A	1001	HEC	C3D-C2D	4.01	1.49	1.37
2	B	1001	HEC	C3D-C2D	3.91	1.49	1.37
2	B	1004	HEC	C3B-C2B	-3.88	1.36	1.40
2	B	1003	HEC	C3D-C2D	3.73	1.48	1.37
2	A	1006	HEC	C3D-C2D	3.63	1.48	1.37
2	B	1002	HEC	C3D-C2D	3.56	1.48	1.37
2	B	1008	HEC	C3D-C2D	3.56	1.48	1.37
2	A	1003	HEC	C3D-C2D	3.45	1.47	1.37
2	B	1006	HEC	C3D-C2D	3.40	1.47	1.37
2	B	1002	HEC	C3B-C4B	3.33	1.49	1.43
2	A	1002	HEC	C3D-C2D	3.31	1.47	1.37
2	A	1002	HEC	C1D-ND	3.25	1.42	1.36
2	A	1001	HEC	C1D-ND	3.22	1.42	1.36
2	B	1002	HEC	C1B-NB	3.16	1.42	1.36
2	A	1004	HEC	C3D-C2D	3.15	1.47	1.37
2	A	1005	HEC	C3D-C2D	3.02	1.46	1.37
2	B	1004	HEC	C3C-C4C	2.84	1.48	1.43
2	A	1002	HEC	C3B-C4B	2.82	1.48	1.43
2	B	1005	HEC	C3D-C2D	2.79	1.45	1.37
2	B	1001	HEC	C1B-NB	2.76	1.41	1.36
2	B	1001	HEC	C1D-ND	2.76	1.41	1.36
2	A	1001	HEC	CMB-C2B	2.75	1.58	1.51
2	B	1004	HEC	C3D-C2D	2.73	1.45	1.37
2	A	1001	HEC	C3B-C4B	2.69	1.47	1.43
2	A	1002	HEC	CMB-C2B	2.65	1.57	1.51
2	A	1008	HEC	C4D-ND	2.63	1.41	1.36
2	B	1002	HEC	C1D-ND	2.60	1.41	1.36
2	A	1006	HEC	C3C-C4C	2.60	1.47	1.43
2	A	1002	HEC	C1B-NB	2.54	1.41	1.36
2	B	1006	HEC	C1A-C2A	2.50	1.48	1.42
2	A	1008	HEC	CMD-C2D	2.44	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	HEC	CMB-C2B	2.43	1.57	1.51
2	A	1004	HEC	CMC-C2C	2.41	1.57	1.51
2	A	1006	HEC	C1A-C2A	2.40	1.48	1.42
2	B	1004	HEC	CMB-C2B	2.38	1.57	1.51
2	A	1005	HEC	CBB-CAB	2.38	1.58	1.49
2	A	1003	HEC	C1D-ND	2.37	1.41	1.36
2	B	1008	HEC	CMC-C2C	2.37	1.57	1.51
2	A	1001	HEC	CMD-C2D	2.36	1.56	1.51
2	A	1008	HEC	C1D-ND	2.33	1.41	1.36
2	A	1001	HEC	CBB-CAB	2.32	1.58	1.49
2	A	1004	HEC	C4D-ND	2.32	1.40	1.36
2	A	1008	HEC	CAD-C3D	2.30	1.55	1.52
2	A	1006	HEC	C4D-ND	2.29	1.40	1.36
2	A	1004	HEC	C3C-C4C	2.26	1.47	1.43
2	B	1004	HEC	C4D-ND	2.26	1.40	1.36
2	A	1002	HEC	C1D-CHD	-2.23	1.34	1.41
2	B	1001	HEC	C3C-C4C	2.22	1.47	1.43
2	B	1003	HEC	CMD-C2D	2.17	1.56	1.51
2	B	1006	HEC	C4D-ND	2.15	1.40	1.36
2	B	1001	HEC	CBB-CAB	2.12	1.57	1.49
2	A	1004	HEC	C1C-NC	2.11	1.40	1.36
2	B	1002	HEC	CMA-C3A	2.09	1.56	1.51
2	B	1008	HEC	CAA-C2A	2.06	1.55	1.52
2	B	1001	HEC	C4D-ND	2.06	1.40	1.36
2	B	1001	HEC	CMA-C3A	2.05	1.56	1.51
2	B	1006	HEC	C2A-C3A	-2.03	1.31	1.37
2	A	1003	HEC	CMB-C2B	2.02	1.56	1.51
2	B	1006	HEC	C3C-C4C	2.02	1.46	1.43
2	A	1004	HEC	CAD-C3D	2.01	1.55	1.52
2	A	1002	HEC	CMA-C3A	2.01	1.56	1.51
2	B	1003	HEC	CBB-CAB	2.01	1.57	1.49

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	HEC	CMC-C2C-C1C	-5.28	120.34	128.46
2	B	1005	HEC	CMB-C2B-C1B	-5.28	120.35	128.46
2	B	1008	HEC	CMB-C2B-C1B	-5.19	120.48	128.46
2	B	1002	HEC	CMB-C2B-C1B	-4.97	120.82	128.46
2	B	1003	HEC	CMB-C2B-C1B	-4.82	121.06	128.46
2	A	1005	HEC	CMB-C2B-C1B	-4.81	121.07	128.46
2	A	1002	HEC	CMB-C2B-C1B	-4.53	121.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	HEC	CMB-C2B-C1B	-4.22	121.98	128.46
2	A	1001	HEC	CMB-C2B-C1B	-4.17	122.06	128.46
2	A	1008	HEC	CMC-C2C-C1C	-4.15	122.09	128.46
2	B	1006	HEC	CMC-C2C-C1C	-4.09	122.18	128.46
2	A	1004	HEC	C1D-C2D-C3D	-4.06	104.17	107.00
2	A	1003	HEC	CMB-C2B-C1B	-4.03	122.27	128.46
2	B	1008	HEC	CMC-C2C-C1C	-3.99	122.33	128.46
2	B	1004	HEC	C1D-C2D-C3D	-3.82	104.34	107.00
2	B	1005	HEC	CMC-C2C-C1C	-3.78	122.66	128.46
2	A	1002	HEC	CAA-CBA-CGA	-3.77	106.34	112.67
2	B	1001	HEC	CMC-C2C-C1C	-3.76	122.69	128.46
2	B	1002	HEC	CMC-C2C-C1C	-3.73	122.73	128.46
2	A	1001	HEC	CMC-C2C-C1C	-3.71	122.76	128.46
2	A	1008	HEC	CMB-C2B-C1B	-3.71	122.77	128.46
2	A	1006	HEC	CMC-C2C-C1C	-3.59	122.94	128.46
2	B	1004	HEC	CMC-C2C-C1C	-3.57	122.98	128.46
2	A	1005	HEC	CMC-C2C-C1C	-3.48	123.11	128.46
2	A	1005	HEC	CMB-C2B-C3B	3.45	129.88	125.82
2	B	1002	HEC	CMC-C2C-C3C	3.22	129.60	125.82
2	B	1002	HEC	CAA-CBA-CGA	-3.20	107.30	112.67
2	B	1002	HEC	C4B-C3B-C2B	-3.19	102.91	106.35
2	A	1005	HEC	CAD-CBD-CGD	-3.13	107.41	112.67
2	A	1006	HEC	CMB-C2B-C1B	-3.04	123.80	128.46
2	B	1002	HEC	CAD-CBD-CGD	2.97	117.66	112.67
2	A	1001	HEC	CAD-CBD-CGD	-2.97	107.69	112.67
2	A	1001	HEC	CMC-C2C-C3C	2.96	129.30	125.82
2	B	1003	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
2	A	1004	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
2	B	1006	HEC	CMB-C2B-C1B	-2.82	124.12	128.46
2	B	1001	HEC	CBD-CAD-C3D	-2.82	107.29	112.49
2	A	1002	HEC	CAD-CBD-CGD	2.78	117.34	112.67
2	A	1001	HEC	C4B-C3B-C2B	-2.78	103.36	106.35
2	B	1008	HEC	CBD-CAD-C3D	-2.76	107.40	112.49
2	B	1005	HEC	CMB-C2B-C3B	2.72	129.02	125.82
2	A	1004	HEC	CMC-C2C-C3C	2.69	128.99	125.82
2	B	1003	HEC	CAA-CBA-CGA	2.58	117.00	112.67
2	B	1006	HEC	CMA-C3A-C2A	2.57	129.78	124.94
2	B	1006	HEC	CMD-C2D-C1D	-2.53	124.57	128.46
2	B	1001	HEC	C1D-C2D-C3D	2.52	108.75	107.00
2	B	1001	HEC	CAD-CBD-CGD	2.50	116.86	112.67
2	B	1001	HEC	CAA-CBA-CGA	2.48	116.83	112.67
2	B	1005	HEC	CMC-C2C-C3C	2.45	128.70	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	HEC	CBA-CAA-C2A	-2.30	108.24	112.48
2	A	1006	HEC	CMA-C3A-C2A	2.28	129.24	124.94
2	A	1004	HEC	CMB-C2B-C3B	2.22	128.43	125.82
2	B	1002	HEC	C1D-C2D-C3D	2.22	108.54	107.00
2	A	1003	HEC	CAA-CBA-CGA	2.20	116.37	112.67
2	B	1008	HEC	CBA-CAA-C2A	-2.14	108.53	112.48
2	A	1006	HEC	CMD-C2D-C1D	-2.12	125.20	128.46
2	A	1003	HEC	CBA-CAA-C2A	-2.12	108.58	112.48
2	B	1006	HEC	CMD-C2D-C3D	2.12	128.94	124.94
2	A	1008	HEC	CMD-C2D-C1D	-2.12	125.21	128.46
2	A	1002	HEC	C4B-C3B-C2B	-2.11	104.07	106.35
2	B	1005	HEC	CMA-C3A-C2A	2.09	128.88	124.94
2	A	1006	HEC	CMB-C2B-C3B	2.08	128.27	125.82
2	A	1005	HEC	CMA-C3A-C2A	2.06	128.82	124.94
2	B	1006	HEC	CMC-C2C-C3C	2.01	128.19	125.82
2	B	1005	HEC	CAD-CBD-CGD	-2.01	109.30	112.67

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	536	TRS	C2-C-C1-O1
7	A	536	TRS	C3-C-C1-O1
7	A	536	TRS	N-C-C1-O1
7	A	536	TRS	C1-C-C3-O3
6	B	533	PG4	C1-C2-O2-C3
6	B	535	PG4	C4-C3-O2-C2
6	B	539	PG4	O2-C3-C4-O3
6	B	533	PG4	O3-C5-C6-O4
6	B	530	PG4	C1-C2-O2-C3
6	B	533	PG4	O2-C3-C4-O3
5	A	533	PG6	O3-C6-C7-O4
6	A	532	PG4	O2-C3-C4-O3
6	A	535	PG4	O2-C3-C4-O3
6	A	535	PG4	O1-C1-C2-O2
6	A	534	PG4	O1-C1-C2-O2
6	B	534	PG4	O1-C1-C2-O2
5	A	533	PG6	C6-C7-O4-C8
6	B	532	PG4	O3-C5-C6-O4
6	A	532	PG4	C6-C5-O3-C4
5	A	533	PG6	O2-C4-C5-O3
7	A	536	TRS	C3-C-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	537	PG4	O1-C1-C2-O2
6	A	531	PG4	C1-C2-O2-C3
6	A	534	PG4	C4-C3-O2-C2
6	B	537	PG4	C1-C2-O2-C3
6	B	535	PG4	C1-C2-O2-C3
6	A	535	PG4	C4-C3-O2-C2
6	B	531	PG4	C1-C2-O2-C3
5	A	529	PG6	C2-C3-O2-C4
7	A	536	TRS	N-C-C2-O2
7	A	536	TRS	C2-C-C3-O3
7	A	536	TRS	N-C-C3-O3
6	B	533	PG4	O1-C1-C2-O2
6	B	531	PG4	O1-C1-C2-O2
6	B	533	PG4	C4-C3-O2-C2
6	A	532	PG4	C5-C6-O4-C7
6	A	531	PG4	C4-C3-O2-C2
7	A	536	TRS	C1-C-C2-O2
6	B	539	PG4	C4-C3-O2-C2
6	B	536	PG4	O1-C1-C2-O2
6	B	538	PG4	O1-C1-C2-O2
6	A	535	PG4	C3-C4-O3-C5
5	A	529	PG6	O2-C4-C5-O3
5	A	533	PG6	C4-C5-O3-C6
6	B	536	PG4	C1-C2-O2-C3

There are no ring outliers.

17 monomers are involved in 38 short contacts:

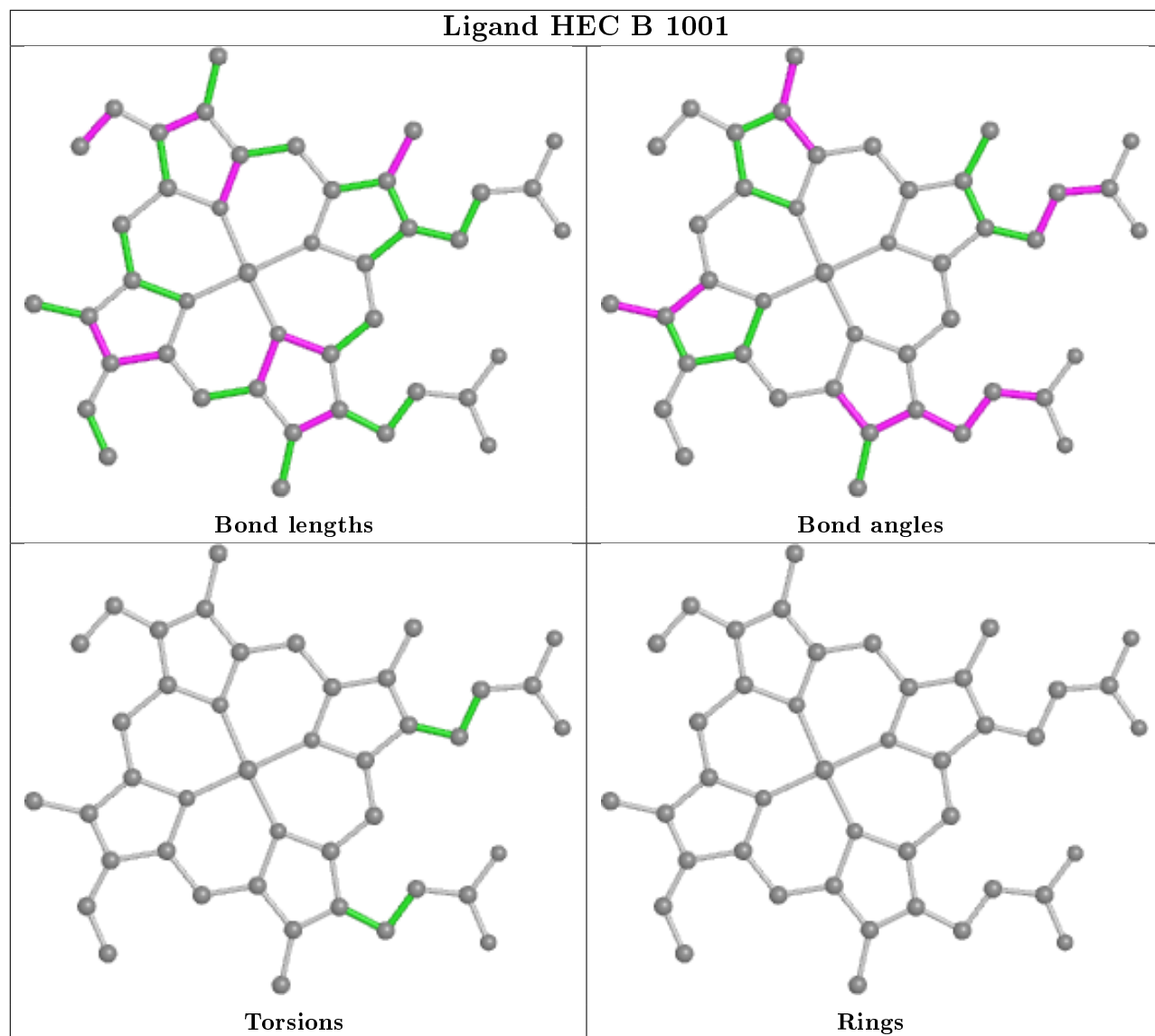
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1004	HEC	1	0
2	B	1008	HEC	1	0
2	A	1001	HEC	2	0
2	A	1003	HEC	1	0
6	B	538	PG4	5	0
2	A	1004	HEC	1	0
6	A	532	PG4	4	0
2	A	1008	HEC	1	0
6	B	533	PG4	2	0
6	A	530	PG4	1	0
6	B	532	PG4	6	0
5	A	533	PG6	2	0
2	B	1002	HEC	1	0

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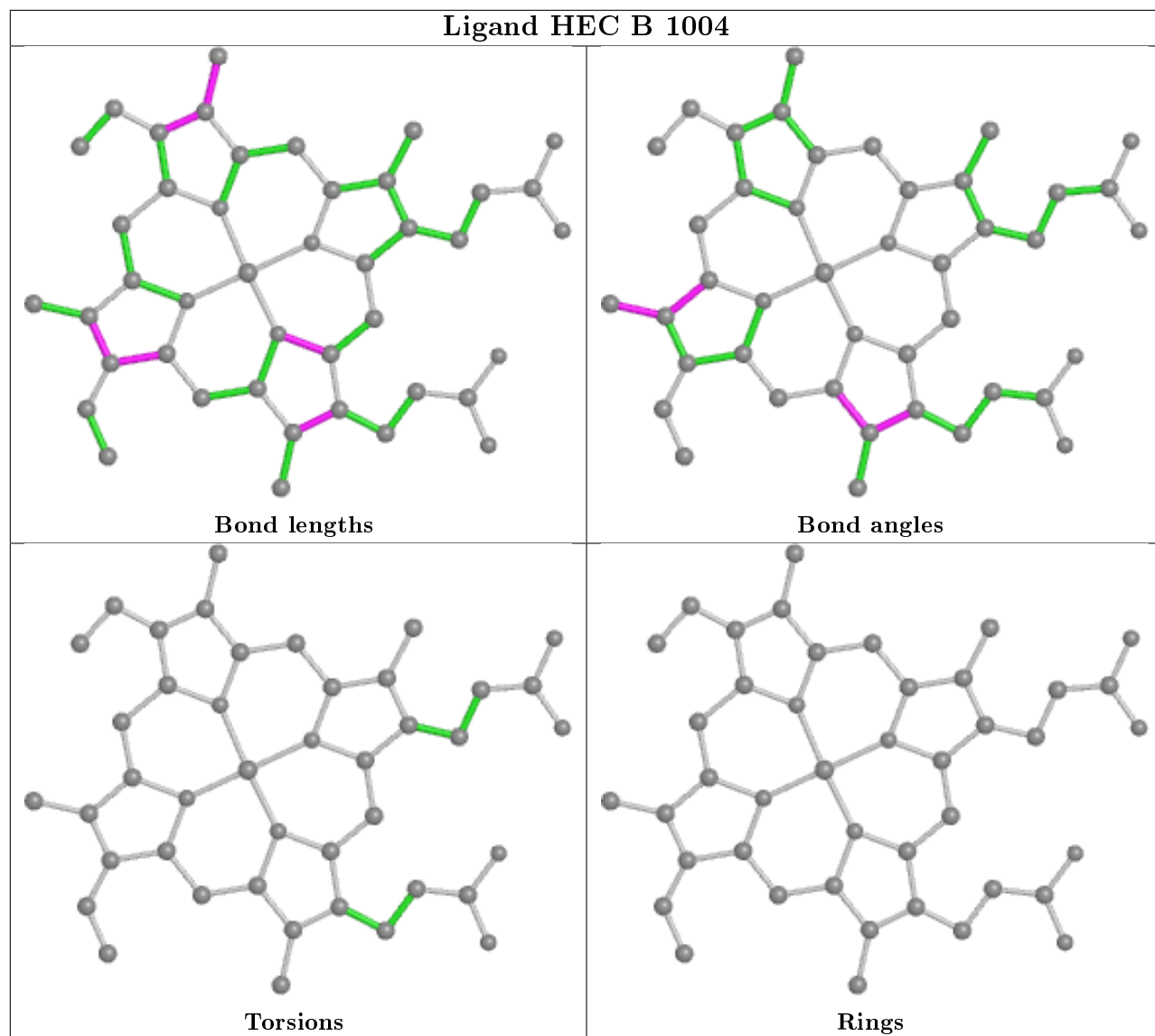
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	530	PG4	5	0
2	B	1003	HEC	1	0
2	A	1002	HEC	2	0
6	B	537	PG4	2	0

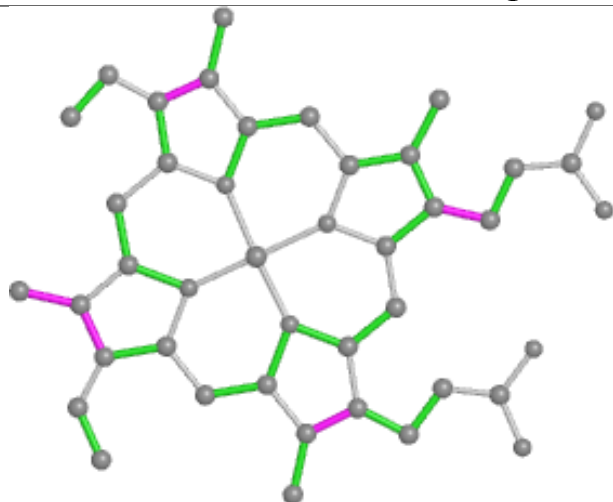
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



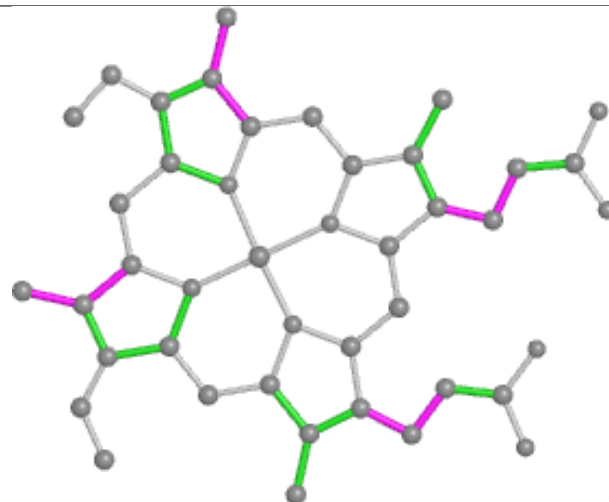




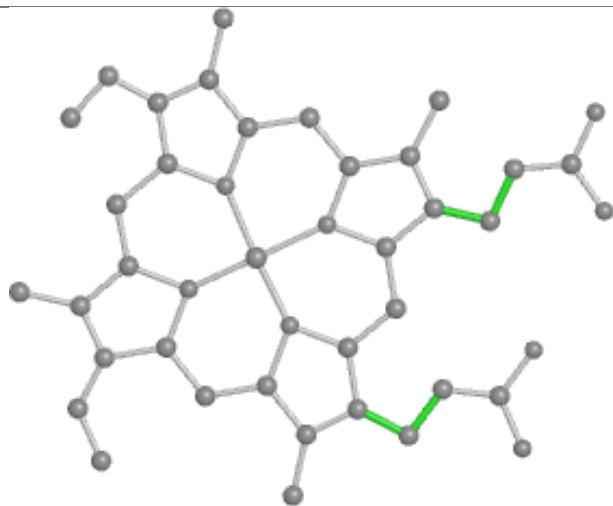
## Ligand HEC B 1008



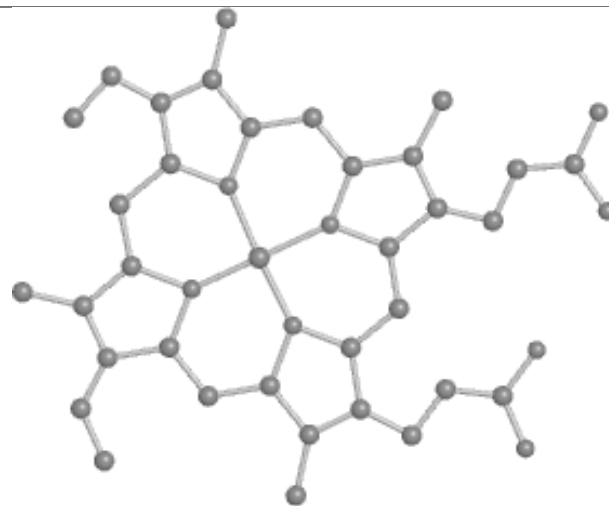
Bond lengths



Bond angles

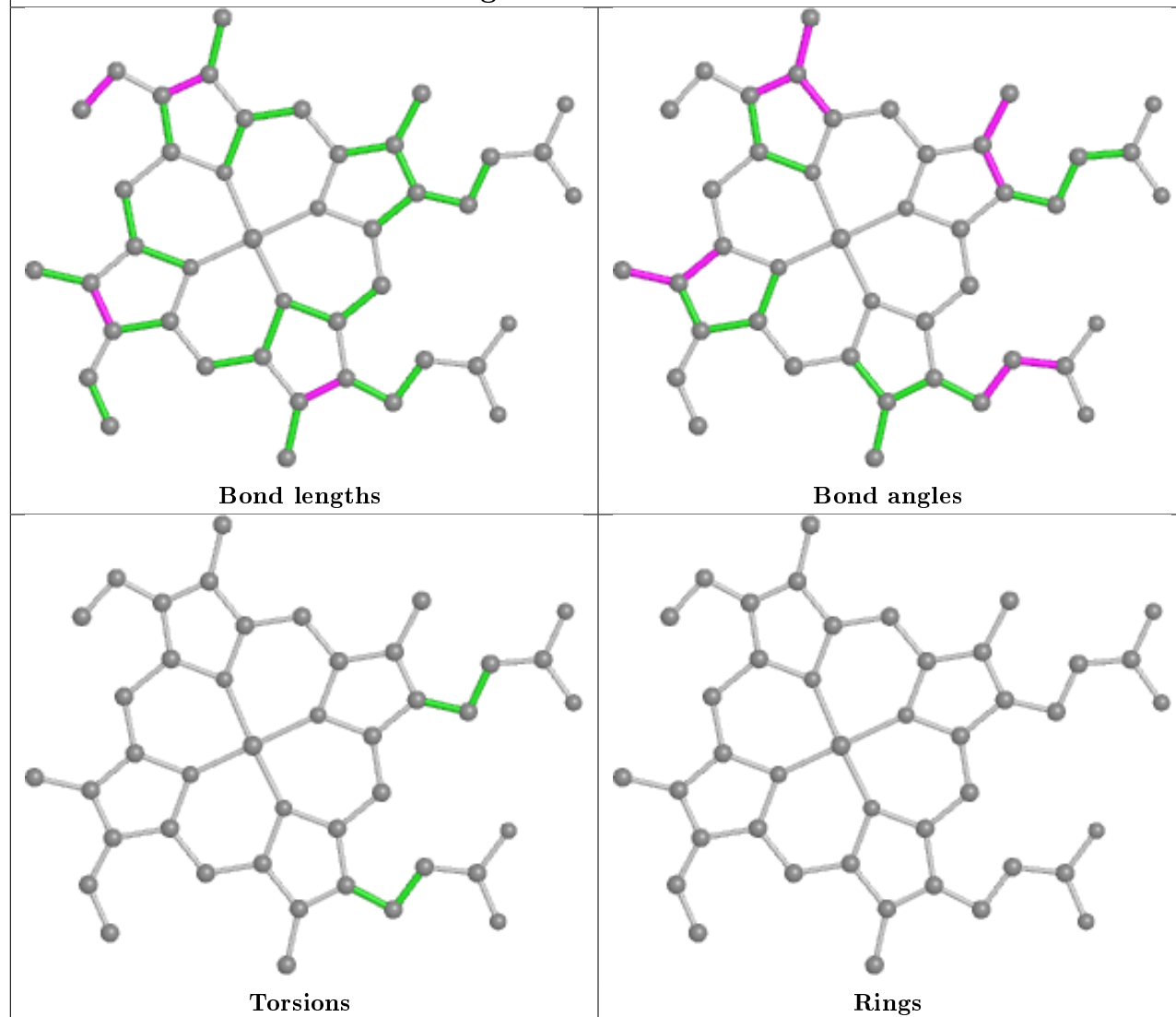


Torsions

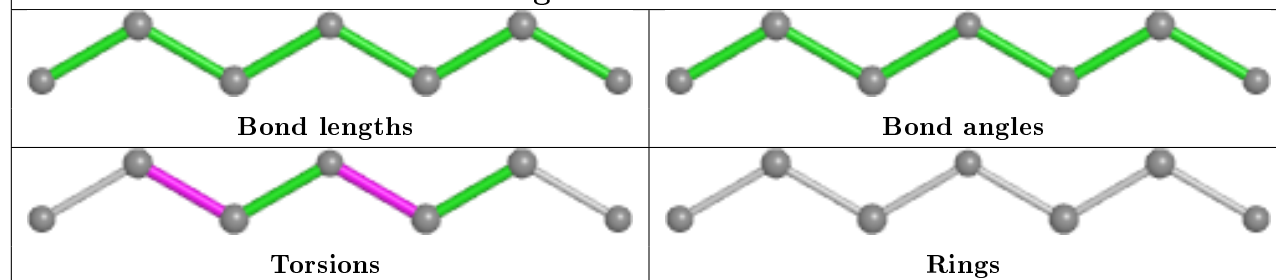


Rings

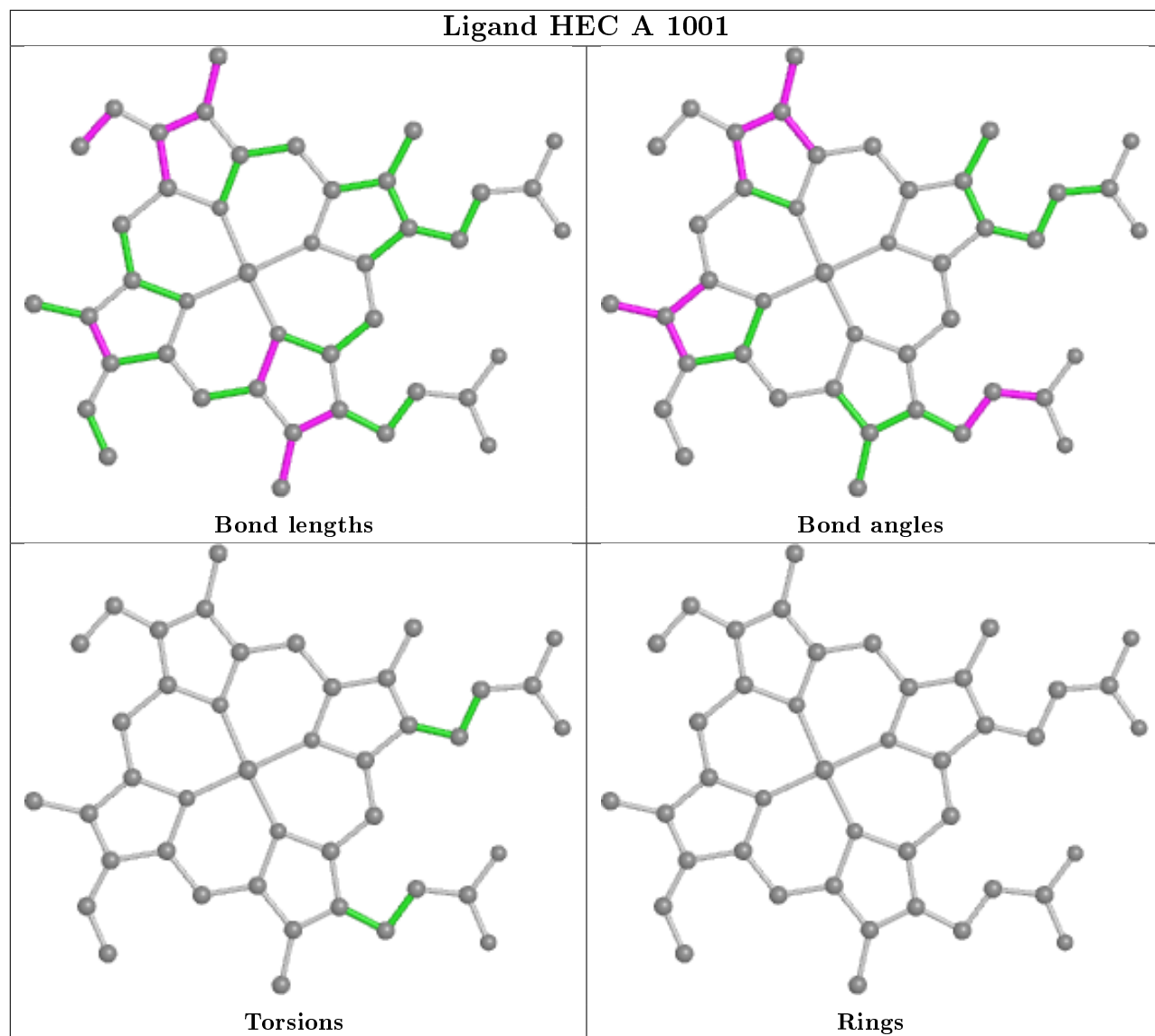
## Ligand HEC A 1005



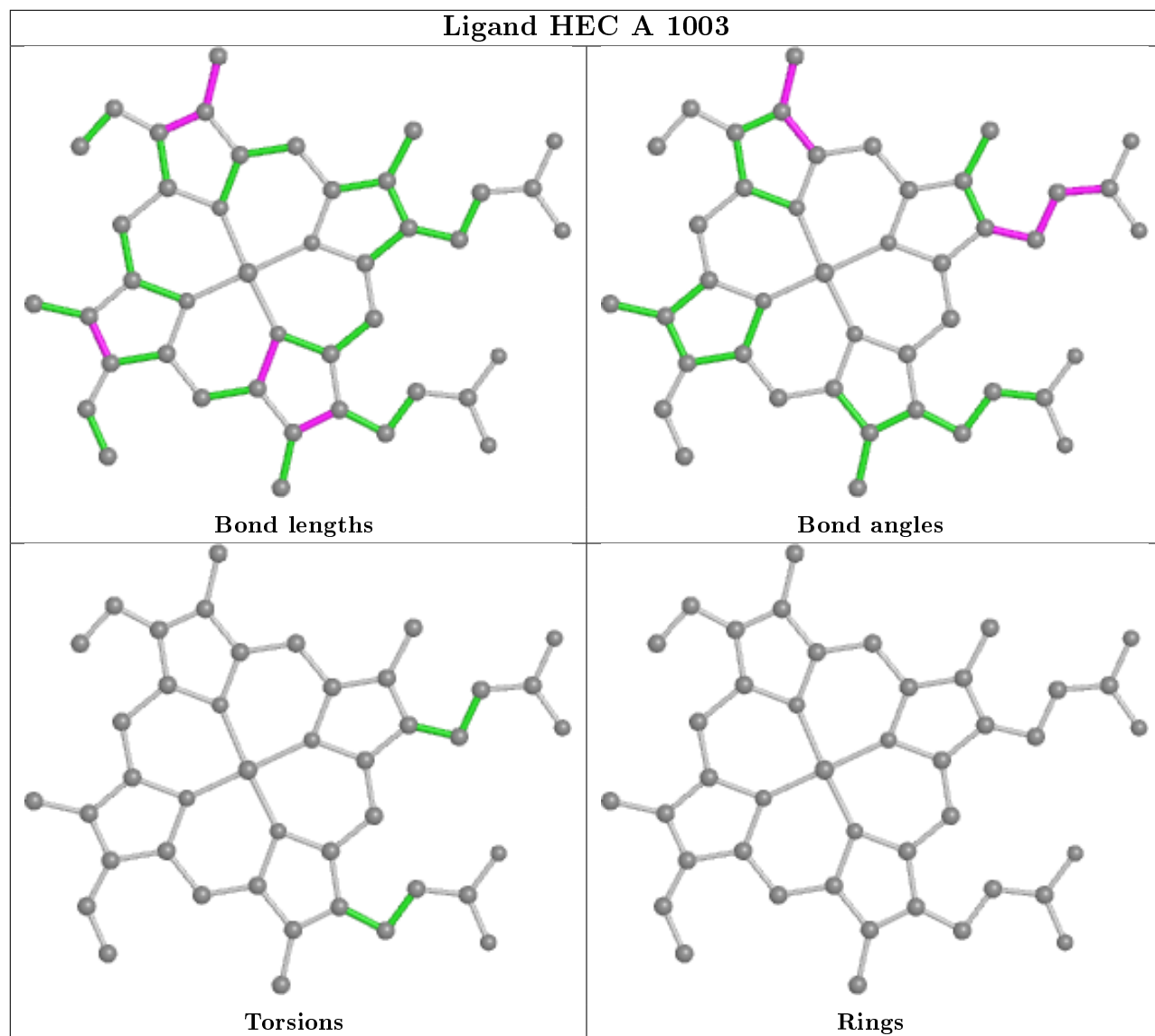
## Ligand PG6 A 529

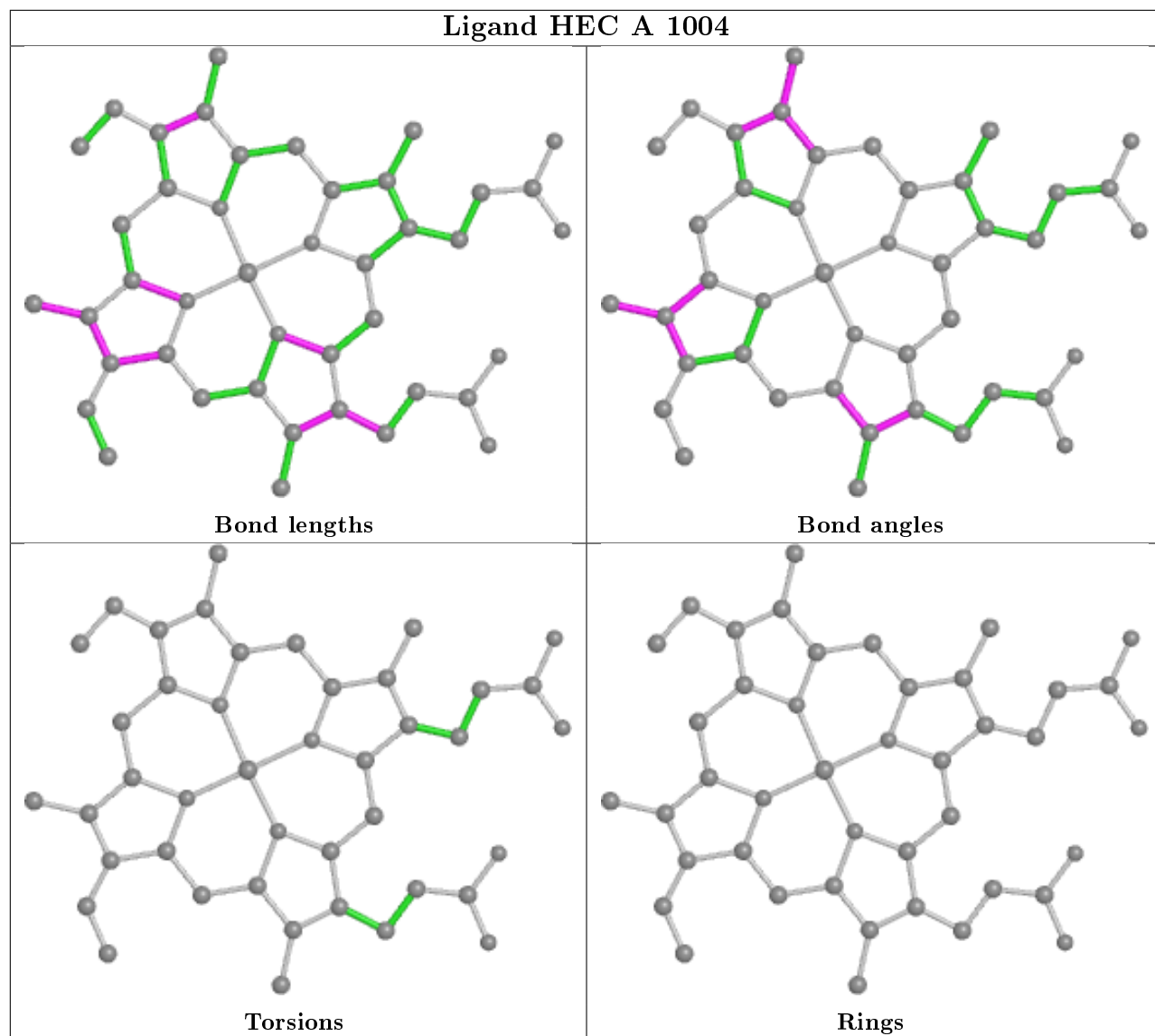


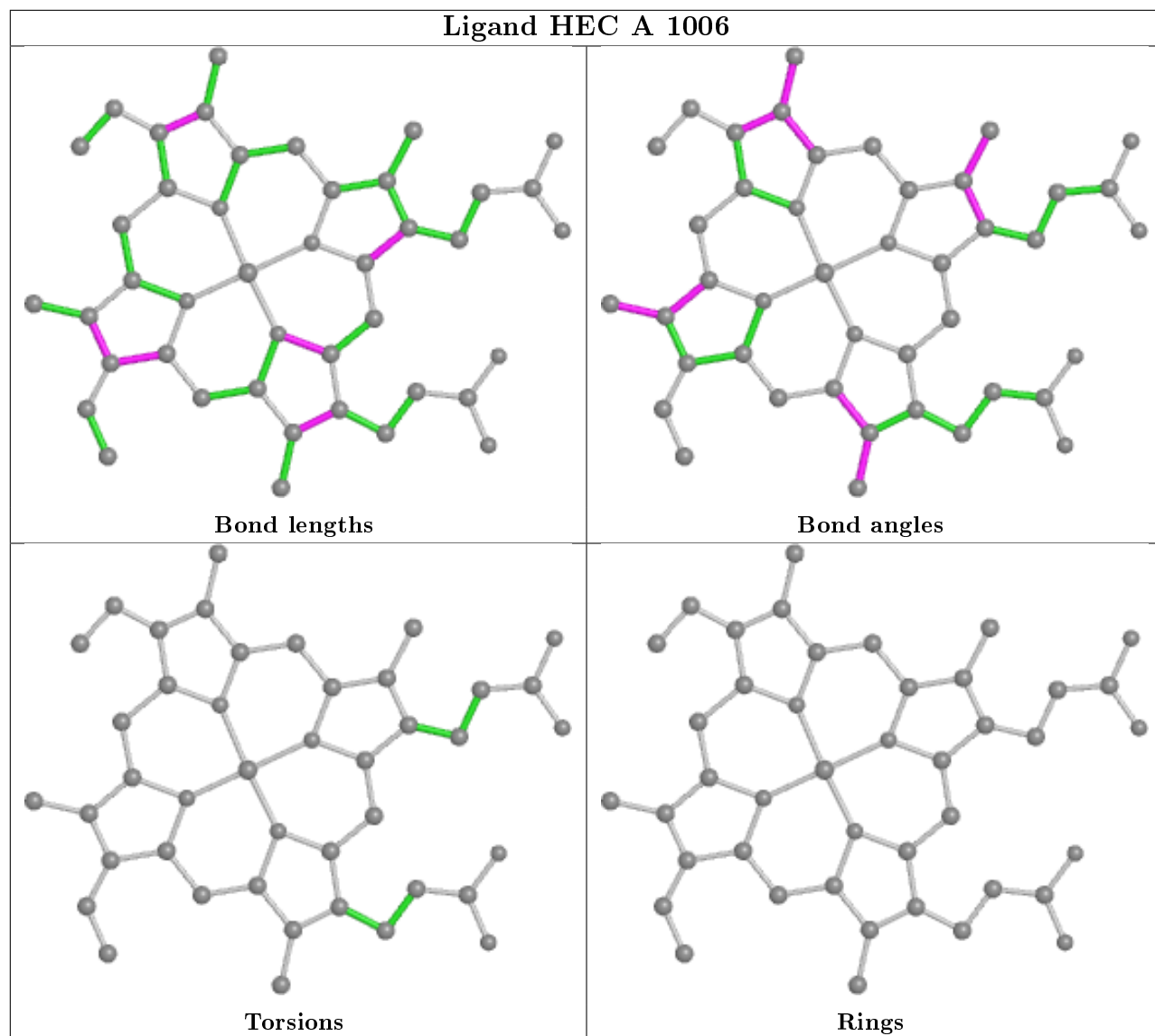
## Ligand HEC A 1001

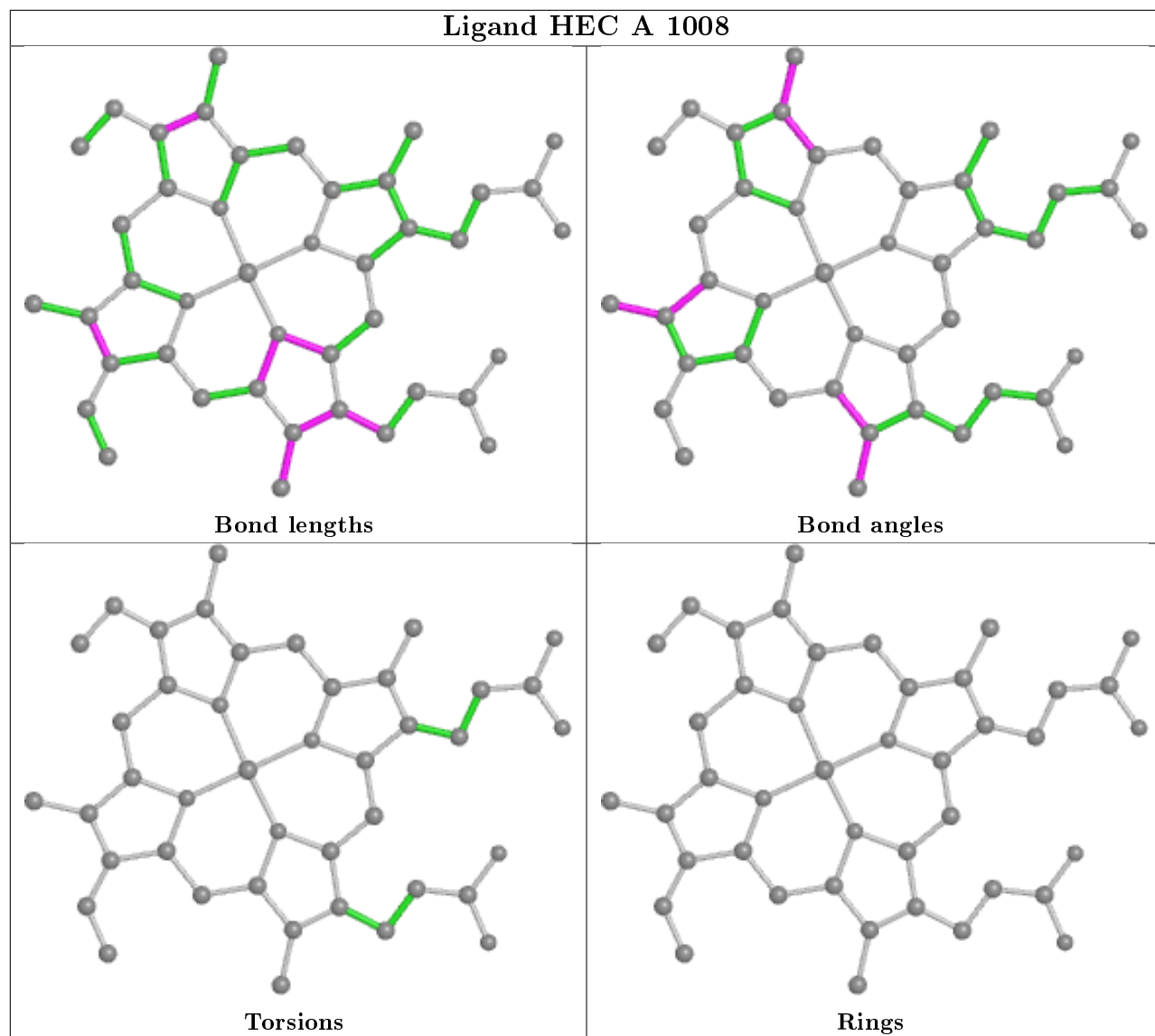


## Ligand HEC A 1003



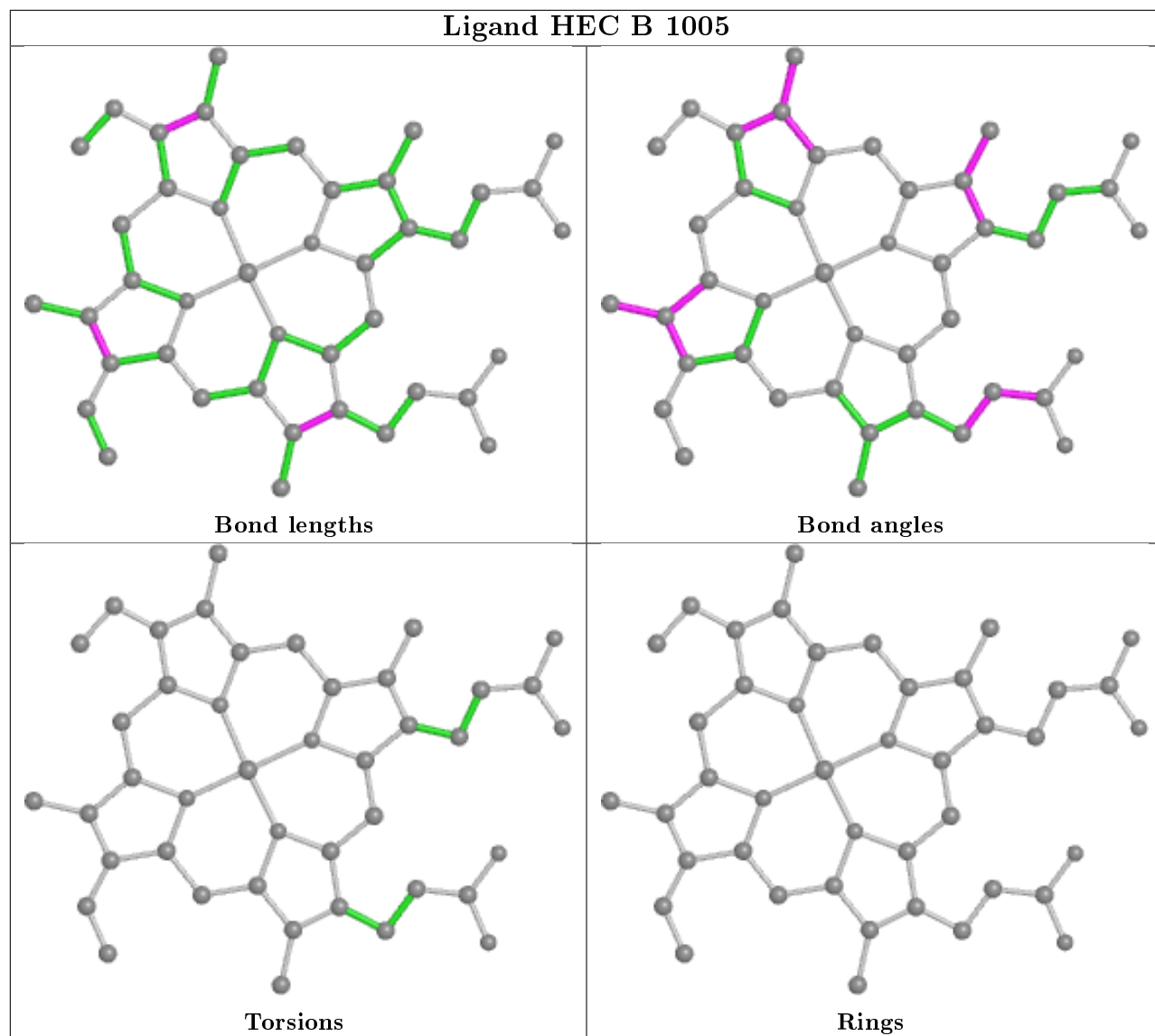




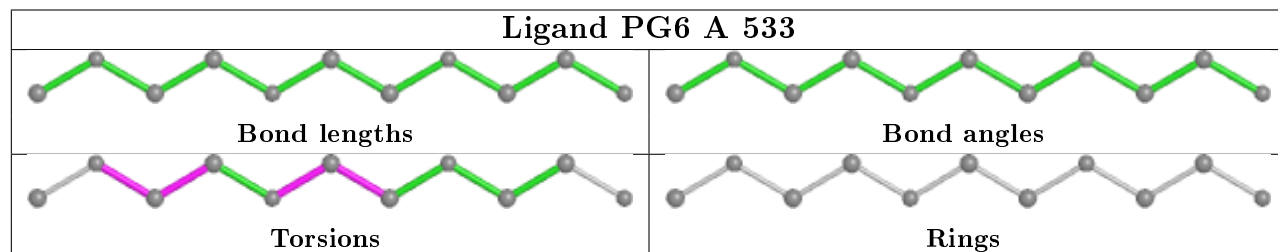




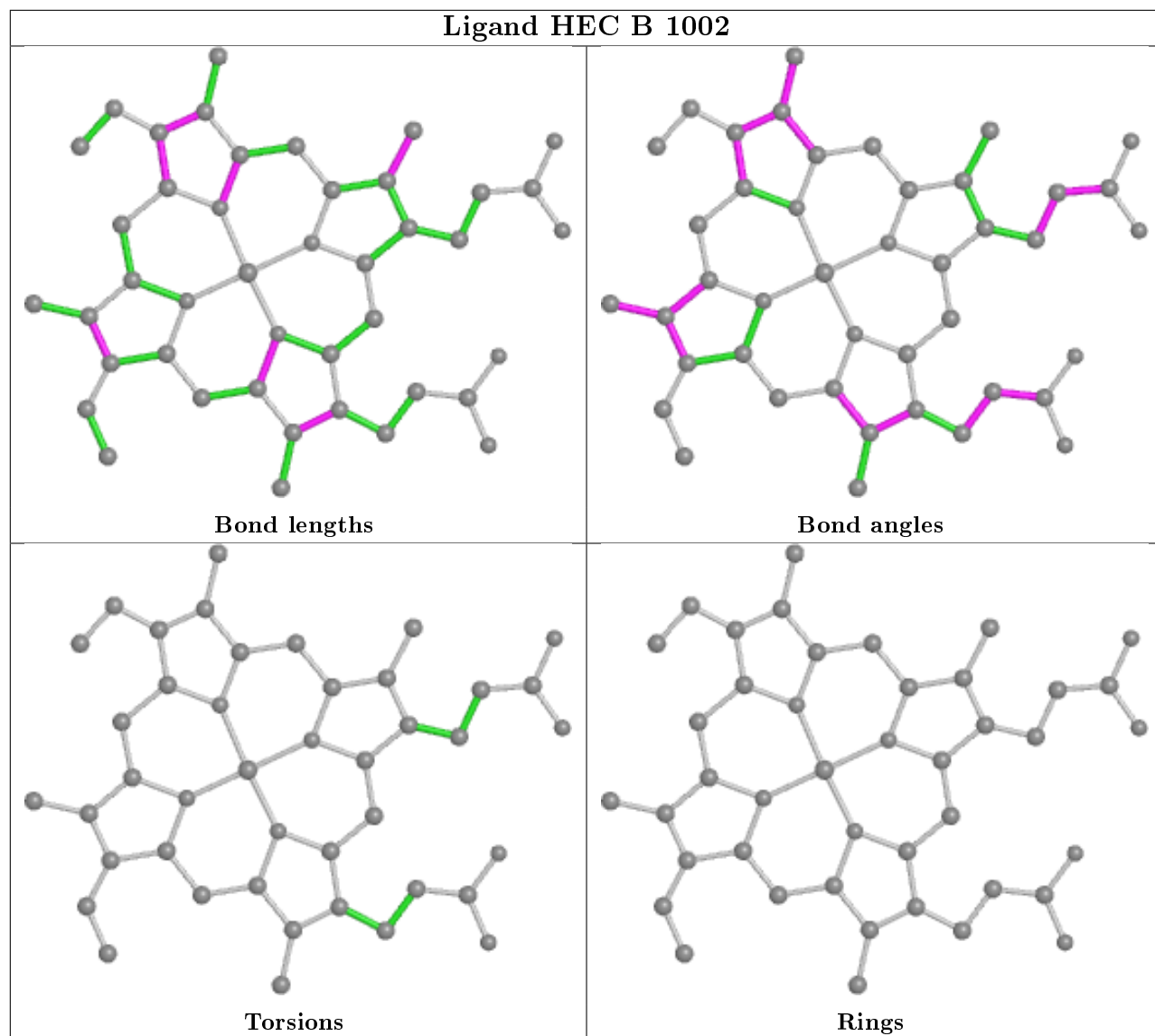
## Ligand HEC B 1005

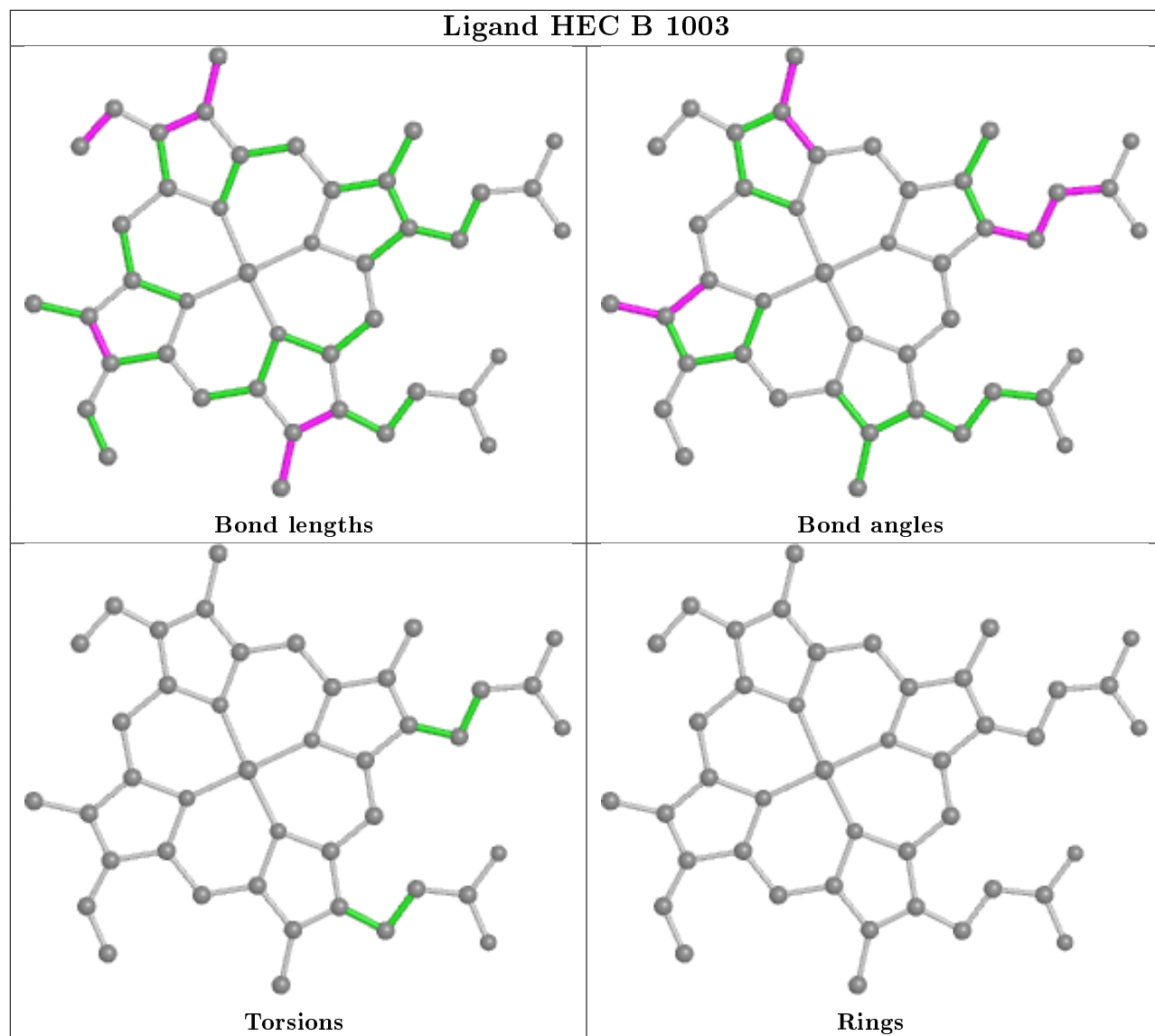


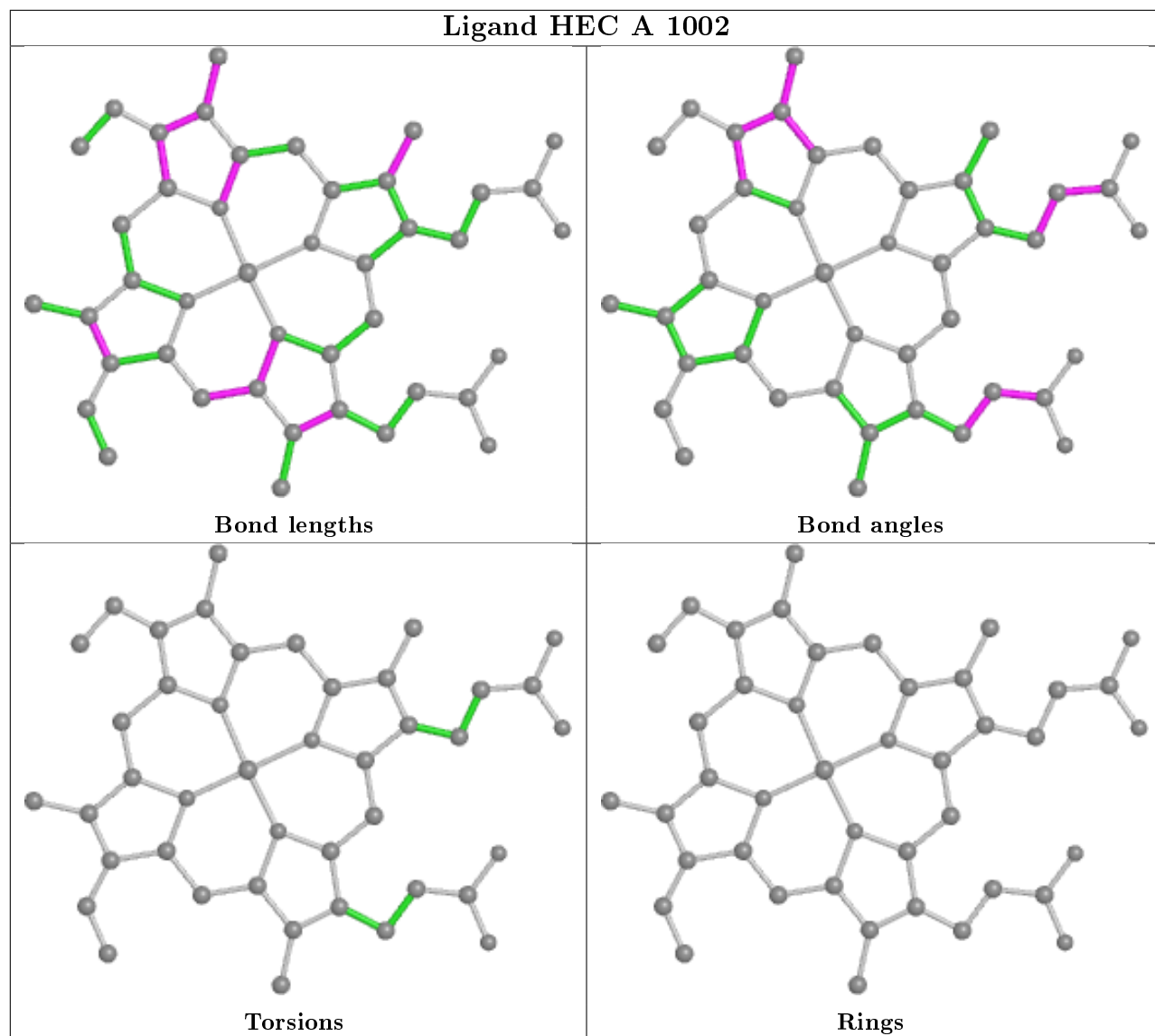
## Ligand PG6 A 533

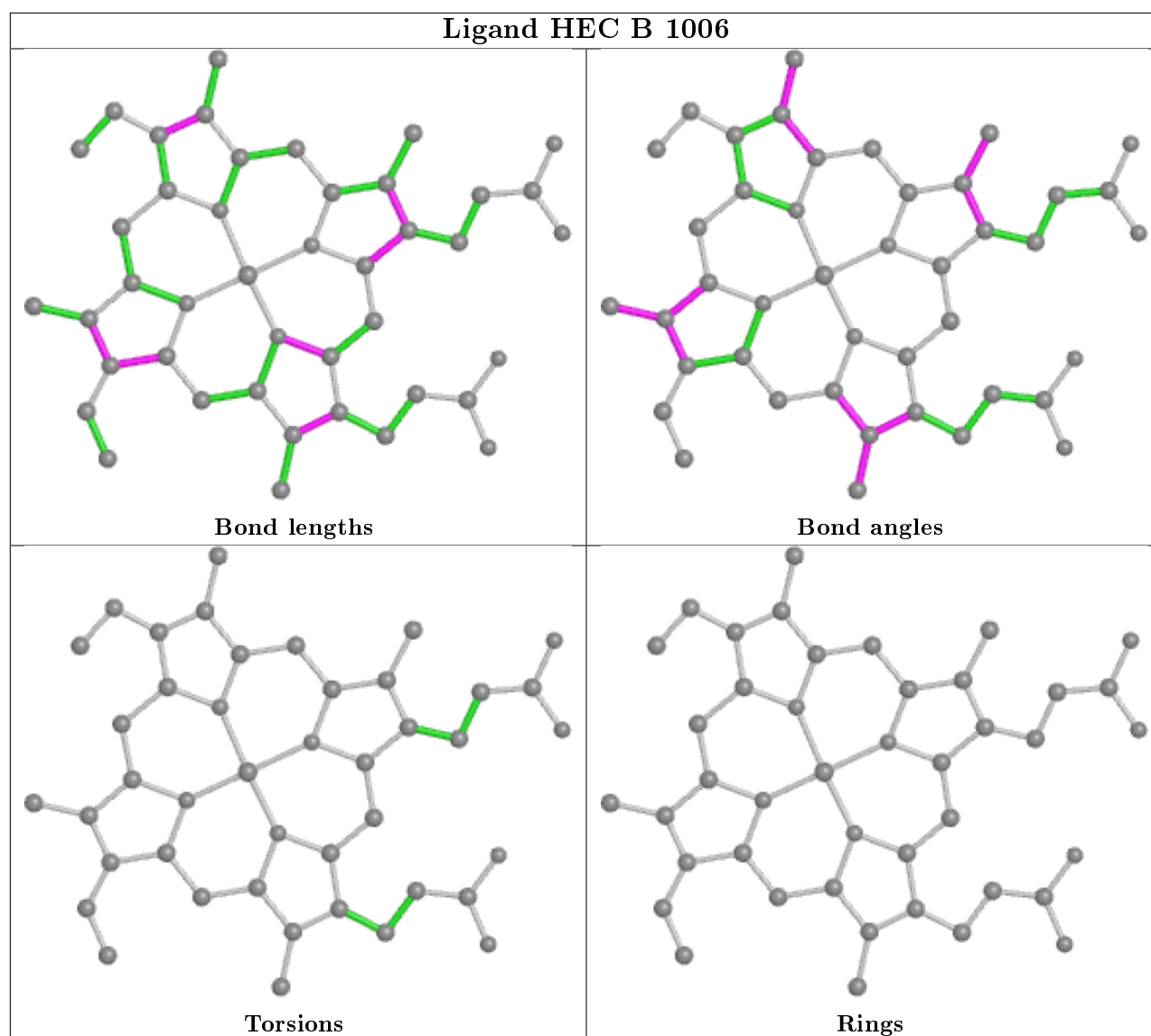


## Ligand HEC B 1002









## 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	518/525 (98%)	-0.65	1 (0%) 95 95	12, 17, 27, 45	1 (0%)
1	B	518/525 (98%)	-0.70	2 (0%) 92 94	11, 15, 26, 43	2 (0%)
All	All	1036/1050 (98%)	-0.67	3 (0%) 94 95	11, 16, 27, 45	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	VAL	6.6
1	B	522	VAL	5.6
1	B	204	GLU	2.4

### 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(Å <sup>2</sup> )	Q<0.9
6	PG4	B	533	11/13	0.51	0.26	27,32,33,34	11
6	PG4	B	532	7/13	0.53	0.21	21,29,31,34	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PG4	A	531	5/13	0.63	0.15	46,47,50,50	0
6	PG4	B	539	5/13	0.64	0.23	39,43,45,46	0
6	PG4	A	532	8/13	0.68	0.19	21,30,32,32	8
5	PG6	A	533	11/18	0.68	0.24	26,33,44,45	11
6	PG4	B	531	5/13	0.69	0.14	50,50,51,51	0
6	PG4	B	535	7/13	0.70	0.19	51,52,55,56	0
6	PG4	B	534	5/13	0.70	0.18	44,47,49,49	0
6	PG4	A	535	8/13	0.73	0.21	58,59,60,60	0
6	PG4	B	536	5/13	0.77	0.12	46,48,51,52	0
6	PG4	B	537	5/13	0.78	0.20	49,50,51,51	0
6	PG4	B	530	6/13	0.78	0.21	21,32,35,36	2
5	PG6	A	529	7/18	0.81	0.15	34,40,43,46	0
6	PG4	A	534	6/13	0.84	0.18	54,56,57,58	0
5	PG6	B	529	5/18	0.86	0.11	35,37,39,40	0
6	PG4	A	530	6/13	0.89	0.19	22,33,35,36	2
7	TRS	A	536	8/8	0.92	0.16	38,47,55,56	8
8	NA	B	540	1/1	0.94	0.07	23,23,23,23	1
6	PG4	B	538	4/13	0.95	0.18	27,29,31,31	4
8	NA	B	542	1/1	0.96	0.07	28,28,28,28	1
8	NA	A	539	1/1	0.97	0.22	19,19,19,19	1
8	NA	A	537	1/1	0.97	0.15	22,22,22,22	1
4	CA	A	528	1/1	0.97	0.10	16,16,16,16	1
2	HEC	A	1008	43/43	0.97	0.08	13,19,29,37	0
4	CA	B	528	1/1	0.98	0.11	15,15,15,15	1
2	HEC	B	1001	43/43	0.98	0.06	15,18,21,23	0
2	HEC	A	1003	43/43	0.98	0.07	11,13,21,33	0
2	HEC	A	1005	43/43	0.98	0.06	11,13,19,27	0
2	HEC	A	1007[A]	43/43	0.98	0.06	10,12,14,15	3
2	HEC	B	1007[A]	43/43	0.98	0.07	10,11,13,13	3
2	HEC	B	1003	43/43	0.98	0.07	11,13,22,33	0
2	HEC	B	1005	43/43	0.98	0.06	9,12,19,27	0
2	HEC	A	1001	43/43	0.98	0.06	14,16,24,27	0
2	HEC	B	1008	43/43	0.98	0.06	12,17,26,34	0
4	CA	A	527	1/1	0.99	0.03	14,14,14,14	0
2	HEC	B	1004	43/43	0.99	0.05	10,11,14,18	0
2	HEC	B	1002	43/43	0.99	0.05	11,14,16,18	0
8	NA	B	541	1/1	0.99	0.12	22,22,22,22	1
2	HEC	A	1004	43/43	0.99	0.05	11,13,17,20	0
2	HEC	A	1006	43/43	0.99	0.05	10,12,13,14	0
3	CYN	B	526	2/2	0.99	0.04	12,12,12,16	0
2	HEC	A	1002	43/43	0.99	0.05	12,14,16,17	0
2	HEC	B	1006	43/43	0.99	0.05	9,10,12,12	0

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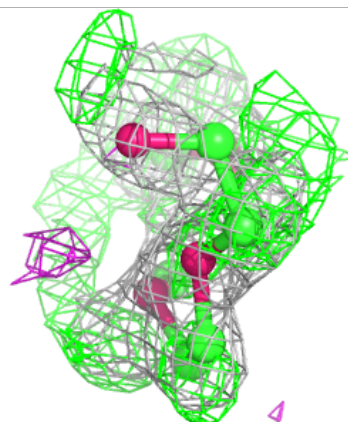
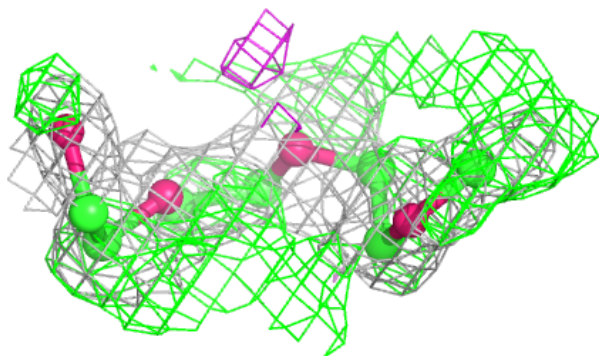
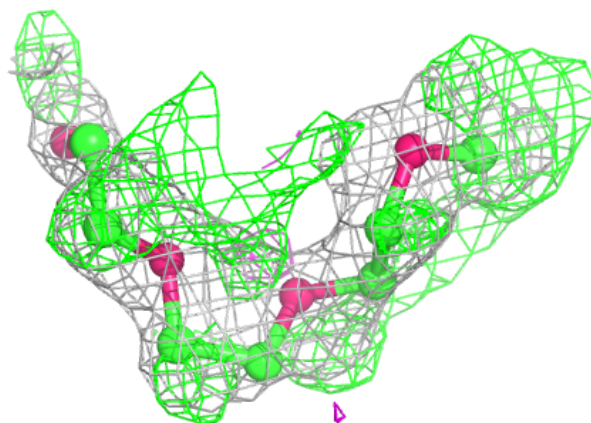
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NA	A	538	1/1	0.99	0.12	36,36,36,36	1
4	CA	B	527	1/1	0.99	0.03	12,12,12,12	0
3	CYN	A	526	2/2	0.99	0.03	13,13,13,16	0

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 PG6 A 533:**

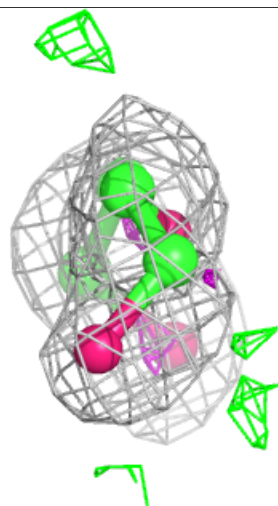
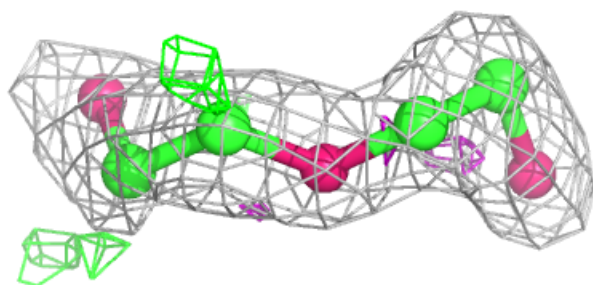
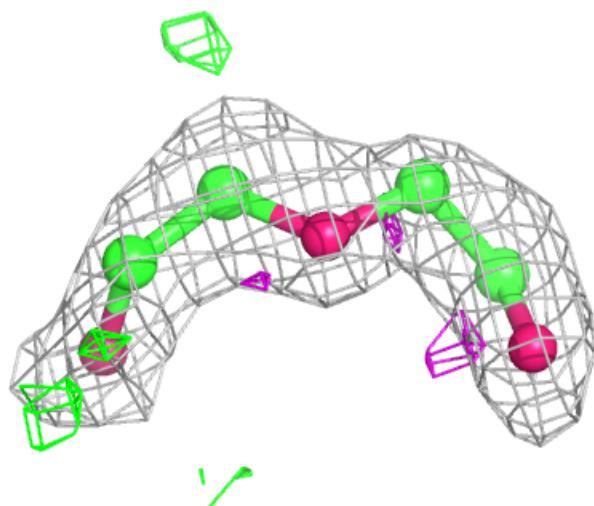
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





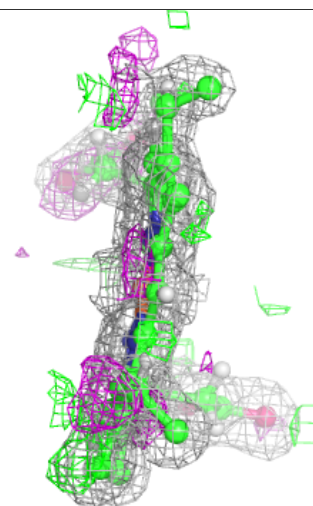
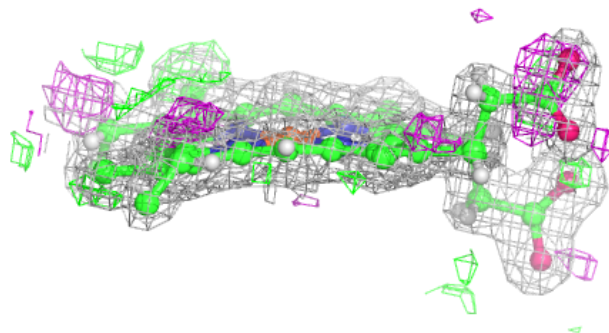
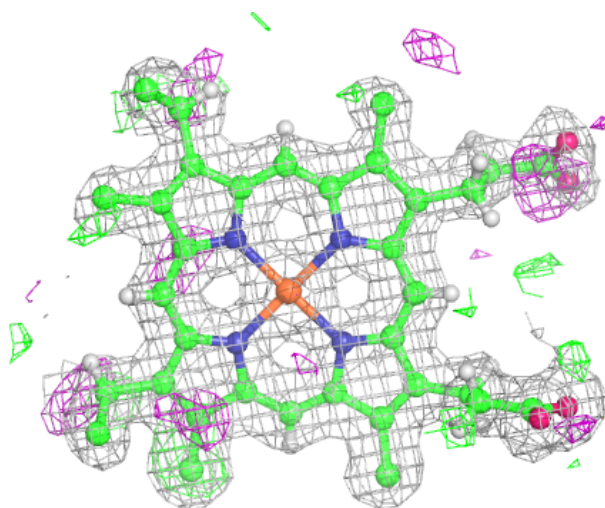
**Electron density around PG6 A 529:**

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



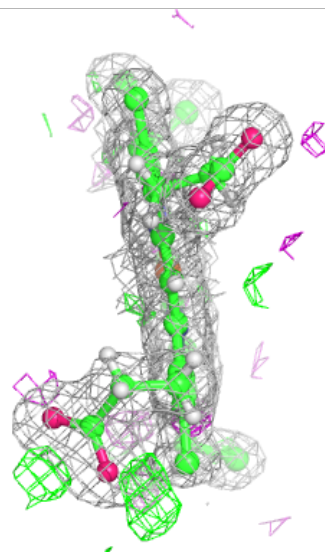
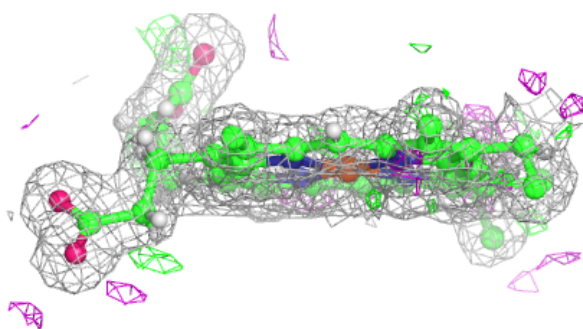
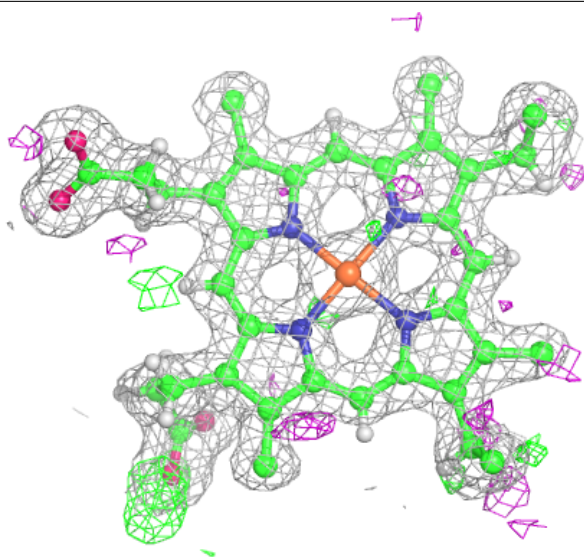
**Electron density around HEC A 1008:**

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



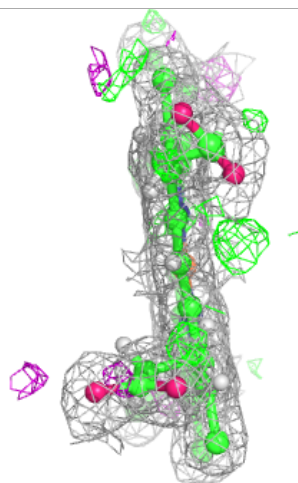
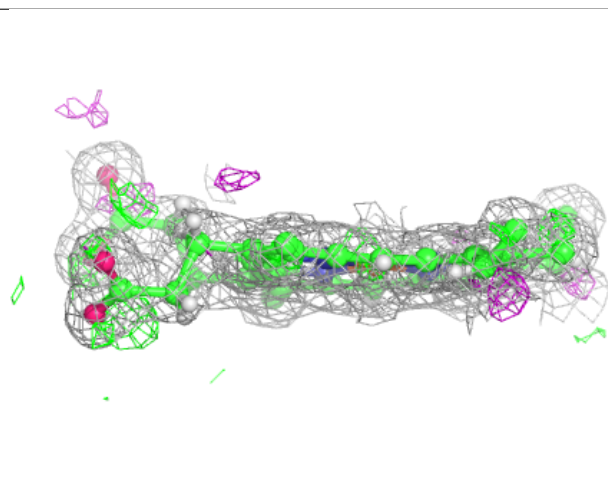
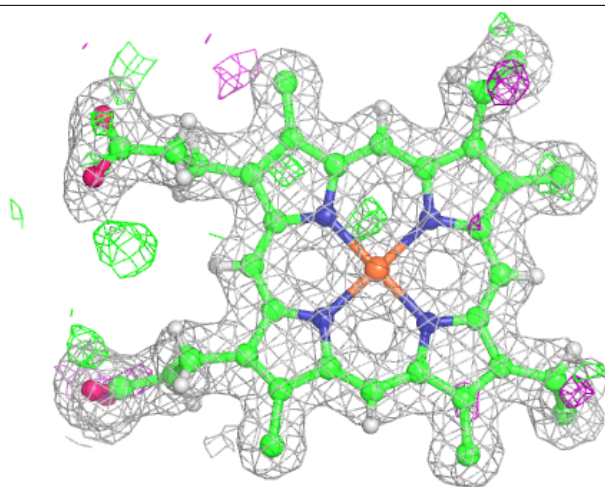
**Electron density around HEC B 1001:**

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



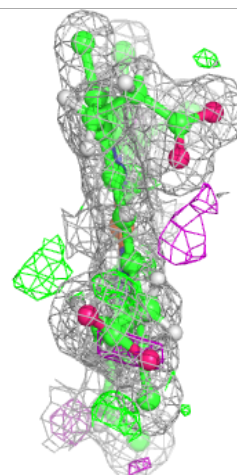
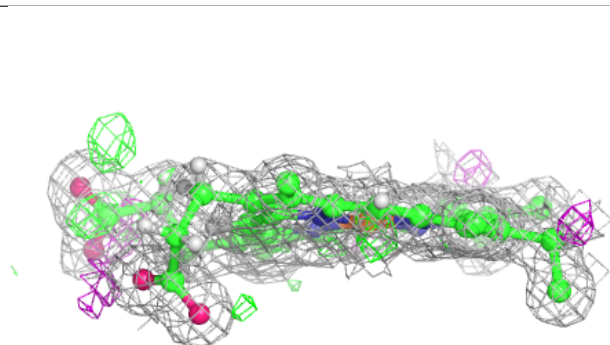
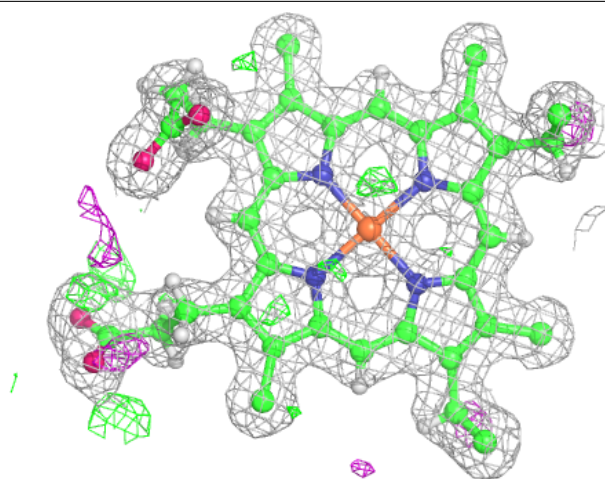
**Electron density around HEC A 1003:**

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



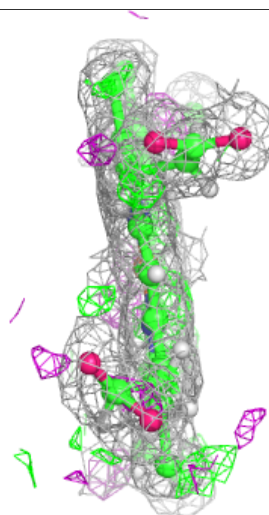
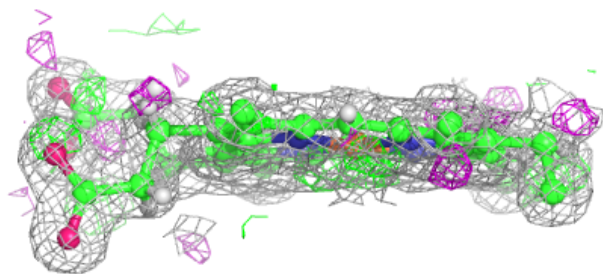
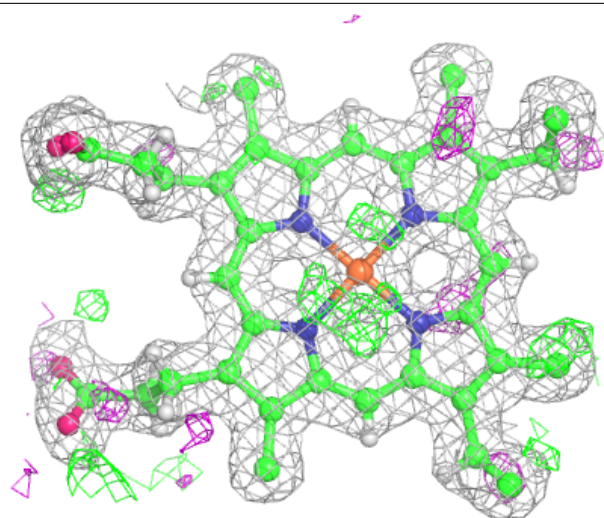
**Electron density around HEC A 1005:**

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



**Electron density around HEC B 1003:**

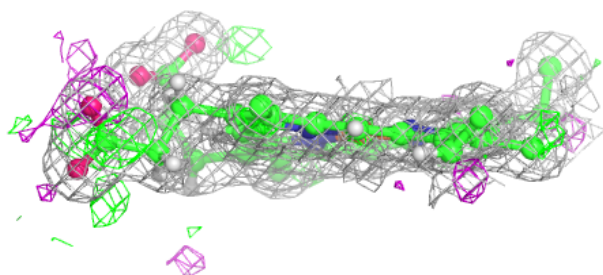
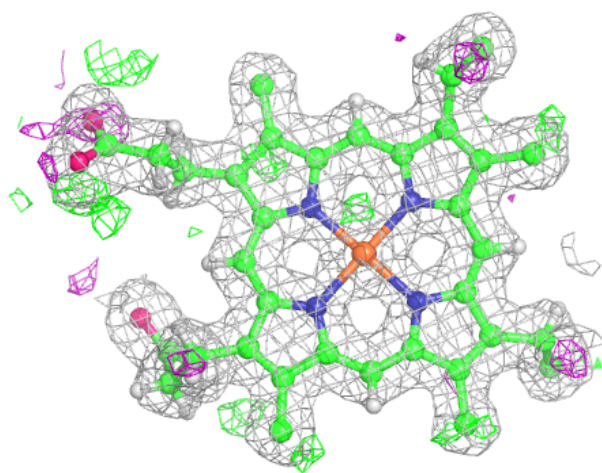
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





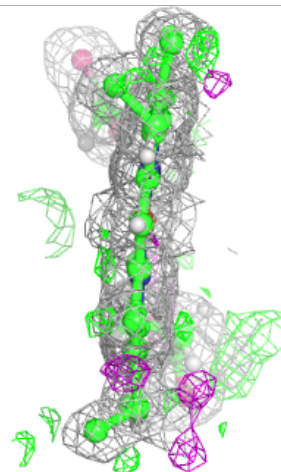
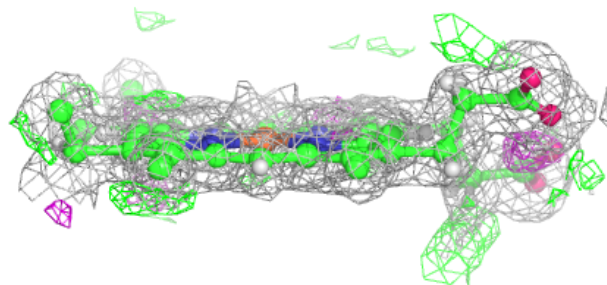
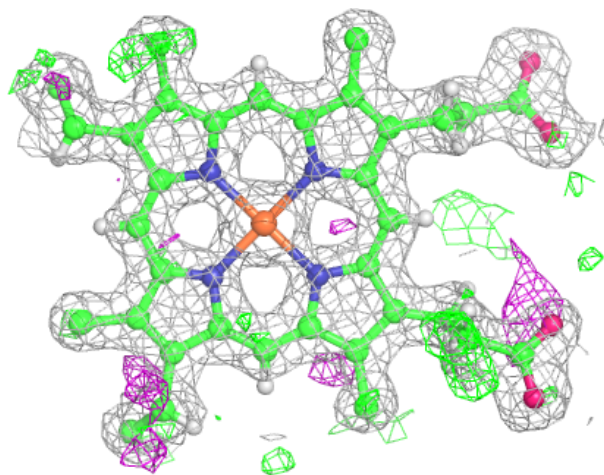
**Electron density around HEC B 1005:**

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



**Electron density around HEC A 1001:**

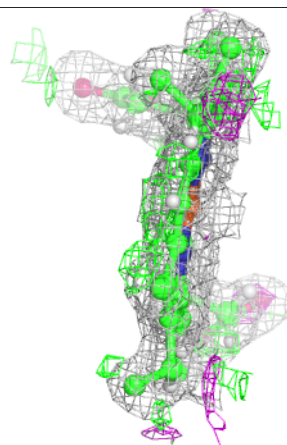
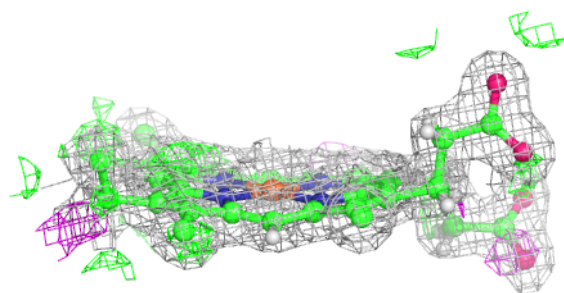
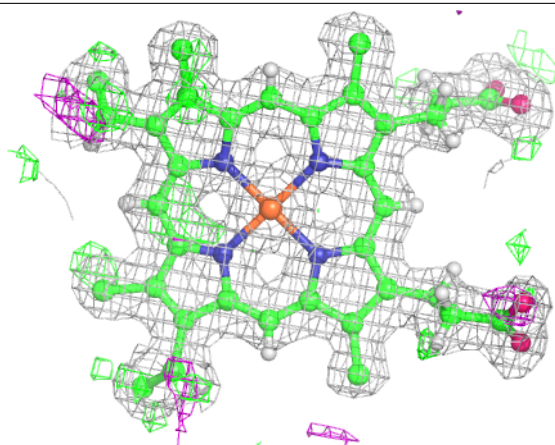
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





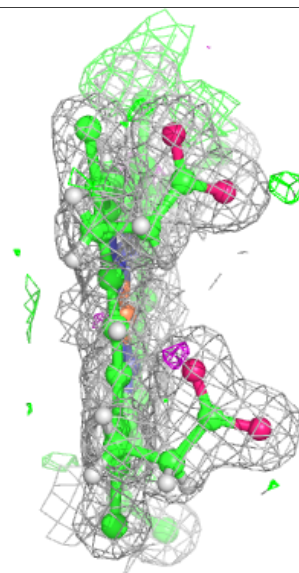
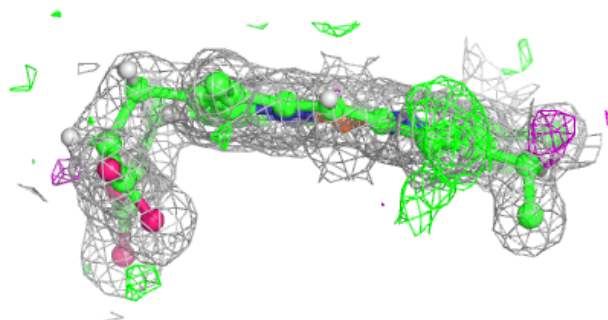
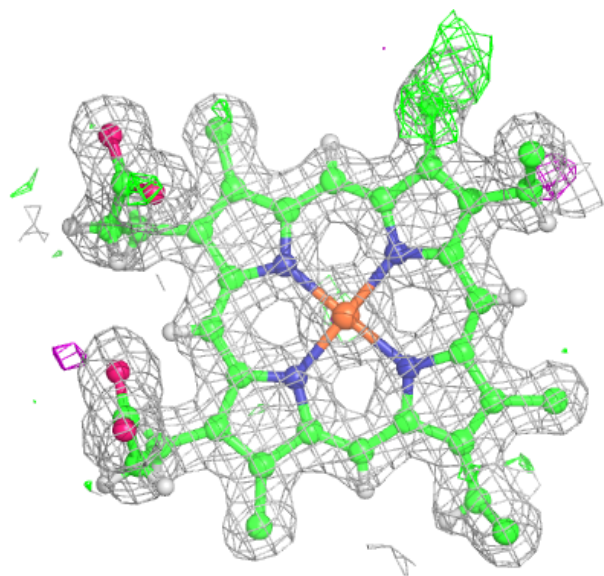
**Electron density around HEC B 1008:**

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



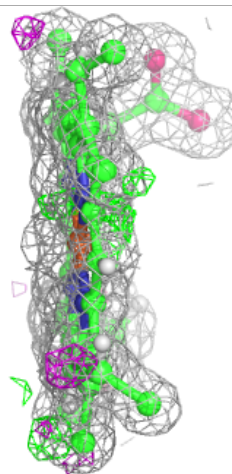
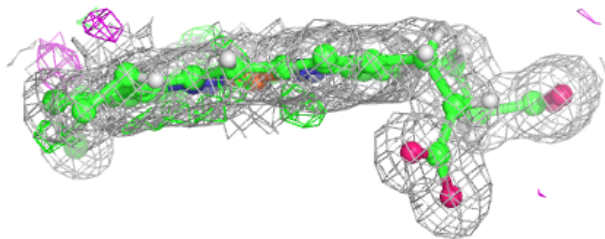
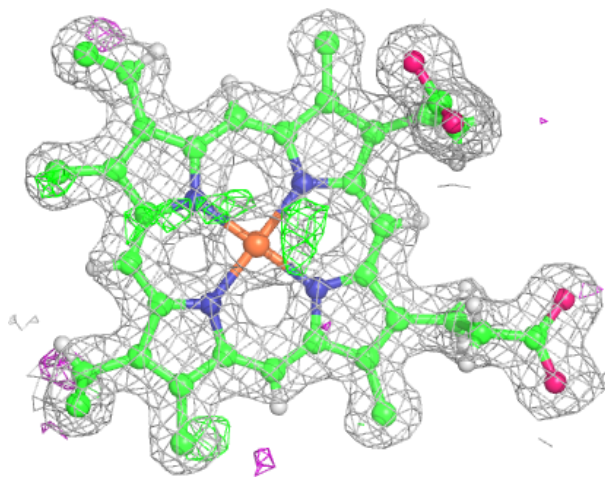
**Electron density around HEC B 1004:**

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



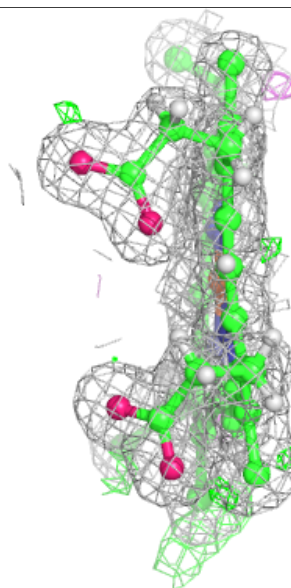
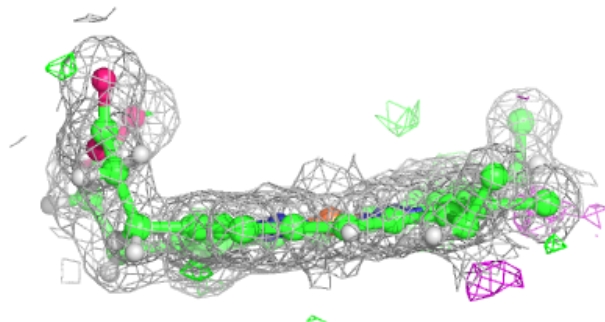
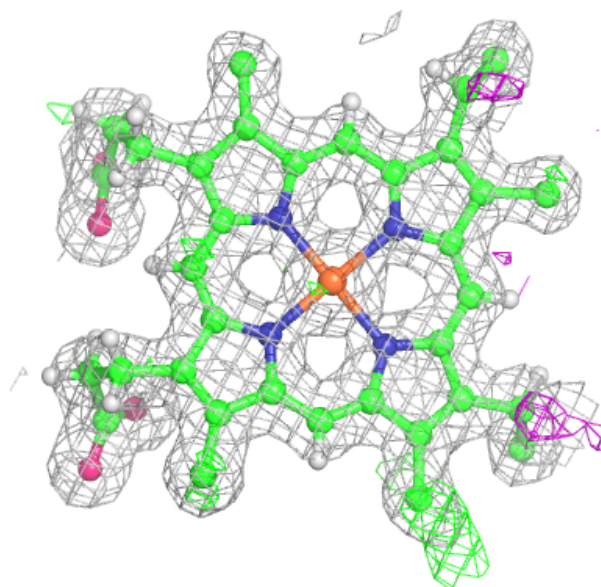
**Electron density around HEC B 1002:**

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



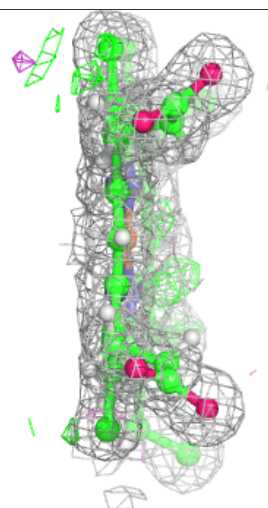
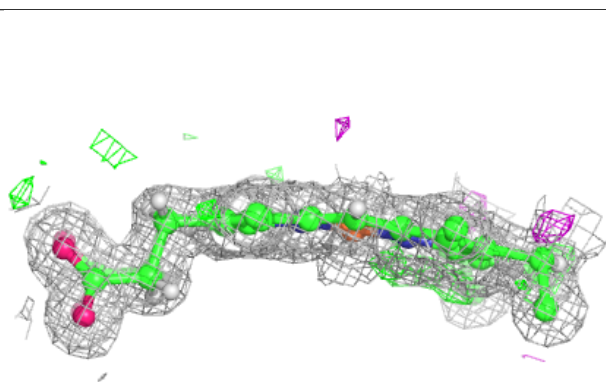
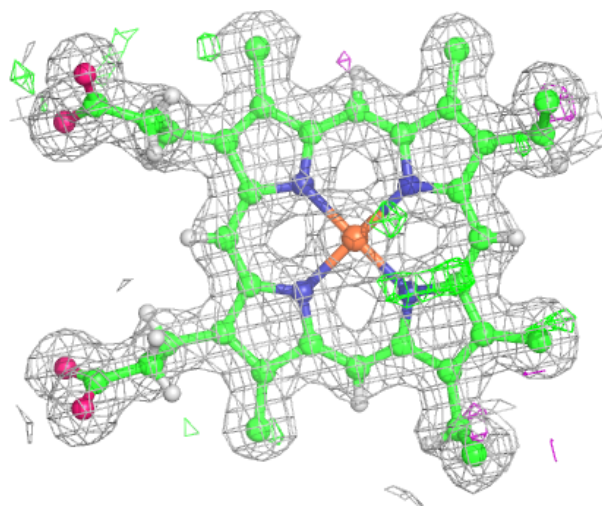
**Electron density around HEC A 1004:**

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



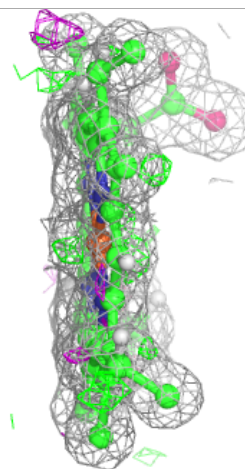
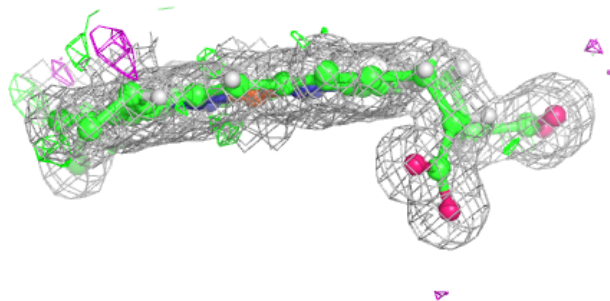
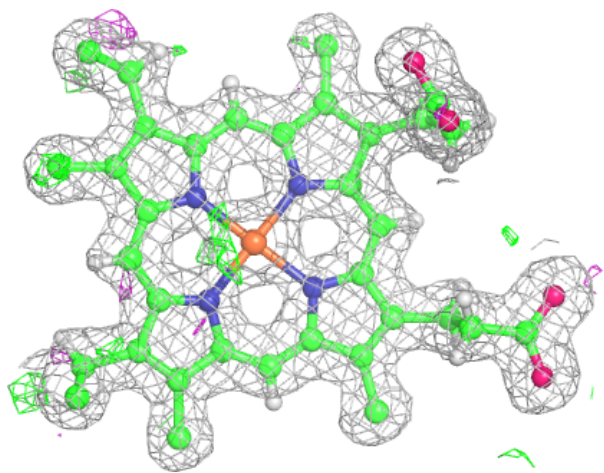
**Electron density around HEC A 1006:**

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



**Electron density around HEC A 1002:**

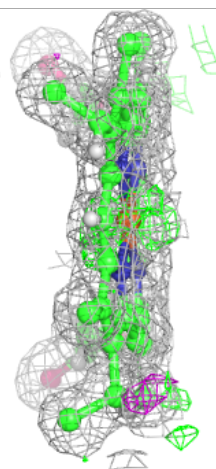
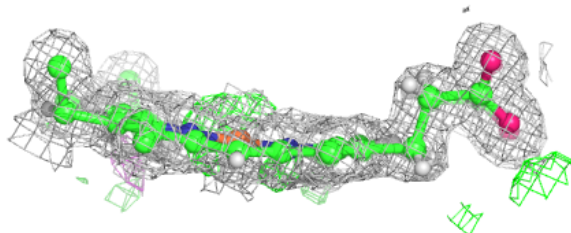
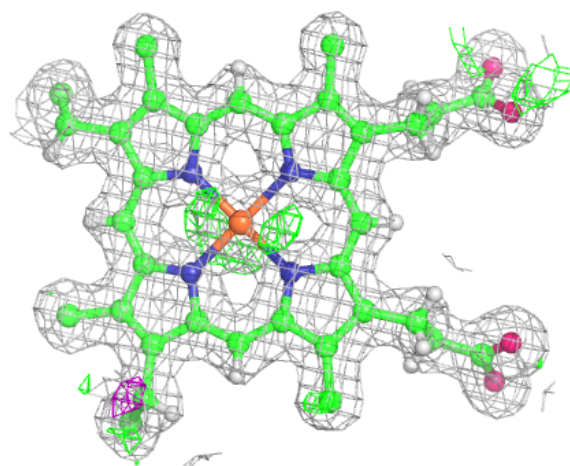
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





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

There are no such residues in this entry.