



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:57 am BST

PDB ID : 3GM6
Title : Structure of the Thioalkalivibrio nitratireducens cytochrome c nitrite reductase in complex with phosphate
Authors : Trofimov, A.A.; Polyakov, K.M.; Boyko, K.M.; Filimonenkov, A.A.; Dorovatsky, P.V.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2009-03-13
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

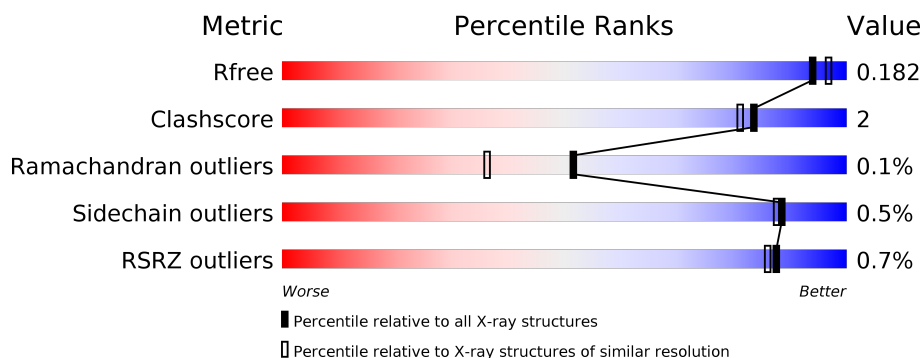
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 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>96%</div> <div>..</div> </div> </div>
1	B	525	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>

2 Entry composition i

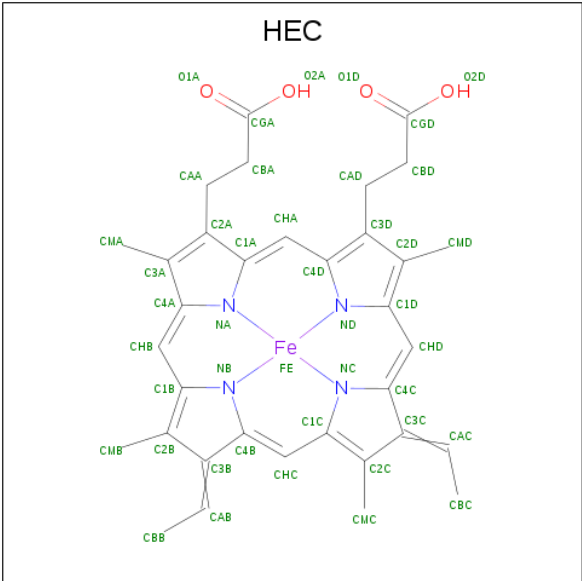
There are 7 unique types of molecules in this entry. The entry contains 15853 atoms, of which 5782 are hydrogens and 0 are deuteriums.

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	521	Total	C	H	N	O	S	0	18	1
			6907	2567	2763	752	788	37			
1	B	521	Total	C	H	N	O	S	0	15	1
			6953	2573	2796	756	792	36			

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



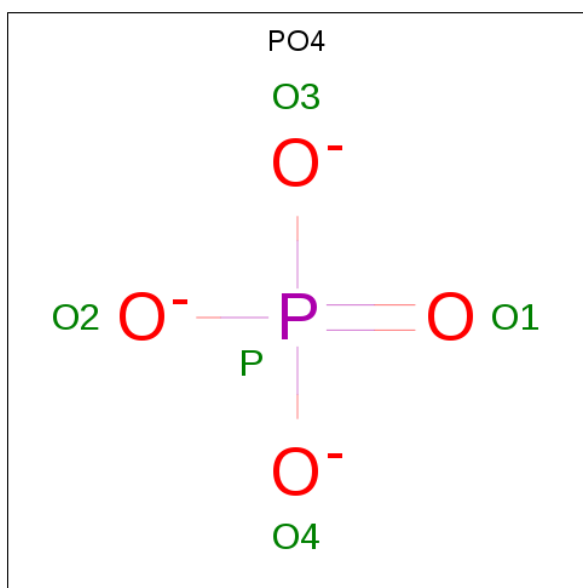
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			57	34	1	14	4	4		

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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	0
			56	34	1	13	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 PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

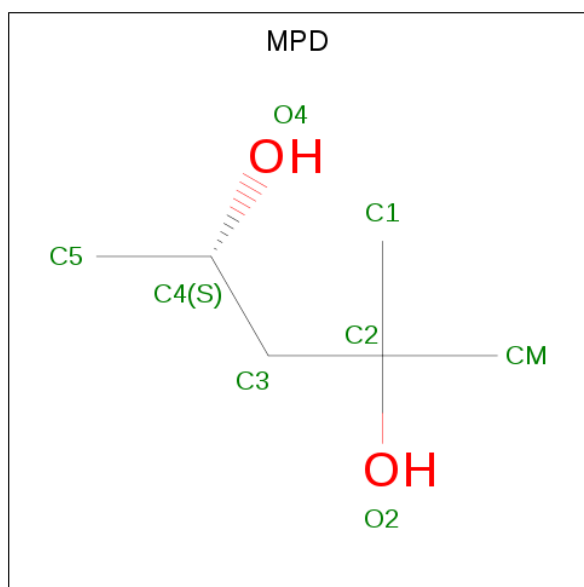


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	506	Total	O	0	0
			506	506		
7	B	532	Total	O	0	0
			532	532		

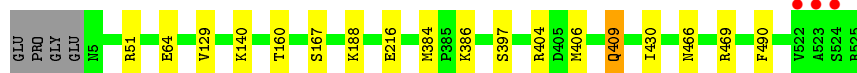
3 Residue-property plots [i](#)

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



- 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, α , β , γ	196.56Å 196.56Å 196.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.80 19.86 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.90-1.80) 97.2 (19.86-1.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.159 , 0.172 0.168 , 0.182	Depositor DCC
R_{free} test set	13222 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15853	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MRD, MPD, CA, PO4, 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	0.77	0/4349	0.72	0/5898
1	B	0.79	0/4350	0.73	3/5901 (0.1%)
All	All	0.78	0/8699	0.73	3/11799 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	404	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	188	LYS	CD-CE-NZ	5.41	124.13	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4144	2763	3815	10	0
1	B	4157	2796	3847	11	0
2	A	344	112	240	13	0
2	B	344	111	240	8	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	28	0	0
5	B	8	0	14	0	0
6	B	8	0	14	1	0
7	A	506	0	0	2	0
7	B	532	0	0	3	0
All	All	10071	5782	8198	41	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 2.

All (41) 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)
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.65	0.78
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.69	0.75
2:A:1001:HEC:HMB1	2:A:1001:HEC:HBB3	1.69	0.74
2:A:1008:HEC:HMB1	2:A:1008:HEC:HBB3	1.70	0.74
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.71	0.72
1:A:399[A]:SER:O	7:A:699:HOH:O	2.11	0.68
2:A:1007:HEC:HMC1	2:A:1007:HEC:HBC3	1.82	0.62
2:B:1001:HEC:HBB3	2:B:1001:HEC:HMB1	1.84	0.58
1:A:360:GLN:HG2	3:A:526:PO4:O3	2.04	0.58
2:B:1007:HEC:HBC3	2:B:1007:HEC:HMC1	1.86	0.58
2:A:1008:HEC:HMC1	2:A:1008:HEC:HBC3	1.85	0.57
1:A:19[A]:THR:HG22	7:A:977:HOH:O	2.04	0.57
2:B:1003:HEC:HMC1	2:B:1003:HEC:HBC3	1.88	0.54
1:A:414[B]:CYS:SG	2:A:1008:HEC:CMC	2.96	0.53
1:B:386:LYS:NZ	7:B:1053:HOH:O	2.42	0.53
2:A:1003:HEC:HBC3	2:A:1003:HEC:HMC1	1.89	0.53
2:B:1004:HEC:HBB3	2:B:1004:HEC:HMB1	1.89	0.52
1:B:64:GLU:HG3	7:B:1061:HOH:O	2.09	0.52
6:B:529:MRD:O4	7:B:556:HOH:O	2.18	0.51
1:A:140:LYS:HG2	1:A:160[A]:THR:HG23	1.93	0.50
1:A:384:MET:HB2	1:A:397:SER:O	2.11	0.50
2:A:1002:HEC:HMC1	2:A:1002:HEC:CBC	2.42	0.47
2:A:1004:HEC:HBB3	2:A:1004:HEC:HMB1	1.95	0.47
2:A:1006:HEC:HMC1	2:A:1006:HEC:HBC3	1.96	0.47
1:A:430:ILE:HG21	1:A:490:PHE:HA	1.97	0.46
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1006:HEC:HMB1	2:A:1006:HEC:HBB3	1.98	0.46
2:A:1001:HEC:HBC3	2:A:1001:HEC:HMC1	1.99	0.45
1:B:167:SER:HB2	1:B:216[B]:GLU:HG3	1.98	0.45
1:B:140:LYS:HG2	1:B:160[A]:THR:HG23	1.97	0.45
1:B:409:GLN:N	1:B:409:GLN:HE21	2.15	0.45
1:A:359:LEU:HD22	1:A:359:LEU:N	2.32	0.44
2:A:1007:HEC:HMB1	2:A:1007:HEC:HBB3	1.99	0.44
1:B:384:MET:HB2	1:B:397:SER:O	2.19	0.43
2:B:1005:HEC:HBC3	2:B:1005:HEC:HMC1	2.01	0.42
1:A:304:ASN:HB2	1:A:326:HIS:HB3	2.01	0.42
1:B:409:GLN:H	1:B:409:GLN:HE21	1.69	0.41
1:B:430:ILE:HG21	1:B:490:PHE:HA	2.03	0.41
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.19	0.41
1:B:129:VAL:HG11	2:B:1004:HEC:HMA1	2.03	0.41
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	537/525 (102%)	505 (94%)	30 (6%)	2 (0%)	34	21
1	B	534/525 (102%)	509 (95%)	25 (5%)	0	100	100
All	All	1071/1050 (102%)	1014 (95%)	55 (5%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277[A]	GLY
1	A	277[B]	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/443 (101%)	447 (100%)	2 (0%)	91	89
1	B	451/443 (102%)	447 (99%)	4 (1%)	78	75
All	All	900/886 (102%)	894 (99%)	6 (1%)	88	81

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	51	ARG
1	B	406[A]	MET
1	B	406[B]	MET
1	B	409	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	340	GLN
1	A	466	ASN
1	B	190	GLN
1	B	340	GLN
1	B	409	GLN
1	B	413	ASN
1	B	466	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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	PO4	B	526	2	4,4,4	1.31	0	6,6,6	0.86	0
2	HEC	B	1001	1	26,50,50	2.22	7 (26%)	18,82,82	1.68	4 (22%)
2	HEC	B	1003	1	26,50,50	2.26	4 (15%)	18,82,82	1.65	5 (27%)
2	HEC	A	1002	1	26,50,50	2.14	7 (26%)	18,82,82	1.60	3 (16%)
2	HEC	B	1005	1	26,50,50	2.27	6 (23%)	18,82,82	1.74	6 (33%)
2	HEC	B	1002	1	26,50,50	2.01	7 (26%)	18,82,82	1.90	4 (22%)
3	PO4	A	526	2	4,4,4	1.29	1 (25%)	6,6,6	1.03	0
2	HEC	B	1007	1	26,50,50	2.45	8 (30%)	18,82,82	2.09	6 (33%)
5	MPD	A	529	-	7,7,7	0.27	0	9,10,10	0.61	0
2	HEC	B	1004	1,3	26,50,50	2.26	6 (23%)	18,82,82	1.55	4 (22%)
2	HEC	A	1006	1	26,50,50	2.39	6 (23%)	18,82,82	1.80	4 (22%)
5	MPD	A	528	-	7,7,7	0.32	0	9,10,10	0.34	0
2	HEC	A	1003	1	26,50,50	2.11	4 (15%)	18,82,82	1.79	5 (27%)
2	HEC	A	1007	1	26,50,50	2.51	5 (19%)	18,82,82	2.03	7 (38%)
6	MRD	B	529	-	7,7,7	0.30	0	9,10,10	0.44	0
2	HEC	B	1006	1	26,50,50	2.36	5 (19%)	18,82,82	1.90	3 (16%)
2	HEC	A	1008	1	26,50,50	2.87	6 (23%)	18,82,82	1.49	4 (22%)
2	HEC	A	1001	1	26,50,50	2.06	9 (34%)	18,82,82	1.45	3 (16%)
2	HEC	A	1005	1	26,50,50	2.43	7 (26%)	18,82,82	1.99	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	B	528	-	7,7,7	0.40	0	9,10,10	0.51	0
2	HEC	A	1004	1,3	26,50,50	2.21	10 (38%)	18,82,82	1.59	3 (16%)
2	HEC	B	1008	1	26,50,50	2.65	4 (15%)	18,82,82	1.66	4 (22%)

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	1002	1	-	0/6/54/54	-
2	HEC	A	1006	1	-	0/6/54/54	-
6	MRD	B	529	-	-	3/5/5/5	-
2	HEC	B	1006	1	-	0/6/54/54	-
2	HEC	B	1001	1	-	0/6/54/54	-
2	HEC	B	1003	1	-	0/6/54/54	-
2	HEC	A	1001	1	-	0/6/54/54	-
5	MPD	A	528	-	-	0/5/5/5	-
2	HEC	B	1007	1	-	0/6/54/54	-
2	HEC	A	1005	1	-	0/6/54/54	-
2	HEC	A	1002	1	-	0/6/54/54	-
5	MPD	A	529	-	-	0/5/5/5	-
2	HEC	B	1004	1,3	-	0/6/54/54	-
2	HEC	A	1004	1,3	-	0/6/54/54	-
5	MPD	B	528	-	-	0/5/5/5	-
2	HEC	B	1008	1	-	0/6/54/54	-
2	HEC	B	1005	1	-	0/6/54/54	-
2	HEC	A	1008	1	-	0/6/54/54	-
2	HEC	A	1003	1	-	0/6/54/54	-
2	HEC	A	1007	1	-	0/6/54/54	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1008	HEC	C3C-C2C	-8.09	1.32	1.40
2	A	1008	HEC	C3B-C2B	-8.08	1.32	1.40
2	A	1005	HEC	C3B-C2B	-8.06	1.32	1.40
2	B	1008	HEC	C3C-C2C	-7.71	1.32	1.40
2	B	1006	HEC	C3C-C2C	-7.22	1.33	1.40
2	A	1007	HEC	C3B-C2B	-7.10	1.33	1.40
2	B	1008	HEC	C3B-C2B	-6.99	1.33	1.40
2	A	1007	HEC	C3C-C2C	-6.97	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	HEC	C3C-C2C	-6.88	1.33	1.40
2	B	1005	HEC	C3B-C2B	-6.86	1.33	1.40
2	B	1007	HEC	C3C-C2C	-6.56	1.33	1.40
2	B	1007	HEC	C3B-C2B	-6.44	1.34	1.40
2	B	1003	HEC	C3B-C2B	-6.33	1.34	1.40
2	A	1003	HEC	C3B-C2B	-5.59	1.34	1.40
2	B	1003	HEC	C3C-C2C	-5.54	1.35	1.40
2	A	1003	HEC	C3C-C2C	-5.38	1.35	1.40
2	B	1001	HEC	C3C-C2C	-5.37	1.35	1.40
2	A	1004	HEC	C3C-C2C	-5.32	1.35	1.40
2	B	1005	HEC	C3C-C2C	-5.29	1.35	1.40
2	B	1004	HEC	C3B-C2B	-5.18	1.35	1.40
2	B	1006	HEC	C3B-C2B	-5.09	1.35	1.40
2	A	1006	HEC	C3B-C2B	-5.05	1.35	1.40
2	A	1005	HEC	C3C-C2C	-4.97	1.35	1.40
2	B	1001	HEC	C3D-C2D	4.93	1.52	1.37
2	B	1001	HEC	C3B-C2B	-4.91	1.35	1.40
2	A	1002	HEC	C3B-C2B	-4.88	1.35	1.40
2	B	1004	HEC	C3D-C2D	4.81	1.51	1.37
2	A	1008	HEC	C3D-C2D	4.79	1.51	1.37
2	B	1002	HEC	C3D-C2D	4.76	1.51	1.37
2	A	1006	HEC	C3D-C2D	4.76	1.51	1.37
2	B	1008	HEC	C3D-C2D	4.73	1.51	1.37
2	A	1004	HEC	C3D-C2D	4.73	1.51	1.37
2	B	1006	HEC	C3D-C2D	4.73	1.51	1.37
2	A	1002	HEC	C3D-C2D	4.36	1.50	1.37
2	A	1002	HEC	C3C-C2C	-4.35	1.36	1.40
2	A	1001	HEC	C3B-C2B	-4.32	1.36	1.40
2	A	1001	HEC	C3D-C2D	4.28	1.50	1.37
2	B	1003	HEC	C3D-C2D	4.25	1.50	1.37
2	B	1004	HEC	C3C-C2C	-4.14	1.36	1.40
2	A	1001	HEC	C3C-C2C	-4.14	1.36	1.40
2	A	1007	HEC	C3D-C2D	4.13	1.49	1.37
2	A	1003	HEC	C3D-C2D	4.07	1.49	1.37
2	A	1004	HEC	C3B-C2B	-4.03	1.36	1.40
2	B	1007	HEC	C3D-C2D	3.93	1.49	1.37
2	B	1002	HEC	C3B-C2B	-3.93	1.36	1.40
2	A	1005	HEC	C3D-C2D	3.77	1.48	1.37
2	A	1008	HEC	C3C-C4C	3.66	1.49	1.43
2	A	1004	HEC	C3B-C4B	3.65	1.49	1.43
2	B	1004	HEC	C3B-C4B	3.64	1.49	1.43
2	B	1002	HEC	C3C-C2C	-3.55	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1005	HEC	C3D-C2D	3.48	1.48	1.37
2	B	1004	HEC	C3C-C4C	3.26	1.49	1.43
2	A	1007	HEC	C3B-C4B	3.26	1.49	1.43
2	B	1006	HEC	C3C-C4C	3.15	1.48	1.43
2	B	1002	HEC	C3B-C4B	3.15	1.48	1.43
2	A	1006	HEC	C3C-C4C	3.10	1.48	1.43
2	B	1007	HEC	C4A-C3A	3.07	1.49	1.42
2	A	1002	HEC	C3B-C4B	3.03	1.48	1.43
2	A	1005	HEC	C3C-C4C	2.91	1.48	1.43
2	B	1007	HEC	C3B-C4B	2.90	1.48	1.43
2	B	1001	HEC	C3C-C4C	2.87	1.48	1.43
2	B	1007	HEC	C3C-C4C	2.79	1.48	1.43
2	B	1008	HEC	C3C-C4C	2.79	1.48	1.43
2	B	1002	HEC	C3C-C4C	2.78	1.48	1.43
2	A	1001	HEC	C1A-C2A	2.78	1.48	1.42
2	A	1001	HEC	C3C-C4C	2.74	1.48	1.43
2	B	1003	HEC	C3C-C4C	2.73	1.48	1.43
2	A	1001	HEC	C3B-C4B	2.72	1.48	1.43
2	A	1005	HEC	C3B-C4B	2.72	1.48	1.43
2	A	1007	HEC	C4A-C3A	2.69	1.48	1.42
2	B	1005	HEC	C3C-C4C	2.59	1.47	1.43
2	A	1006	HEC	C3B-C4B	2.56	1.47	1.43
2	A	1006	HEC	C1D-ND	2.52	1.41	1.36
2	A	1008	HEC	C1D-ND	2.51	1.41	1.36
2	A	1002	HEC	C3C-C4C	2.46	1.47	1.43
2	A	1004	HEC	C3C-C4C	2.44	1.47	1.43
2	A	1004	HEC	CAD-C3D	2.38	1.55	1.52
2	B	1006	HEC	C1D-ND	2.37	1.41	1.36
2	B	1007	HEC	CMD-C2D	2.36	1.56	1.51
2	A	1002	HEC	C1D-ND	2.31	1.40	1.36
2	B	1002	HEC	C4A-C3A	2.31	1.47	1.42
2	A	1004	HEC	C1A-C2A	2.28	1.47	1.42
2	A	1005	HEC	C4A-C3A	2.26	1.47	1.42
2	B	1005	HEC	CMA-C3A	2.25	1.56	1.51
3	A	526	PO4	P-O1	-2.19	1.45	1.50
2	B	1005	HEC	C3B-C4B	2.18	1.47	1.43
2	A	1003	HEC	C3C-C4C	2.15	1.47	1.43
2	A	1001	HEC	CMA-C3A	2.14	1.56	1.51
2	A	1004	HEC	C4D-ND	2.13	1.40	1.36
2	A	1005	HEC	C1A-C2A	2.13	1.47	1.42
2	B	1001	HEC	C1D-ND	2.13	1.40	1.36
2	A	1004	HEC	C4A-C3A	2.12	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	HEC	CMD-C2D	2.10	1.56	1.51
2	B	1001	HEC	CMA-C3A	2.09	1.56	1.51
2	B	1002	HEC	CMB-C2B	2.08	1.56	1.51
2	B	1007	HEC	C1A-C2A	2.07	1.47	1.42
2	A	1002	HEC	CMB-C2B	2.07	1.56	1.51
2	B	1004	HEC	C4A-C3A	2.06	1.47	1.42
2	A	1008	HEC	C4D-ND	2.05	1.40	1.36
2	A	1001	HEC	CBB-CAB	2.02	1.57	1.49
2	A	1001	HEC	C4A-C3A	2.01	1.47	1.42
2	A	1004	HEC	CAA-C2A	2.01	1.55	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	HEC	CMC-C2C-C1C	-5.17	120.52	128.46
2	A	1002	HEC	CMC-C2C-C1C	-5.07	120.67	128.46
2	B	1006	HEC	CMC-C2C-C1C	-5.00	120.78	128.46
2	A	1005	HEC	CMB-C2B-C1B	-4.52	121.52	128.46
2	B	1001	HEC	CMC-C2C-C1C	-4.46	121.61	128.46
2	A	1006	HEC	CMC-C2C-C1C	-4.42	121.68	128.46
2	B	1007	HEC	CMB-C2B-C1B	-4.34	121.79	128.46
2	A	1004	HEC	CMB-C2B-C1B	-4.28	121.88	128.46
2	A	1005	HEC	CMC-C2C-C1C	-4.27	121.89	128.46
2	A	1007	HEC	CMC-C2C-C1C	-4.15	122.09	128.46
2	B	1002	HEC	CAA-CBA-CGA	-3.92	106.10	112.67
2	B	1007	HEC	CMC-C2C-C1C	-3.91	122.45	128.46
2	A	1007	HEC	CMB-C2B-C1B	-3.88	122.50	128.46
2	B	1005	HEC	CMB-C2B-C1B	-3.83	122.58	128.46
2	A	1001	HEC	CMC-C2C-C1C	-3.80	122.62	128.46
2	B	1008	HEC	CMC-C2C-C1C	-3.76	122.68	128.46
2	B	1008	HEC	CMB-C2B-C1B	-3.56	122.99	128.46
2	A	1003	HEC	CMC-C2C-C1C	-3.52	123.05	128.46
2	B	1005	HEC	CMC-C2C-C1C	-3.50	123.08	128.46
2	B	1007	HEC	CBD-CAD-C3D	-3.47	106.08	112.49
2	B	1004	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
2	B	1004	HEC	CMB-C2B-C1B	-3.40	123.23	128.46
2	A	1007	HEC	C1D-C2D-C3D	-3.31	104.69	107.00
2	A	1004	HEC	CMB-C2B-C3B	3.27	129.66	125.82
2	B	1003	HEC	CMB-C2B-C1B	-3.23	123.50	128.46
2	B	1003	HEC	CMC-C2C-C1C	-3.19	123.56	128.46
2	A	1006	HEC	C1D-C2D-C3D	-3.15	104.80	107.00
2	A	1008	HEC	CMC-C2C-C1C	-3.15	123.63	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1007	HEC	CBA-CAA-C2A	-3.05	106.86	112.48
2	A	1002	HEC	C1D-C2D-C3D	-3.03	104.89	107.00
2	A	1001	HEC	CAD-CBD-CGD	-3.01	107.63	112.67
2	B	1004	HEC	CMB-C2B-C3B	2.98	129.32	125.82
2	A	1003	HEC	CMB-C2B-C1B	-2.95	123.93	128.46
2	B	1003	HEC	C1D-C2D-C3D	-2.92	104.96	107.00
2	A	1004	HEC	CMC-C2C-C1C	-2.90	124.00	128.46
2	B	1006	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
2	B	1002	HEC	C1D-C2D-C3D	-2.80	105.05	107.00
2	A	1003	HEC	CAA-CBA-CGA	2.79	117.35	112.67
2	A	1005	HEC	CAD-CBD-CGD	-2.78	108.01	112.67
2	A	1005	HEC	CMB-C2B-C3B	2.78	129.09	125.82
2	A	1003	HEC	C1D-C2D-C3D	-2.69	105.13	107.00
2	A	1005	HEC	CAA-CBA-CGA	-2.66	108.20	112.67
2	A	1006	HEC	CMB-C2B-C1B	-2.66	124.37	128.46
2	A	1007	HEC	CAD-CBD-CGD	2.65	117.12	112.67
2	B	1001	HEC	CMB-C2B-C1B	-2.59	124.48	128.46
2	A	1003	HEC	CBA-CAA-C2A	-2.59	107.71	112.48
2	A	1008	HEC	CMB-C2B-C1B	-2.53	124.57	128.46
2	B	1005	HEC	CAA-CBA-CGA	-2.50	108.48	112.67
2	A	1008	HEC	CBA-CAA-C2A	-2.49	107.88	112.48
2	B	1003	HEC	CAA-CBA-CGA	2.48	116.83	112.67
2	A	1007	HEC	CMA-C3A-C2A	2.47	129.61	124.94
2	B	1002	HEC	CMB-C2B-C1B	-2.43	124.73	128.46
2	B	1001	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
2	A	1001	HEC	CMB-C2B-C1B	-2.36	124.83	128.46
2	B	1008	HEC	CBA-CAA-C2A	-2.35	108.14	112.48
2	B	1005	HEC	CAD-CBD-CGD	-2.35	108.73	112.67
2	A	1007	HEC	CBA-CAA-C2A	-2.34	108.16	112.48
2	B	1001	HEC	CBA-CAA-C2A	-2.32	108.20	112.48
2	A	1007	HEC	CBD-CAD-C3D	-2.32	108.21	112.49
2	A	1006	HEC	CBD-CAD-C3D	-2.29	108.26	112.49
2	B	1003	HEC	CBA-CAA-C2A	-2.26	108.31	112.48
2	B	1007	HEC	CMA-C3A-C2A	2.26	129.20	124.94
2	A	1008	HEC	CMA-C3A-C2A	2.26	129.20	124.94
2	B	1007	HEC	C1D-C2D-C3D	-2.15	105.50	107.00
2	B	1008	HEC	CAD-CBD-CGD	-2.11	109.13	112.67
2	B	1005	HEC	CBD-CAD-C3D	-2.11	108.59	112.49
2	B	1004	HEC	CBA-CAA-C2A	-2.08	108.64	112.48
2	B	1005	HEC	CMB-C2B-C3B	2.08	128.26	125.82
2	A	1002	HEC	CAA-CBA-CGA	-2.06	109.21	112.67
2	B	1006	HEC	CBA-CAA-C2A	-2.04	108.72	112.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

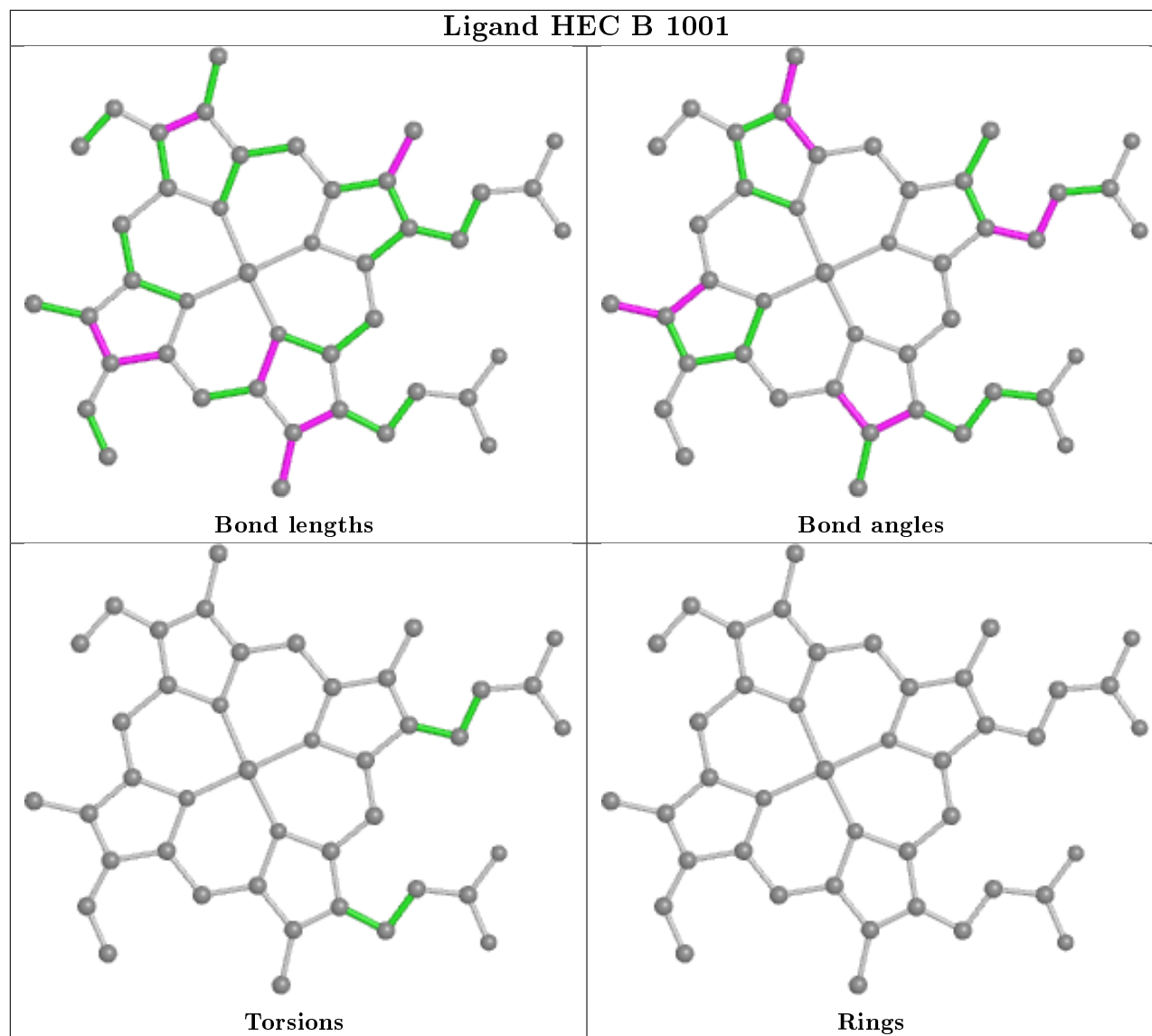
Mol	Chain	Res	Type	Atoms
6	B	529	MRD	O2-C2-C3-C4
6	B	529	MRD	CM-C2-C3-C4
6	B	529	MRD	C1-C2-C3-C4

There are no ring outliers.

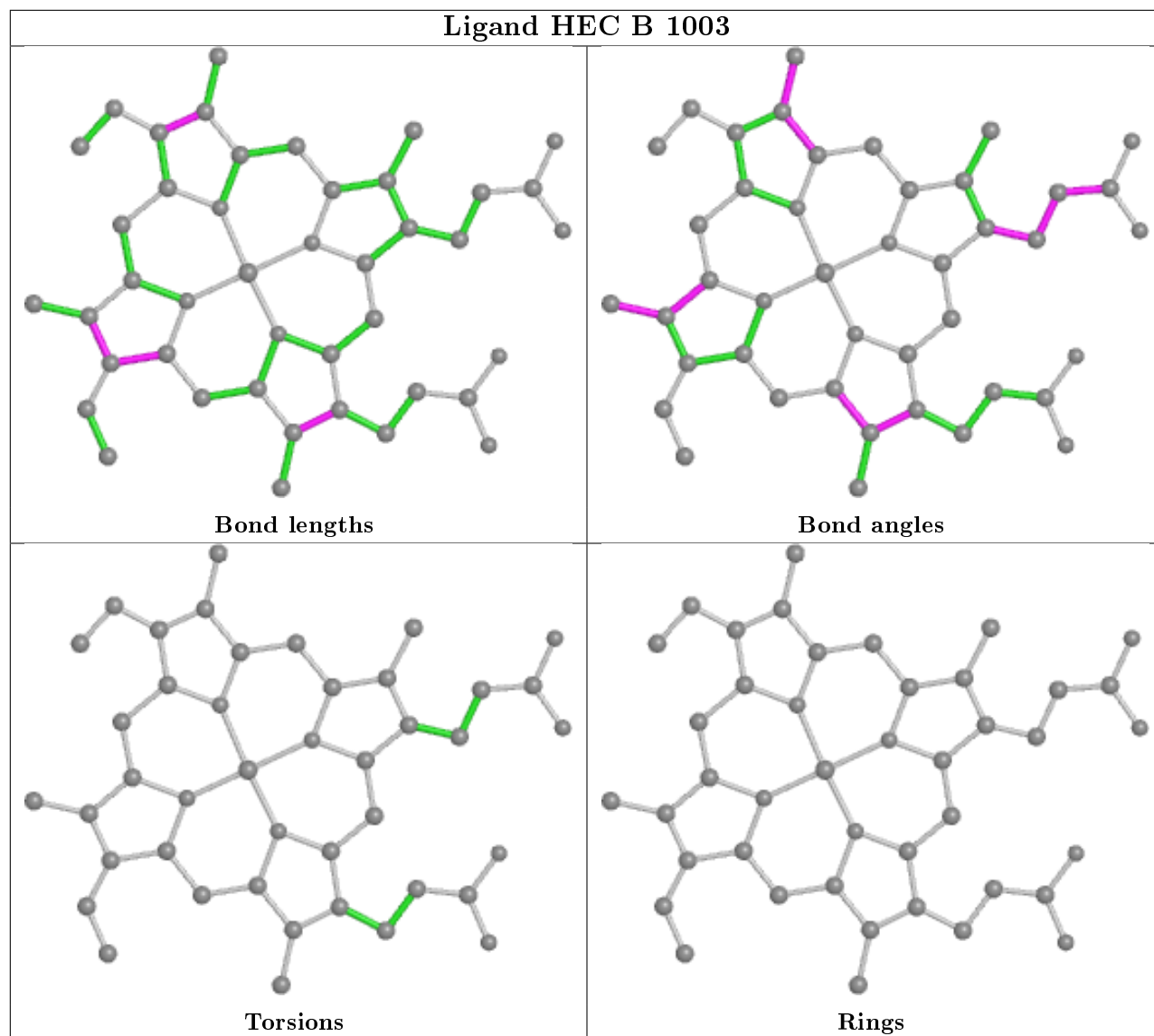
16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	HEC	1	0
2	B	1003	HEC	1	0
2	A	1002	HEC	2	0
2	B	1005	HEC	1	0
2	B	1002	HEC	1	0
3	A	526	PO4	1	0
2	B	1007	HEC	1	0
2	B	1004	HEC	2	0
2	A	1006	HEC	2	0
2	A	1003	HEC	1	0
2	A	1007	HEC	2	0
6	B	529	MRD	1	0
2	A	1008	HEC	3	0
2	A	1001	HEC	2	0
2	A	1004	HEC	1	0
2	B	1008	HEC	1	0

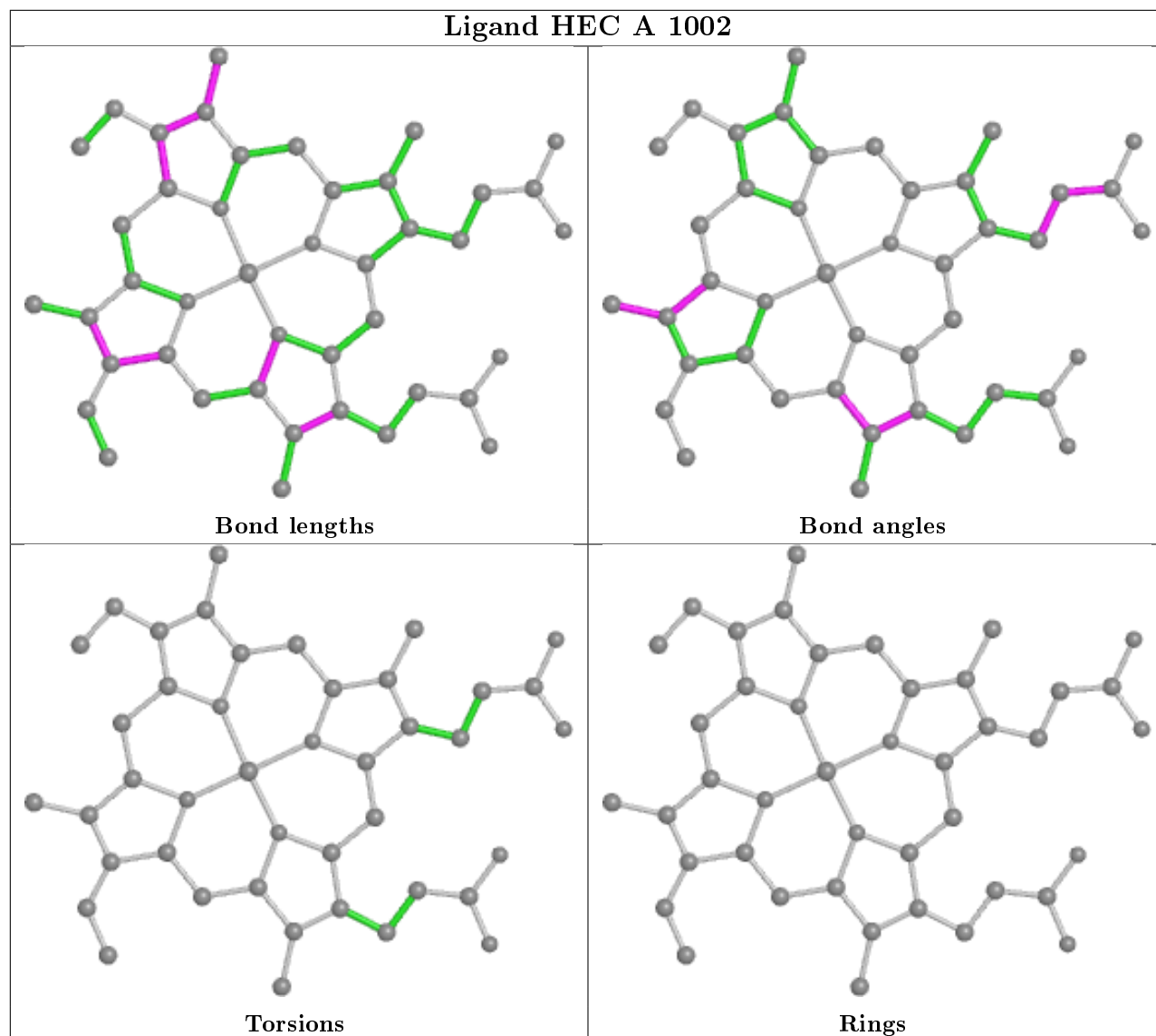
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

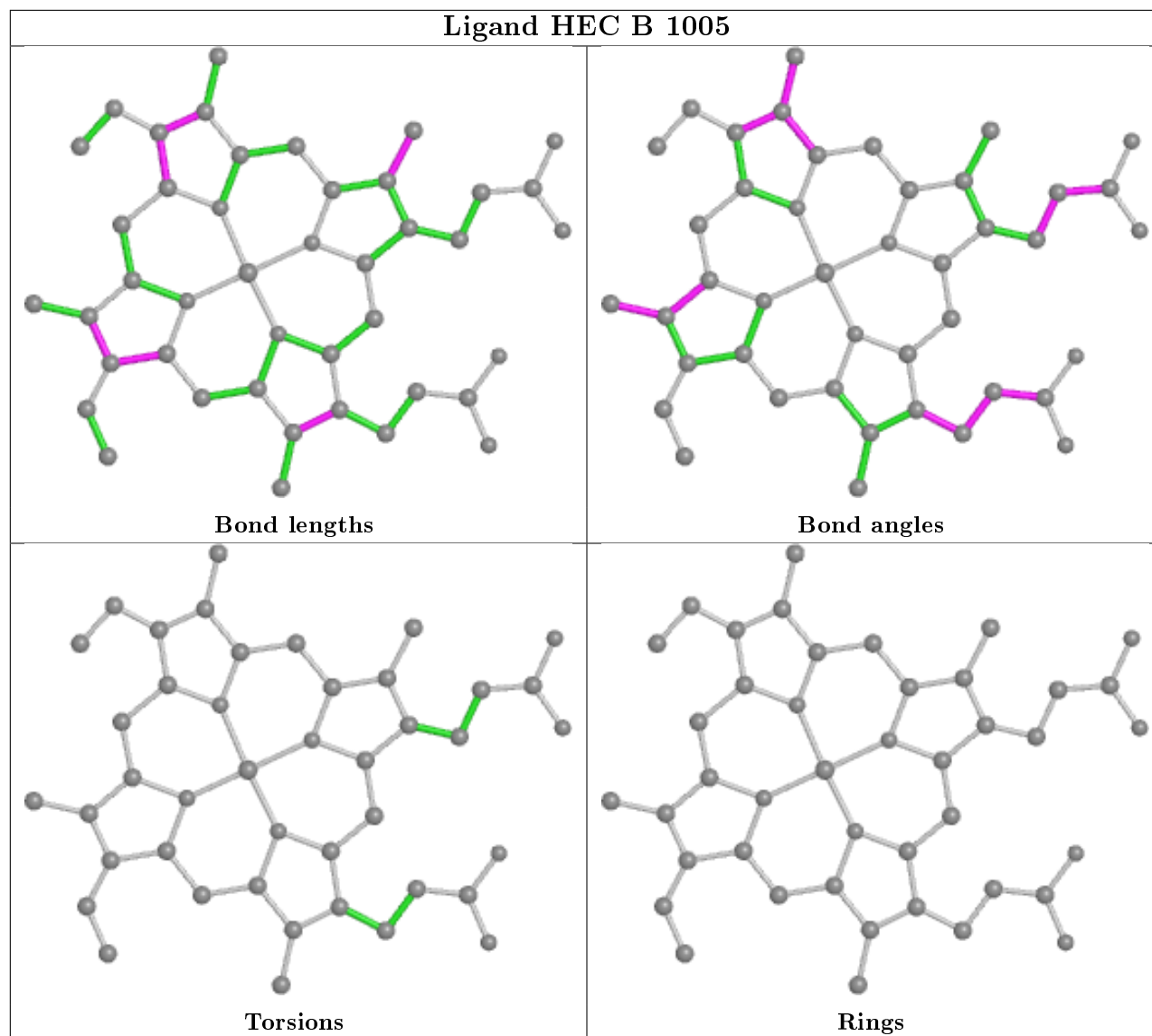


Ligand HEC B 1003

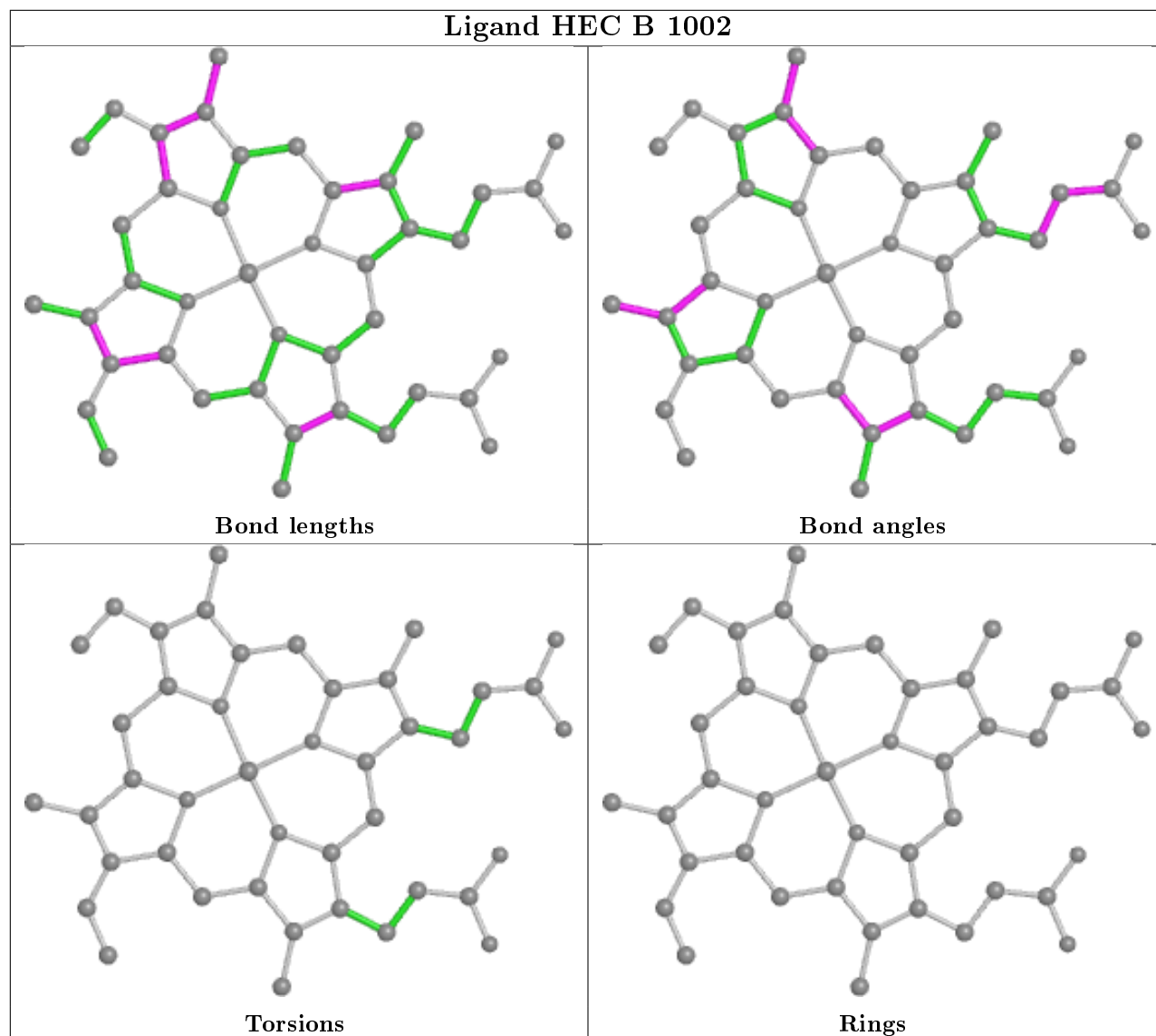


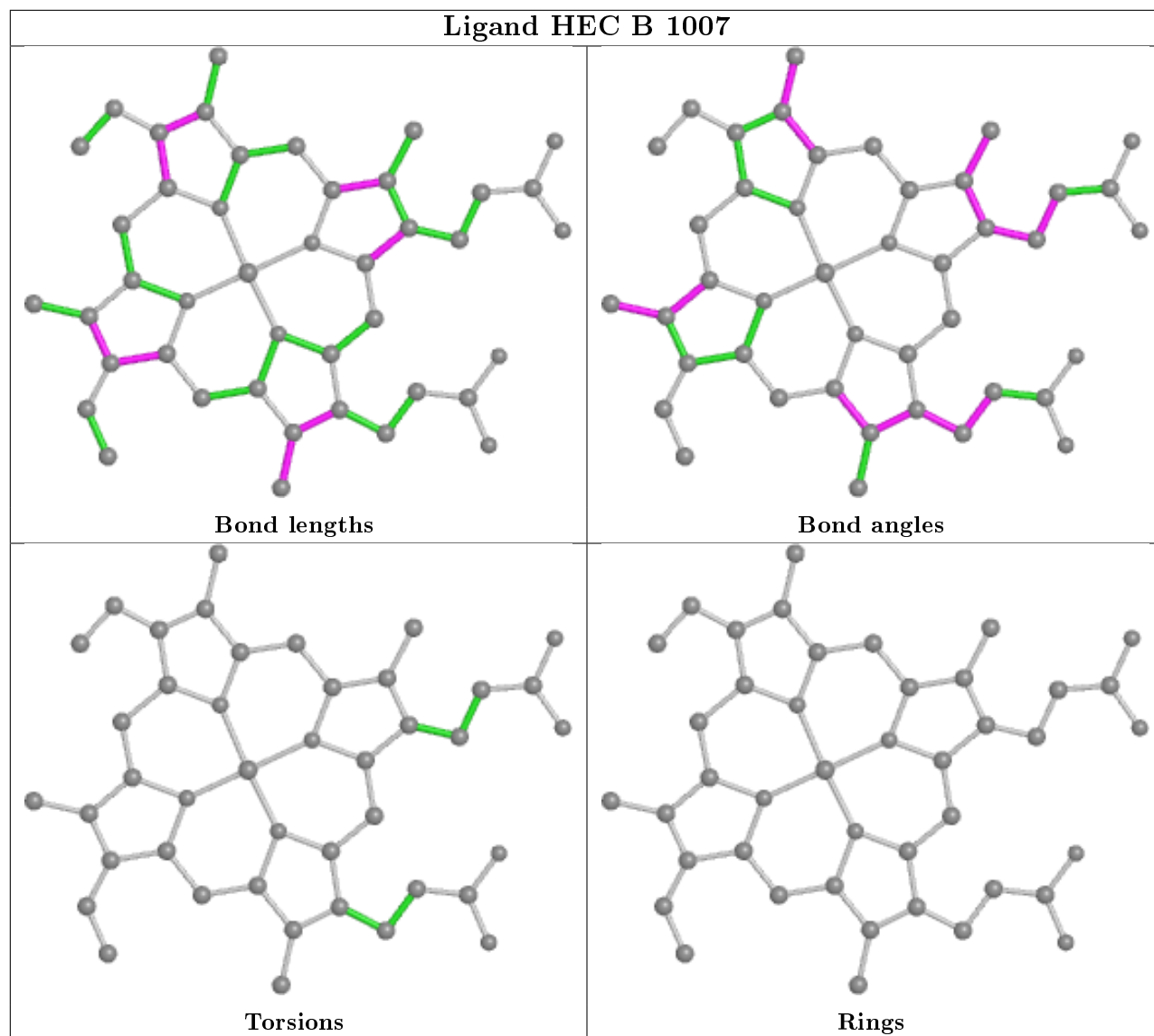
Ligand HEC A 1002



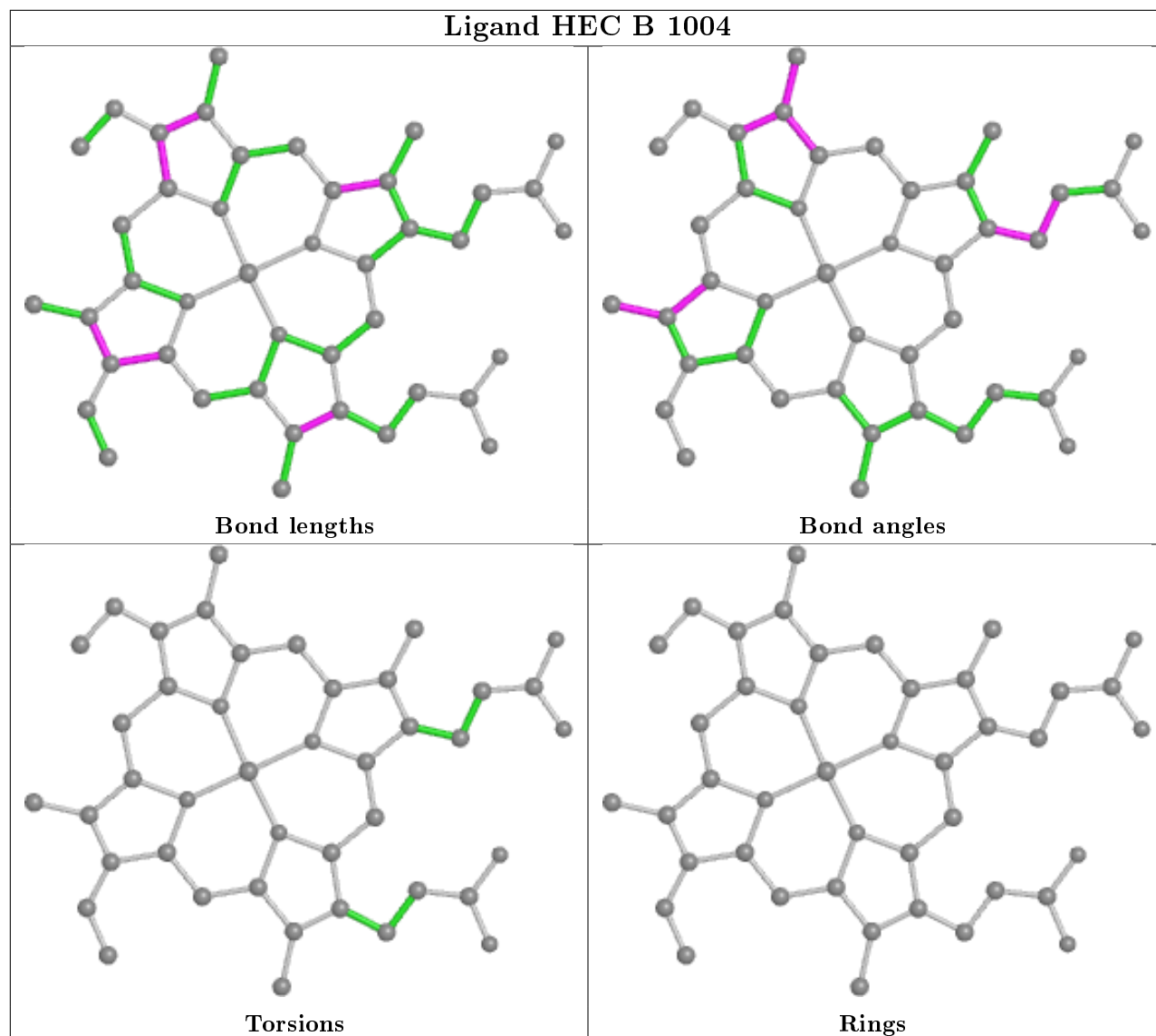


Ligand HEC B 1002

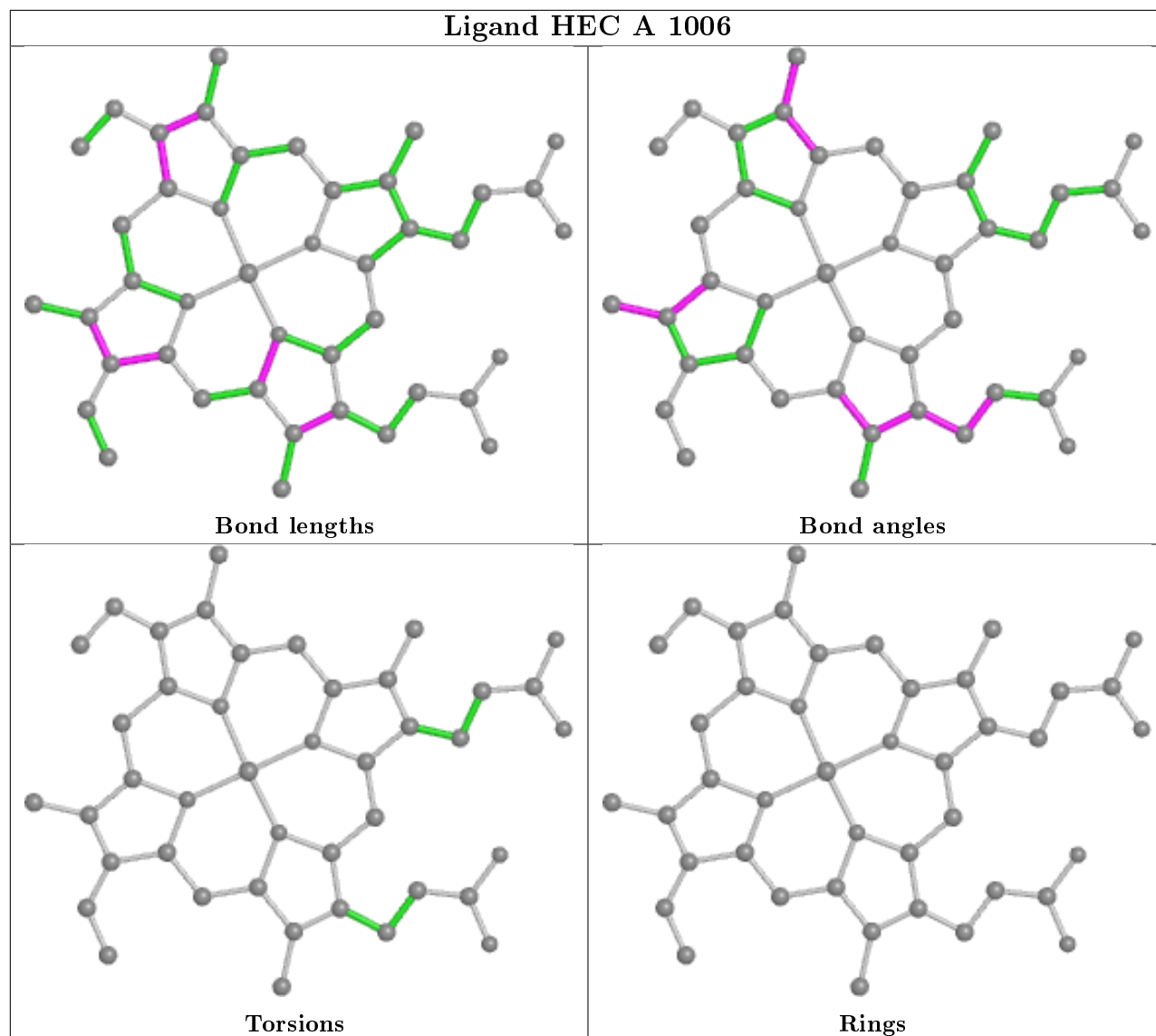




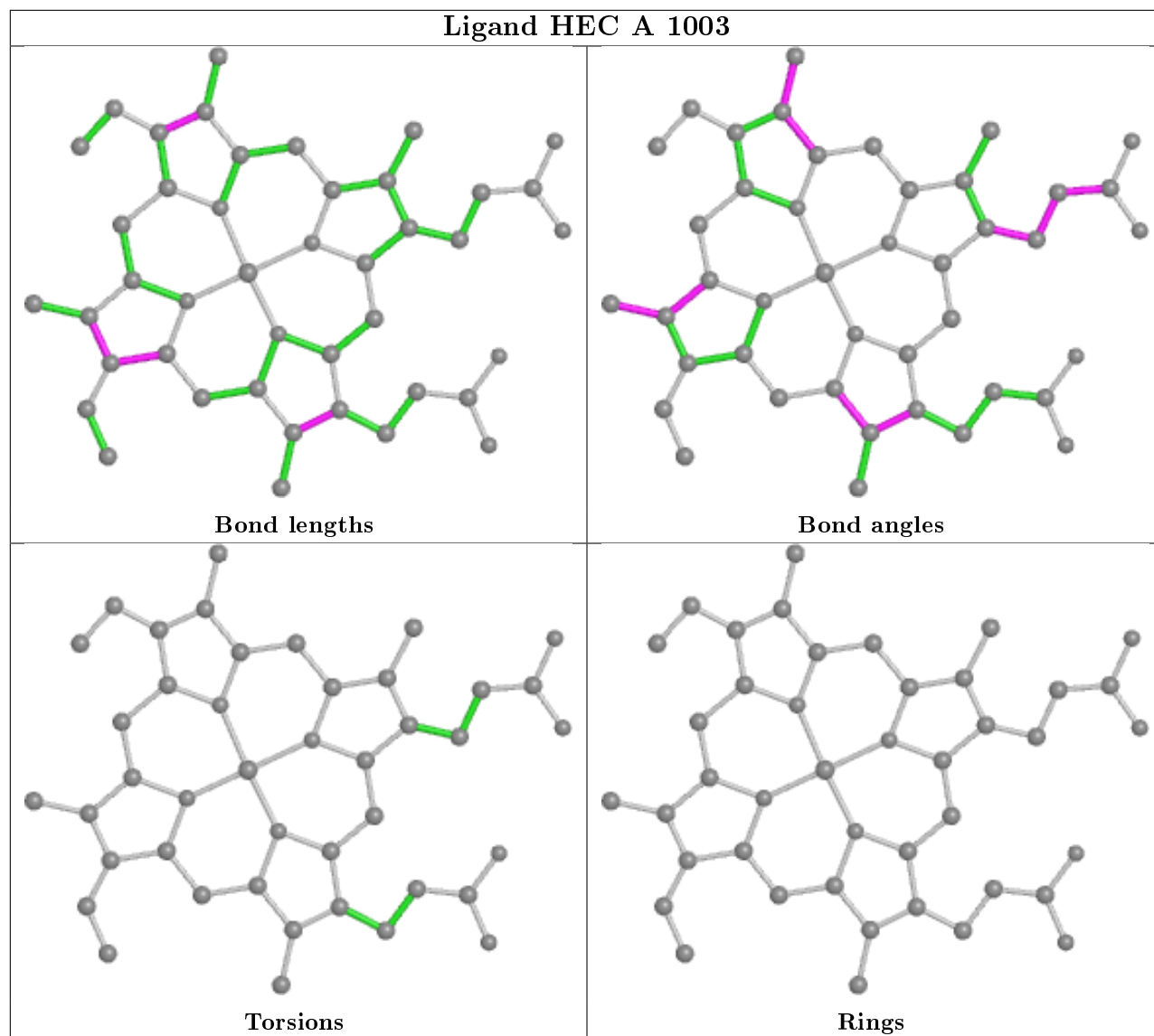
Ligand HEC B 1004



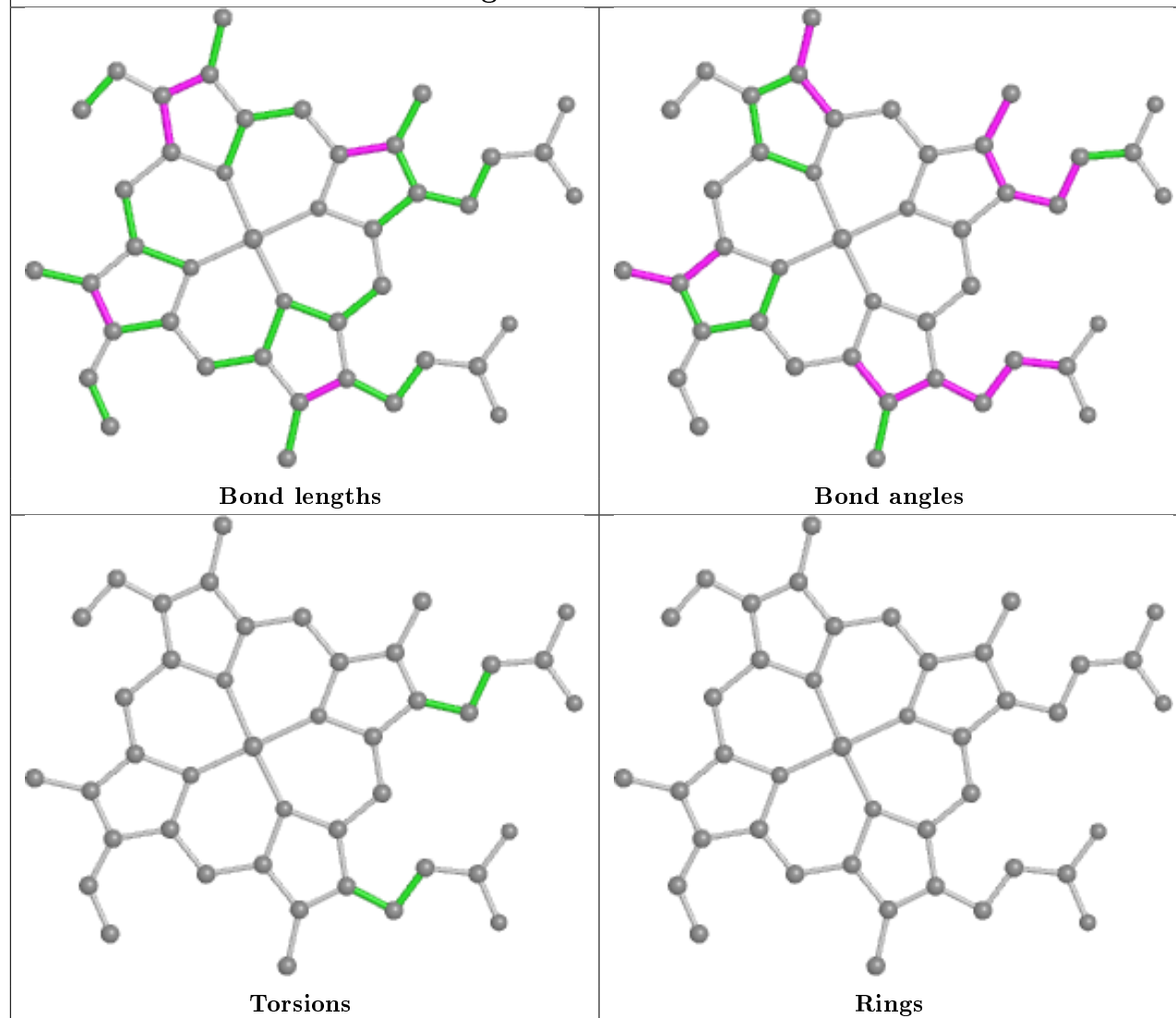
Ligand HEC A 1006



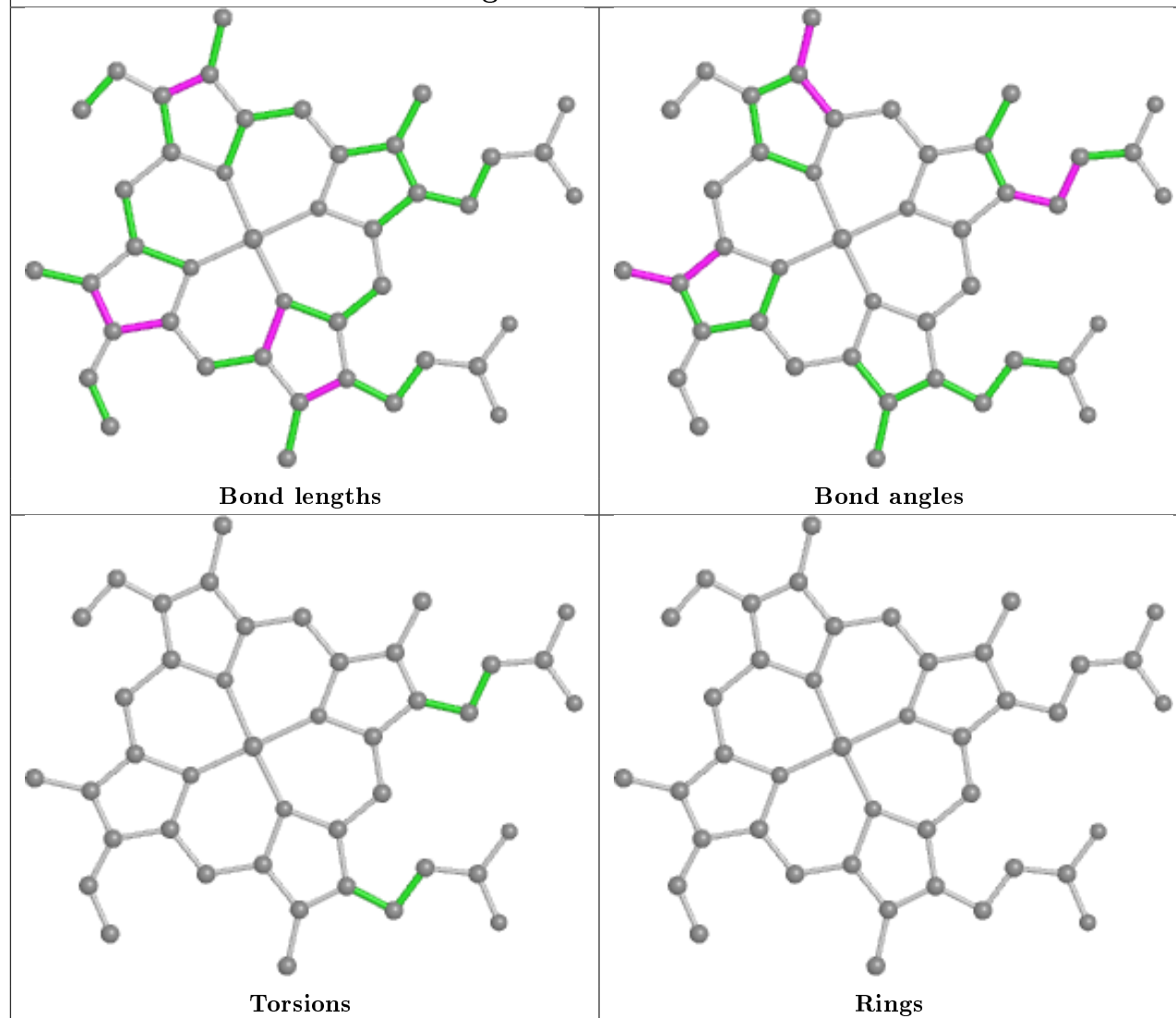
Ligand HEC A 1003



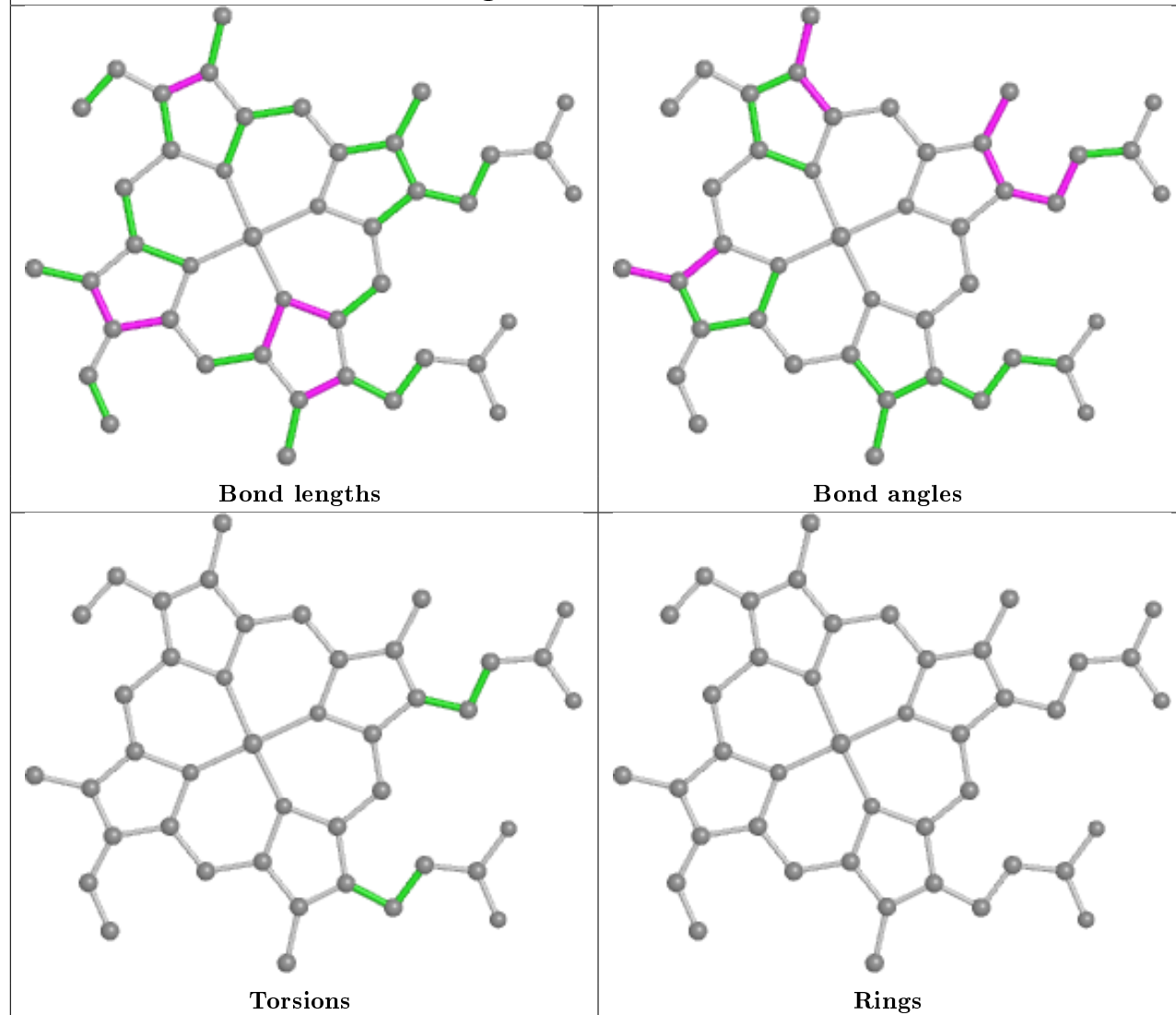
Ligand HEC A 1007



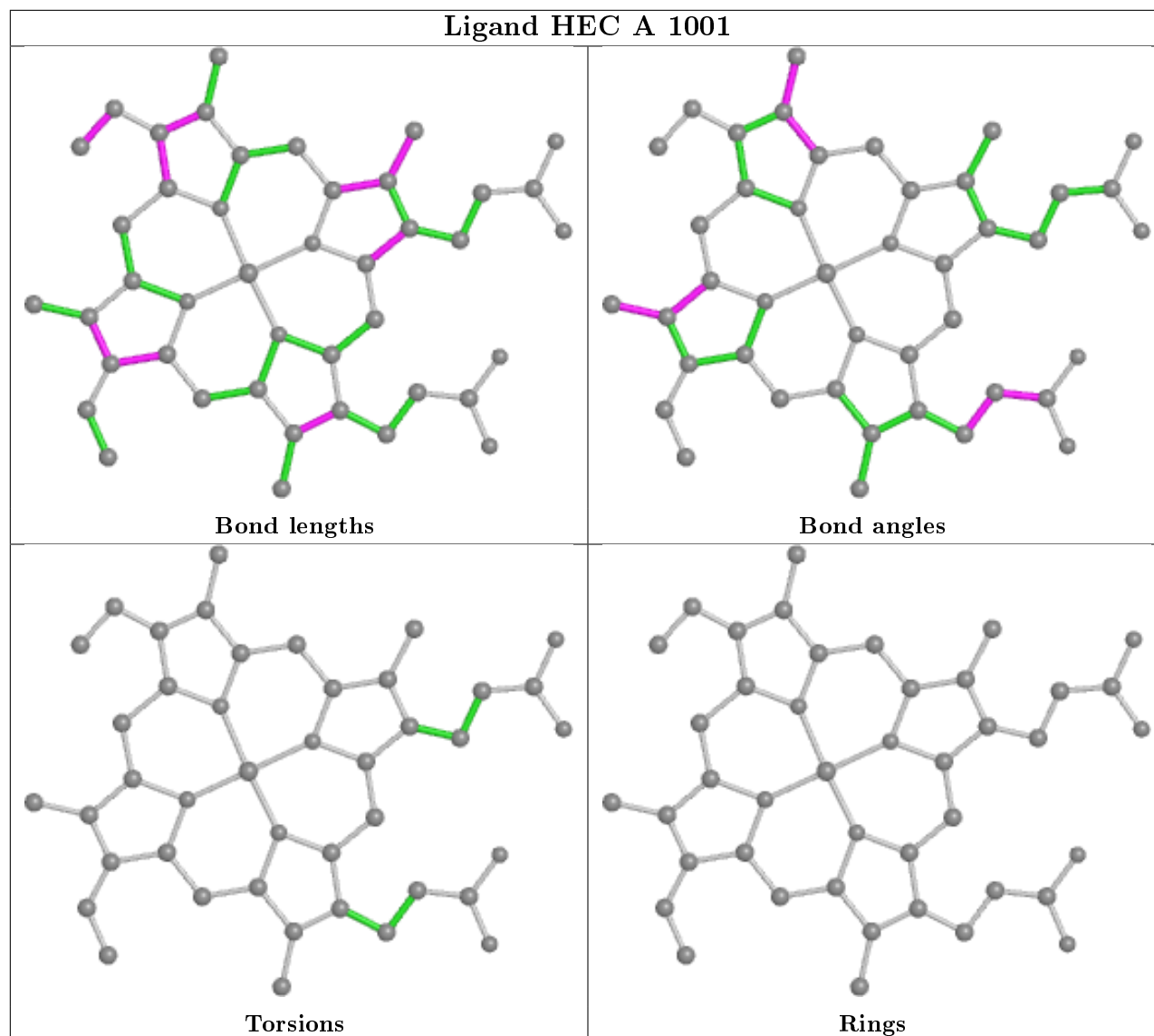
Ligand HEC B 1006

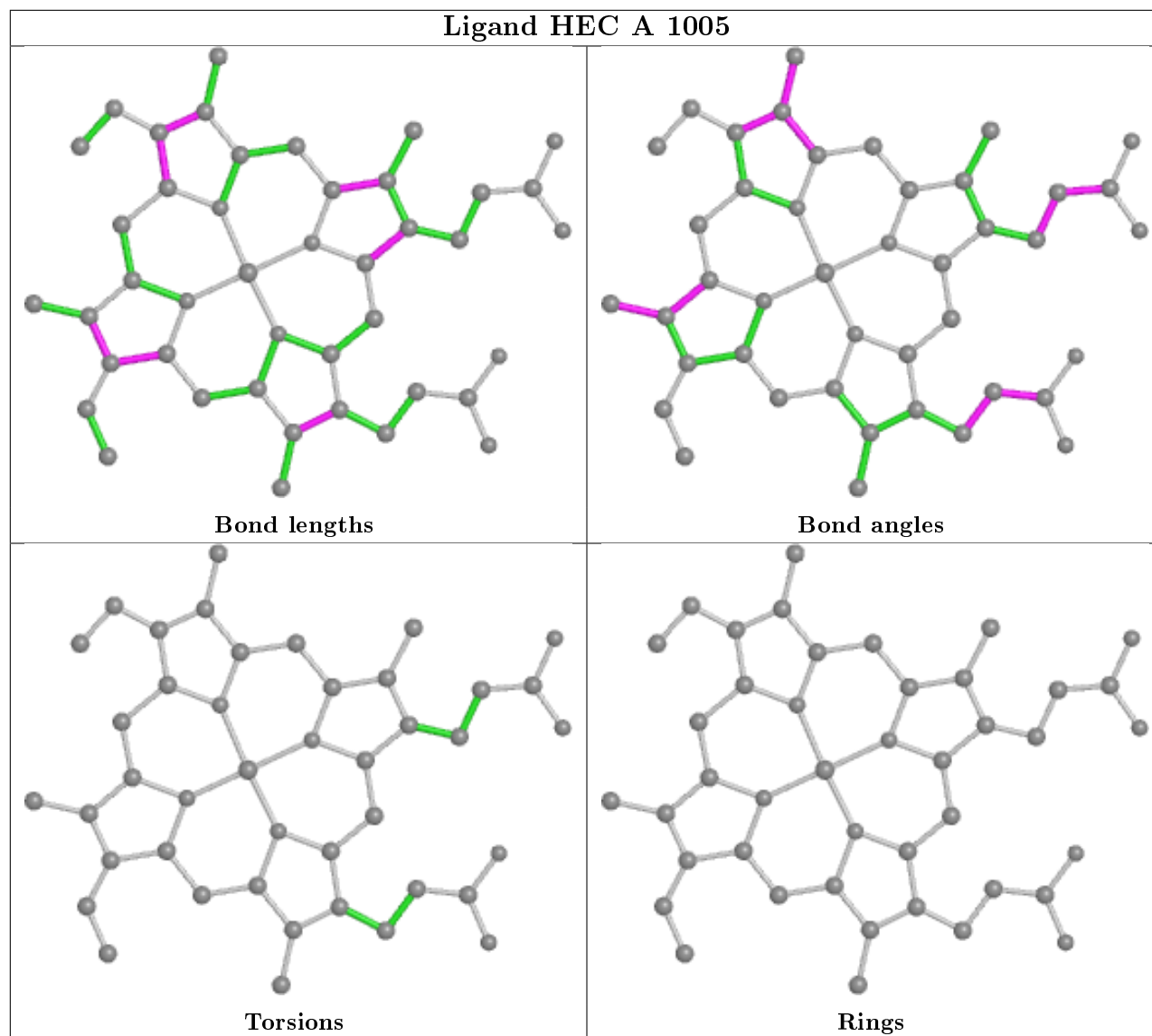


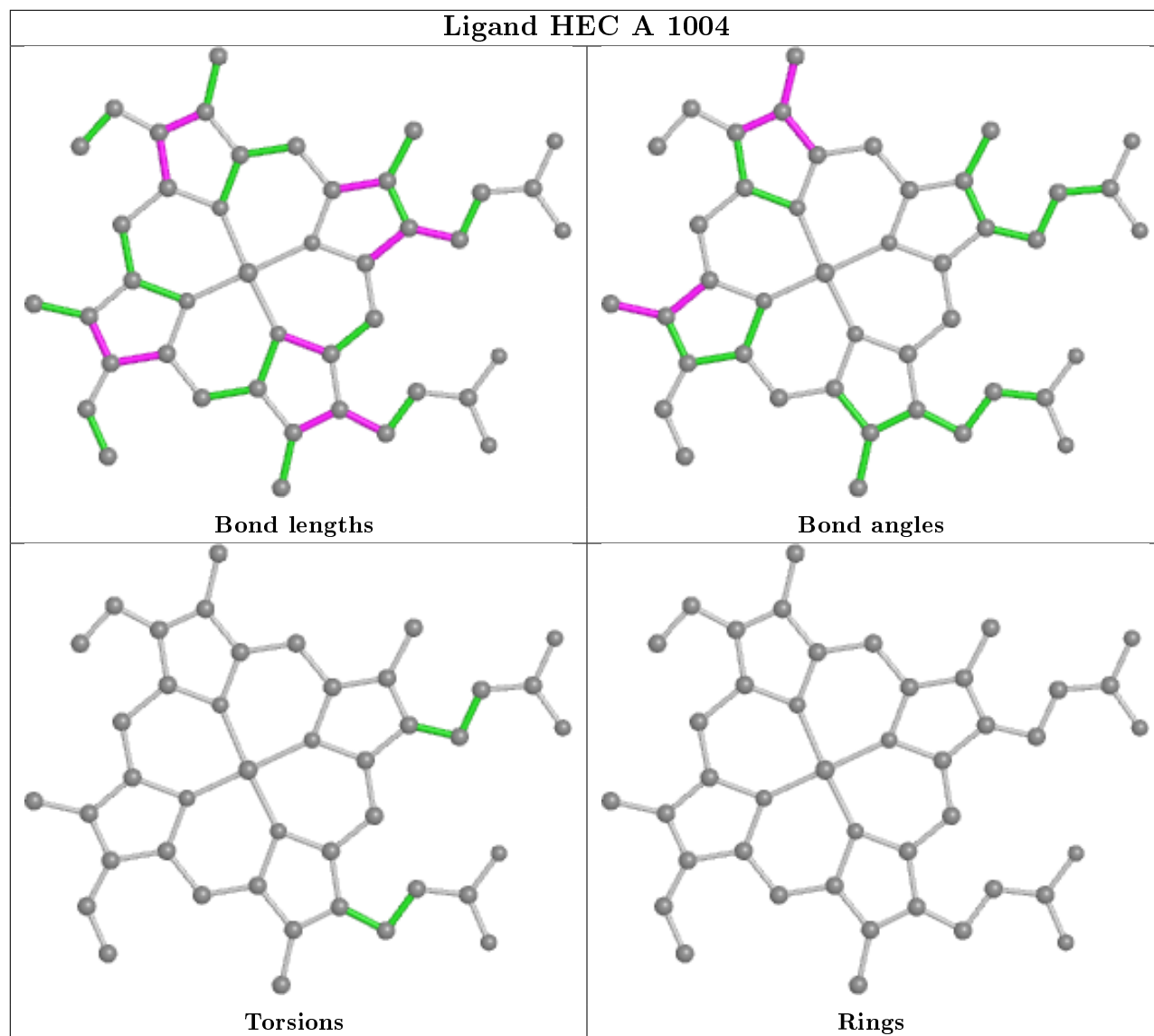
Ligand HEC A 1008

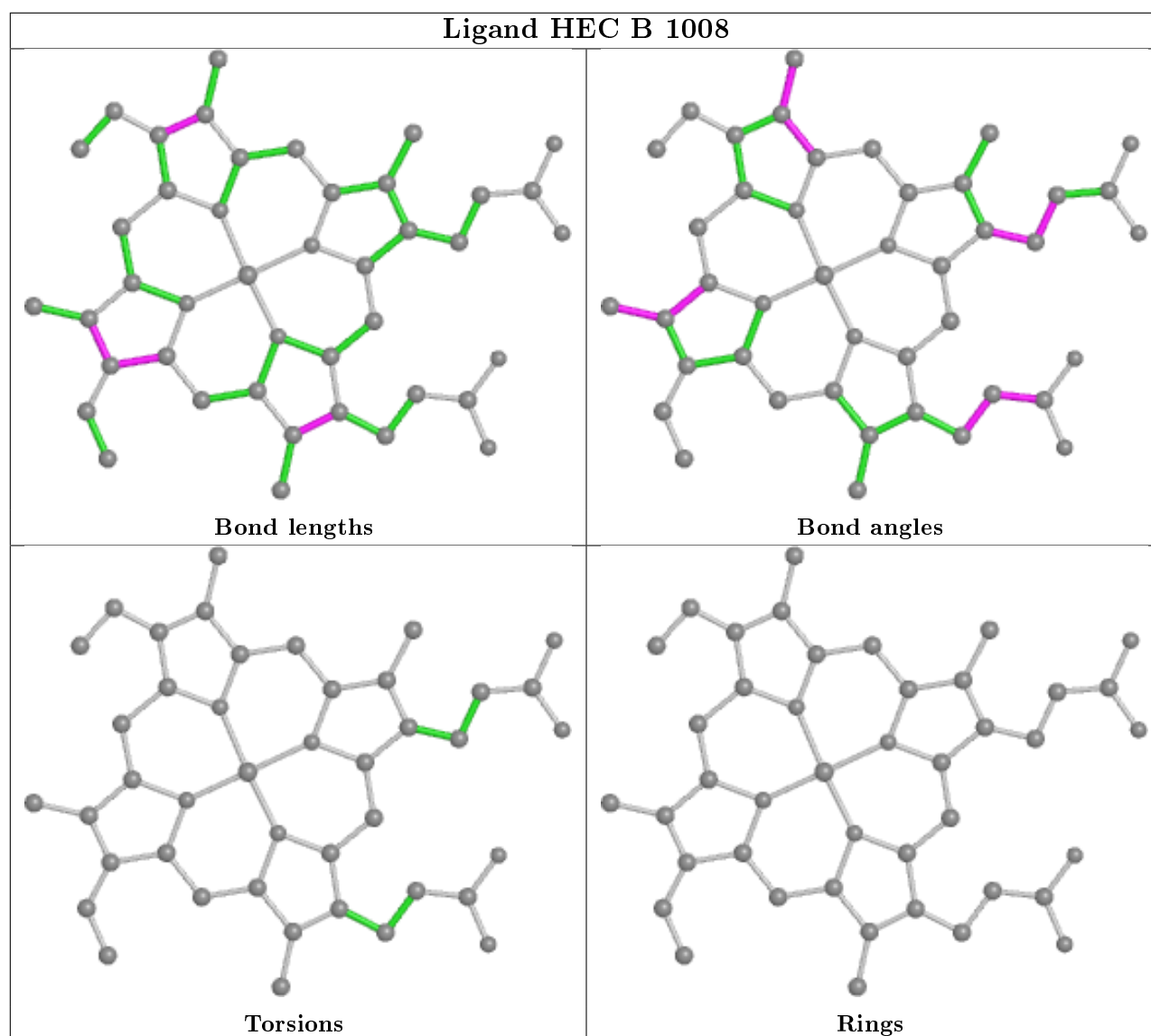


Ligand HEC A 1001









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, 95th 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 ²)	Q<0.9
1	A	521/525 (99%)	-0.73	4 (0%) 86 84	11, 17, 26, 52	0
1	B	521/525 (99%)	-0.74	3 (0%) 89 87	11, 16, 27, 50	0
All	All	1042/1050 (99%)	-0.73	7 (0%) 87 86	11, 16, 27, 52	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	4.8
1	A	524	SER	3.8
1	B	524	SER	3.6
1	A	523	ALA	3.0
1	A	525	ARG	2.4
1	A	522	VAL	2.2
1	B	522	VAL	2.1

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](#)

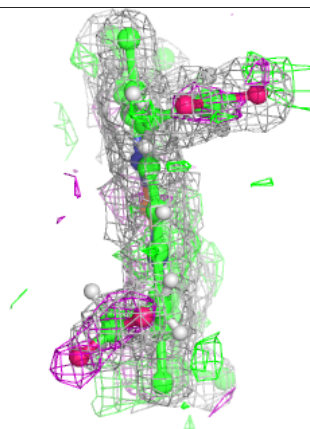
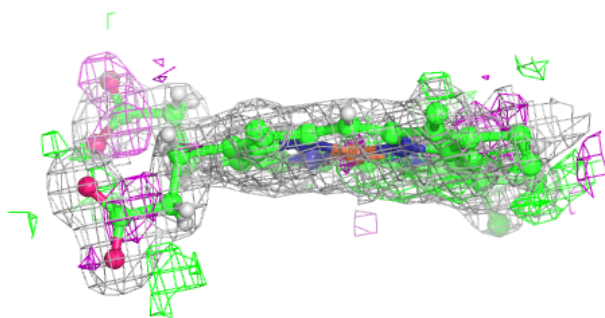
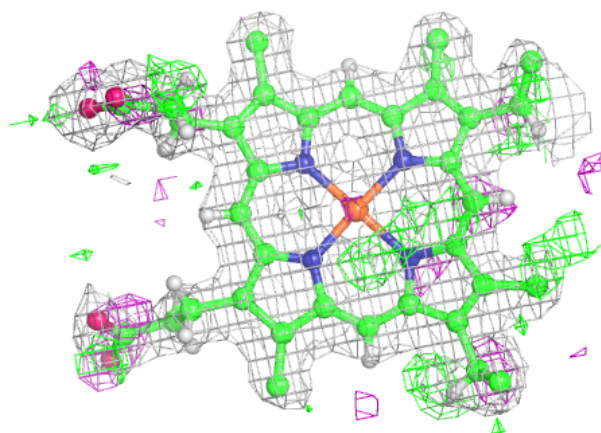
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MPD	A	529	8/8	0.72	0.32	30,31,32,33	8
6	MRD	B	529	8/8	0.77	0.26	24,26,27,27	8
2	HEC	A	1008	43/43	0.95	0.12	14,19,32,43	0
2	HEC	B	1008	43/43	0.95	0.12	14,19,32,42	0
2	HEC	A	1003	43/43	0.97	0.10	9,13,23,32	0
2	HEC	B	1003	43/43	0.97	0.10	9,13,22,30	0
2	HEC	B	1001	43/43	0.97	0.10	16,20,24,25	0
5	MPD	B	528	8/8	0.97	0.07	16,19,19,20	0
5	MPD	A	528	8/8	0.97	0.07	18,20,21,21	0
2	HEC	B	1002	43/43	0.98	0.10	10,15,17,18	0
2	HEC	A	1007	43/43	0.98	0.09	10,13,15,18	0
2	HEC	B	1007	43/43	0.98	0.10	10,12,14,17	0
2	HEC	B	1006	43/43	0.98	0.07	7,11,13,14	0
3	PO4	B	526	5/5	0.98	0.06	10,13,15,17	0
2	HEC	A	1001	43/43	0.98	0.09	14,16,20,24	0
2	HEC	A	1005	43/43	0.98	0.08	9,12,19,25	0
2	HEC	A	1006	43/43	0.98	0.07	8,11,13,14	0
2	HEC	A	1004	43/43	0.98	0.06	12,13,15,16	0
2	HEC	B	1005	43/43	0.98	0.08	8,13,20,26	0
4	CA	A	527	1/1	0.99	0.03	14,14,14,14	0
3	PO4	A	526	5/5	0.99	0.05	14,15,16,17	0
2	HEC	B	1004	43/43	0.99	0.06	11,13,14,16	0
2	HEC	A	1002	43/43	0.99	0.10	11,14,16,18	0
4	CA	B	527	1/1	1.00	0.04	14,14,14,14	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.

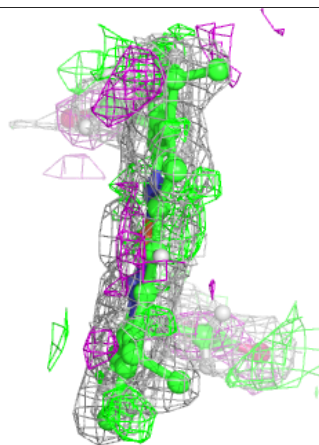
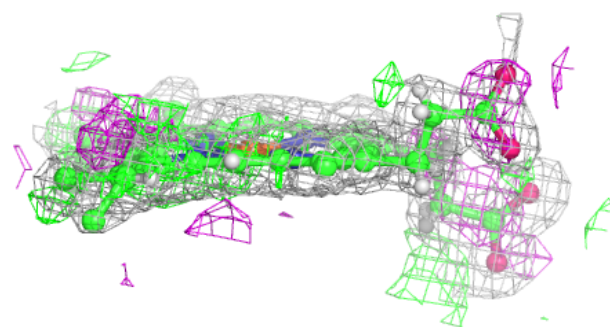
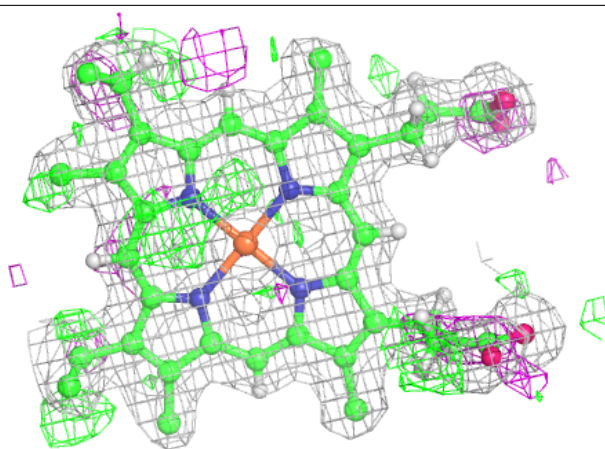
Electron density around HEC A 1008:

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



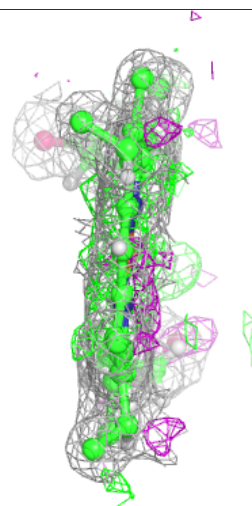
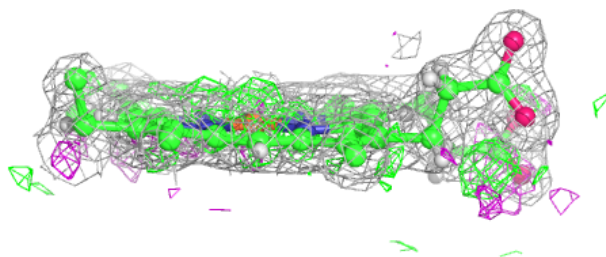
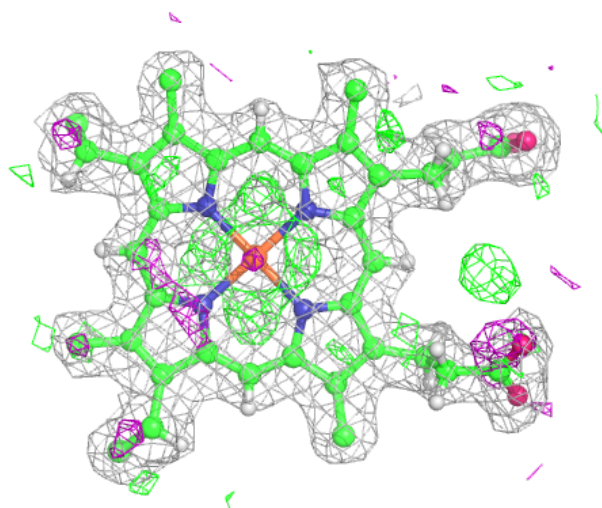
Electron density around HEC B 1008:

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



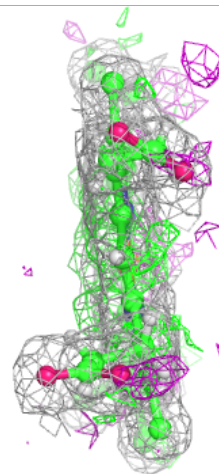
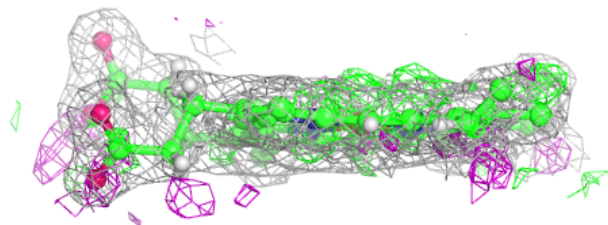
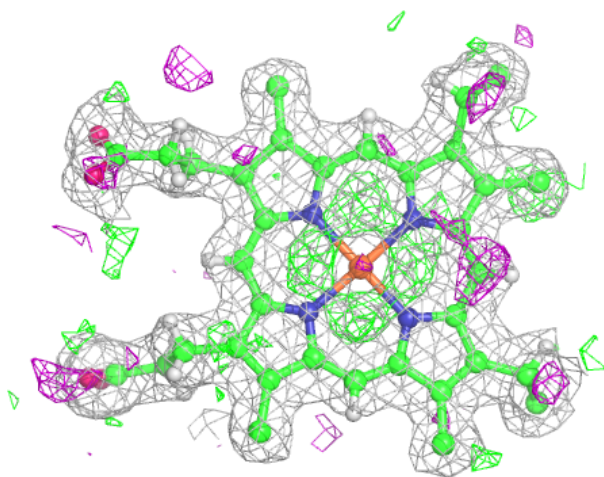
Electron density around HEC A 1003:

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



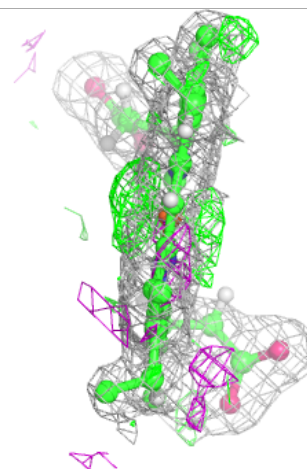
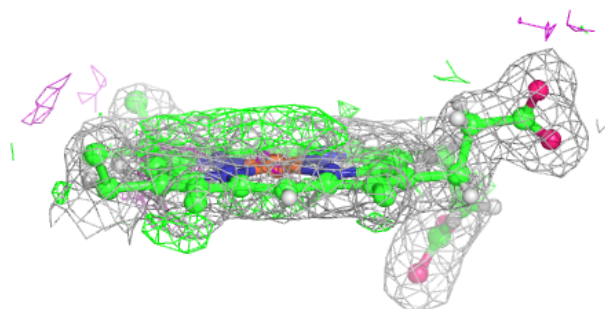
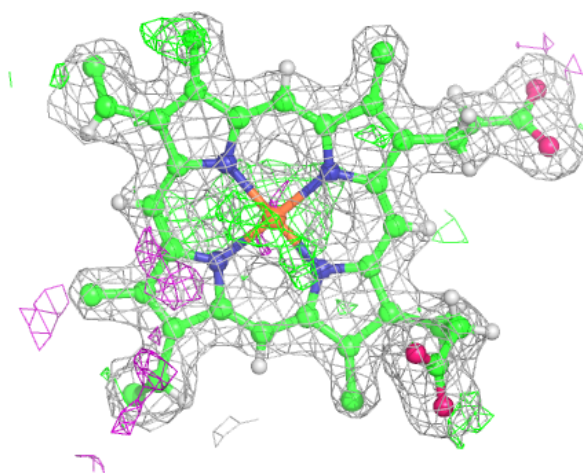
Electron density around HEC B 1003:

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



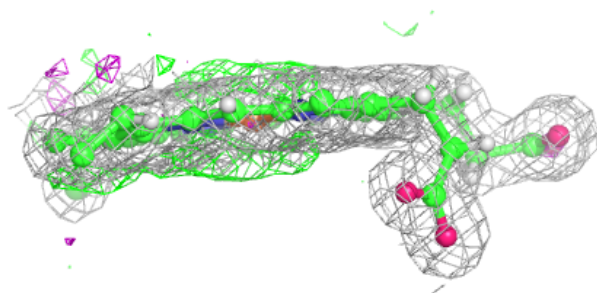
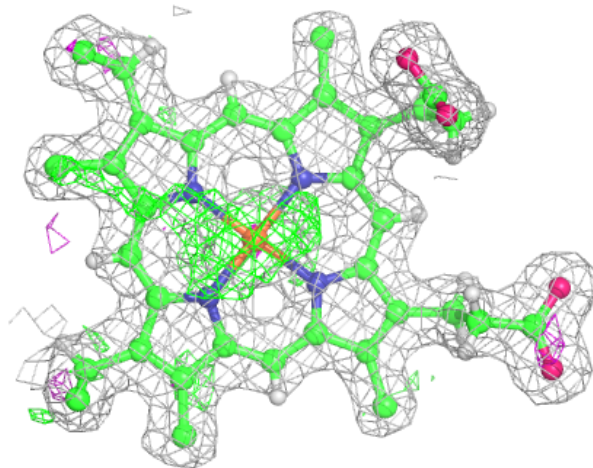
Electron density around HEC B 1001:

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



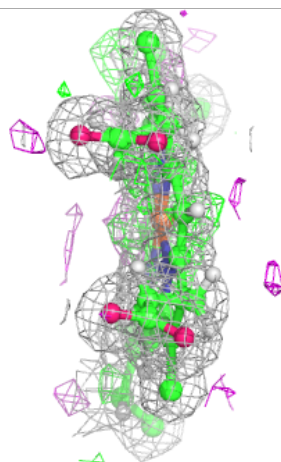
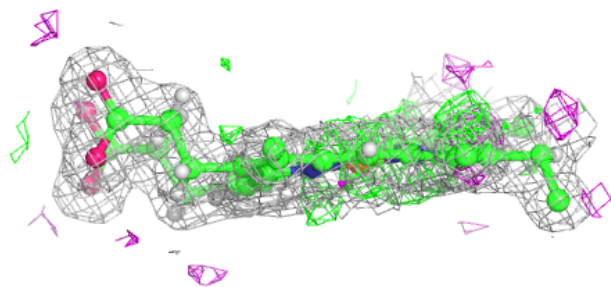
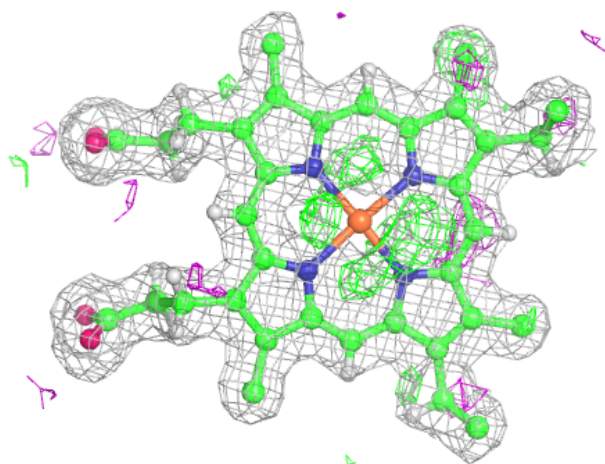
Electron density around HEC B 1002:

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



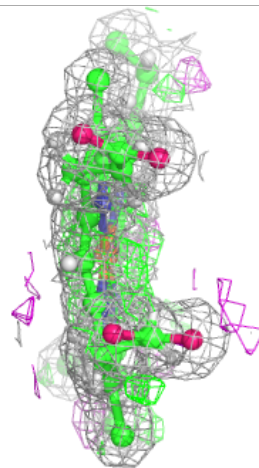
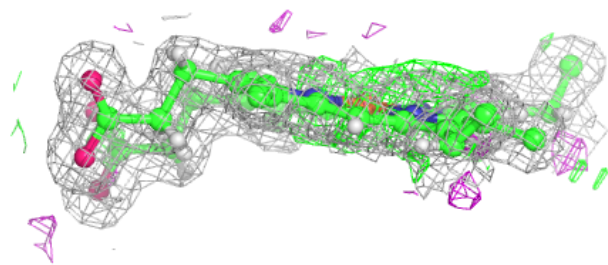
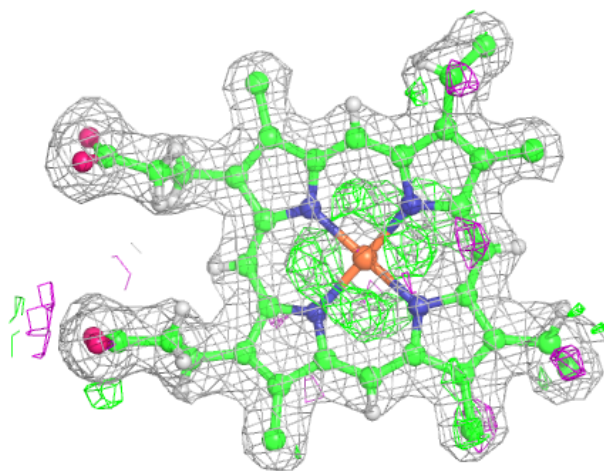
Electron density around HEC A 1007:

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



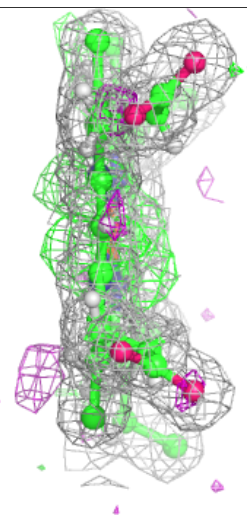
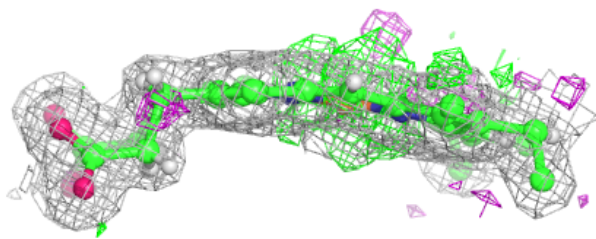
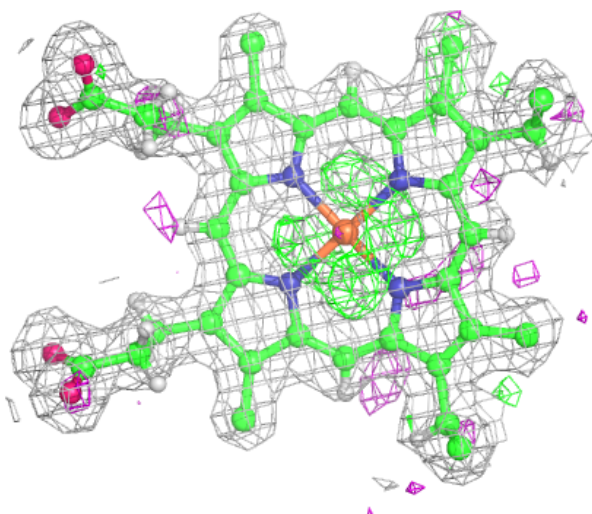
Electron density around HEC B 1007:

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



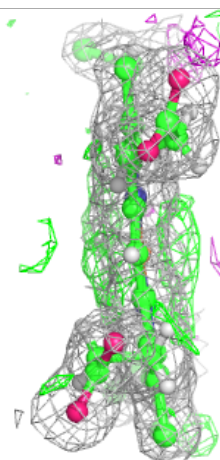
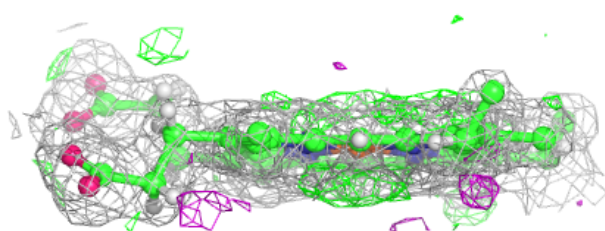
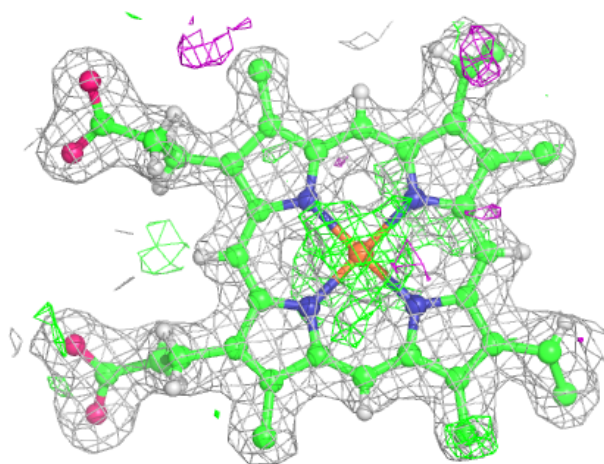
Electron density around HEC B 1006:

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



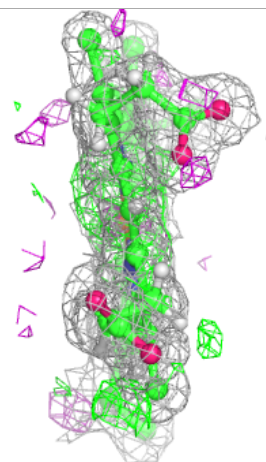
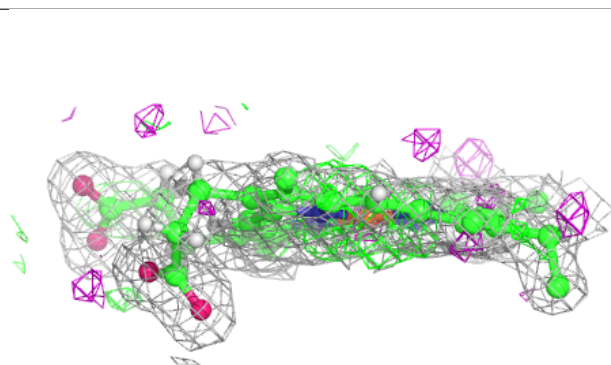
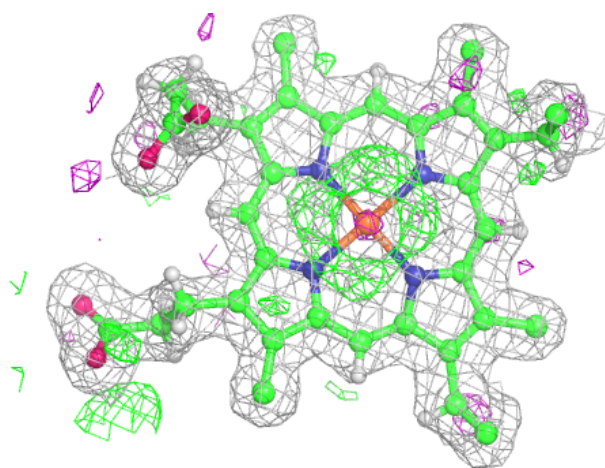
Electron density around HEC A 1001:

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



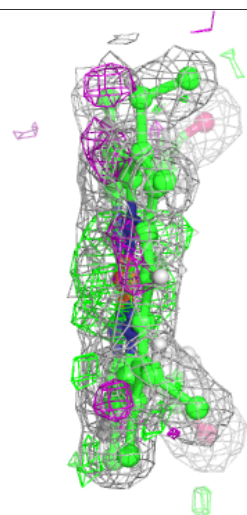
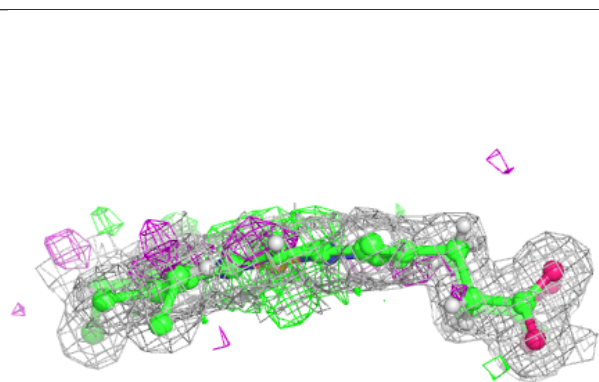
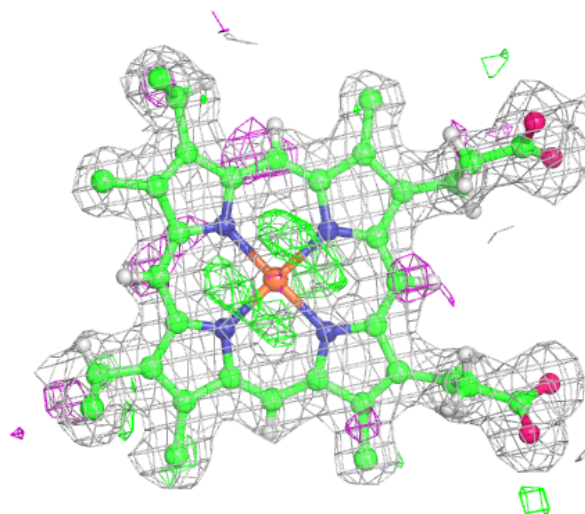
Electron density around HEC A 1005:

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



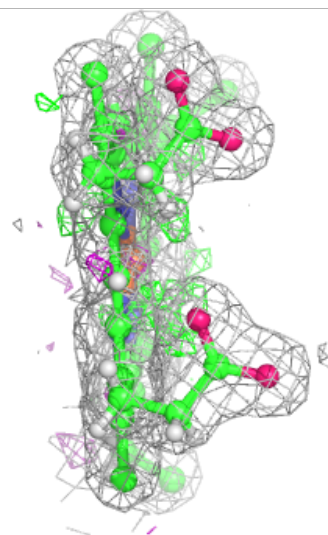
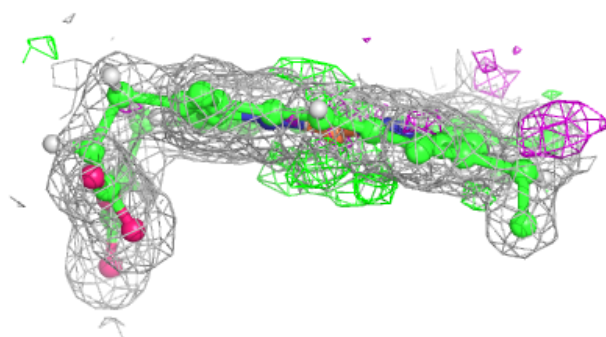
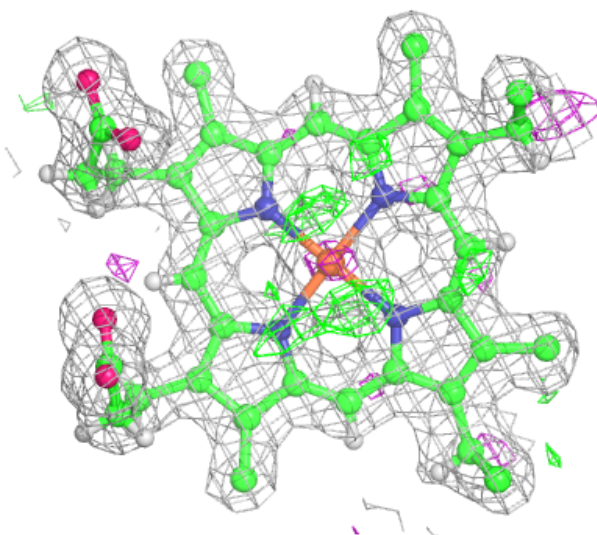
Electron density around HEC A 1006:

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



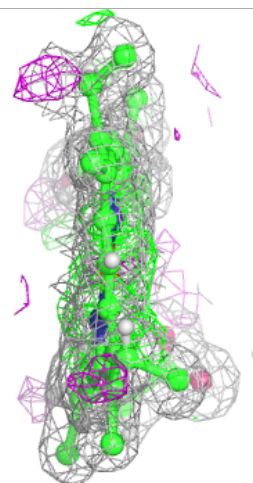
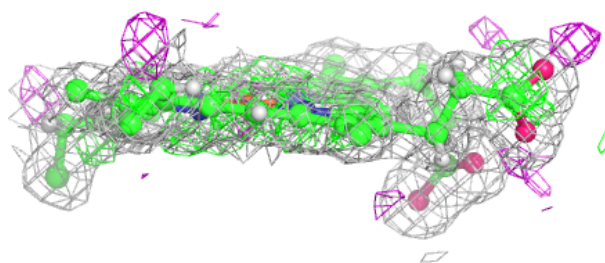
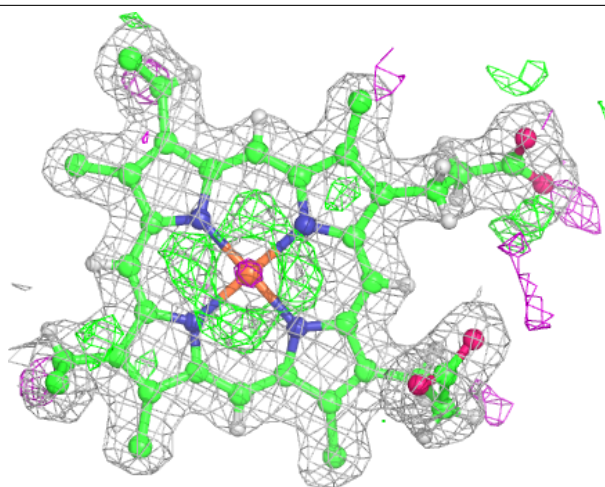
Electron density around HEC A 1004:

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



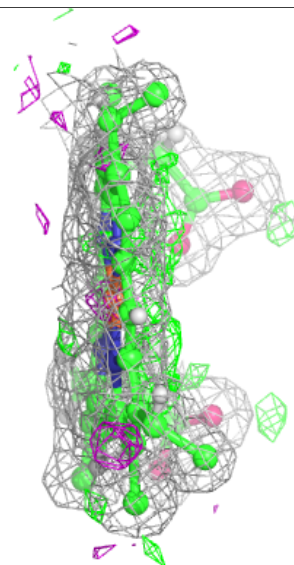
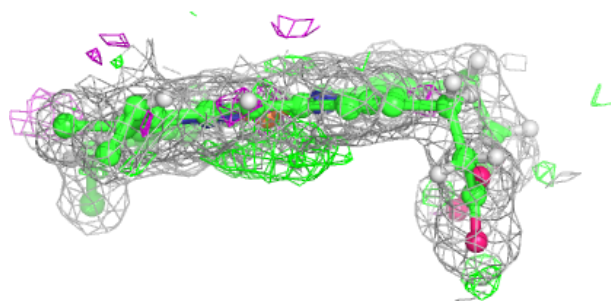
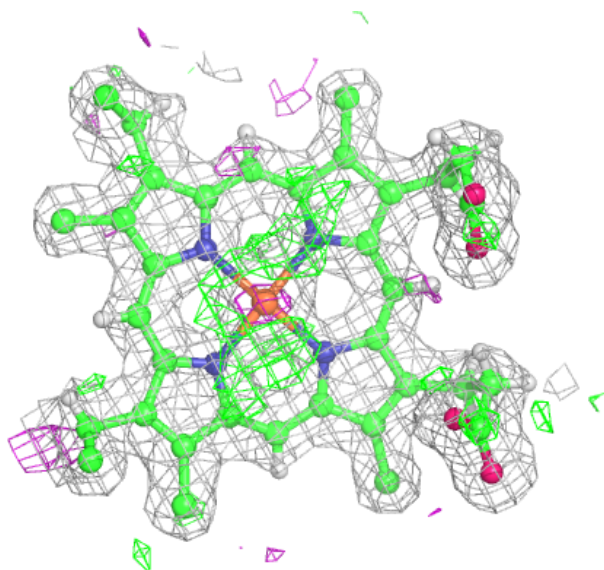
Electron density around HEC B 1005:

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



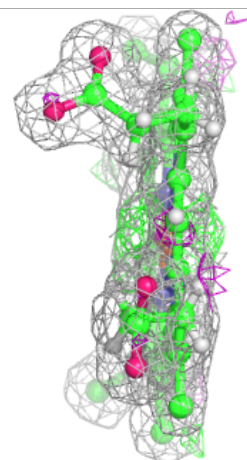
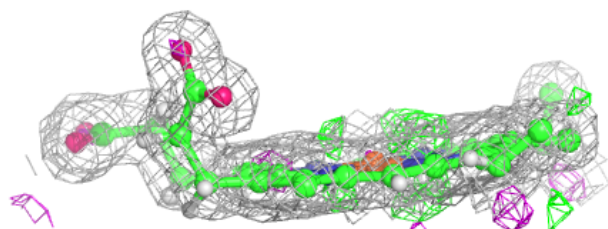
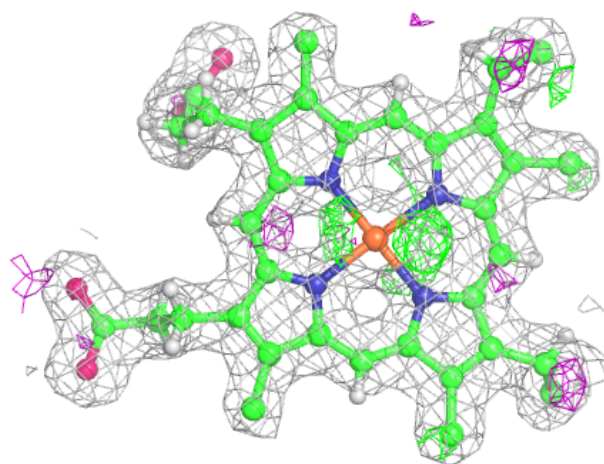
Electron density around HEC B 1004:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.