



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:47 PM EDT

PDB ID : 2ZO5 / pdb_00002zo5
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase in a complex with azide
Authors : Polyakov, K.M.; Boyko, K.M.; Slutsky, A.; Tikhonova, T.V.; Antipov, A.N.; Zvyagilskaya, R.A.; Popov, A.N.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.
Deposited on : 2008-05-05
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

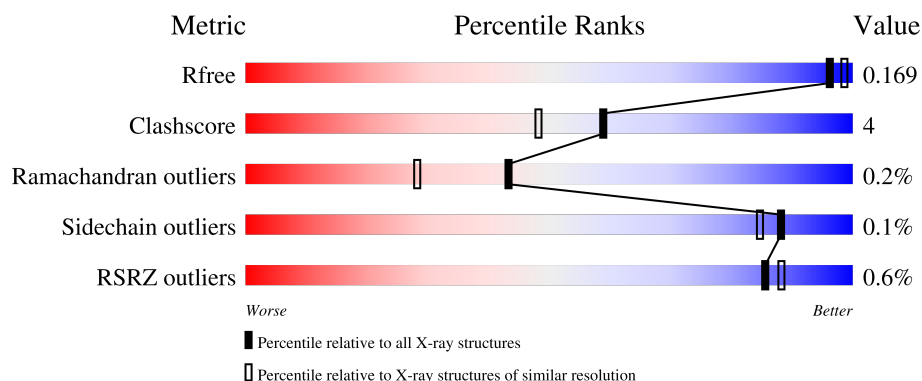
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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% 6% %
1	B	525	% 92% 7% %

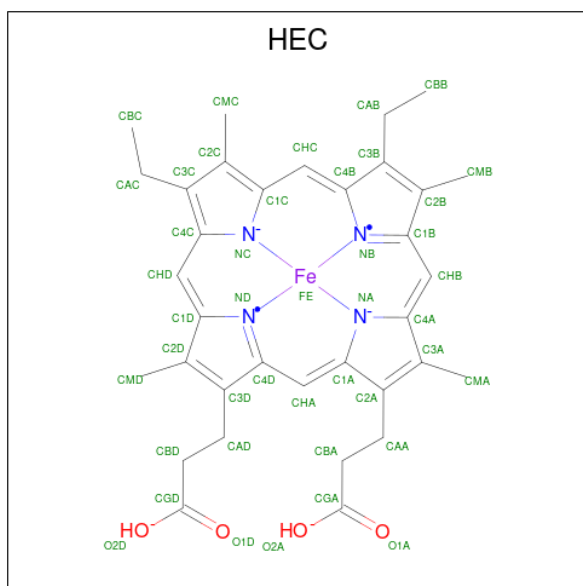
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	1001	X	-	-	-
2	HEC	A	1002	X	-	-	-
2	HEC	A	1003	X	-	-	-
2	HEC	A	1004	X	-	-	-
2	HEC	A	1005	X	-	-	-
2	HEC	A	1006	X	-	-	-
2	HEC	A	1007[A]	X	-	-	-
2	HEC	A	1007[B]	X	-	-	-
2	HEC	A	1008	X	-	-	-
2	HEC	B	1001	X	-	-	-
2	HEC	B	1002	X	-	-	-
2	HEC	B	1003	X	-	-	-
2	HEC	B	1004	X	-	-	-
2	HEC	B	1005	X	-	-	-
2	HEC	B	1006	X	-	-	-
2	HEC	B	1007[A]	X	-	-	-
2	HEC	B	1007[B]	X	-	-	-
3	AZI	A	526	-	X	-	-
3	AZI	A	530	-	X	-	-
3	AZI	B	526	-	X	-	-
3	AZI	B	530	-	X	-	-
6	PG4	B	1014	-	-	X	-
8	TRS	B	1012	-	X	-	-

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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 2 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



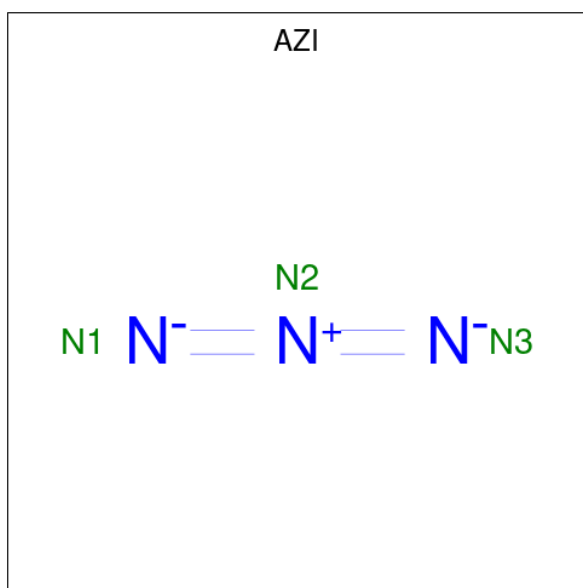
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 79	C 36	Fe 1	H 32	N 4	O 6	18	1

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	A	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	A	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	A	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	1
			79	36	1	32	4	6		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	18	0
			73	34	1	30	4	4		

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



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

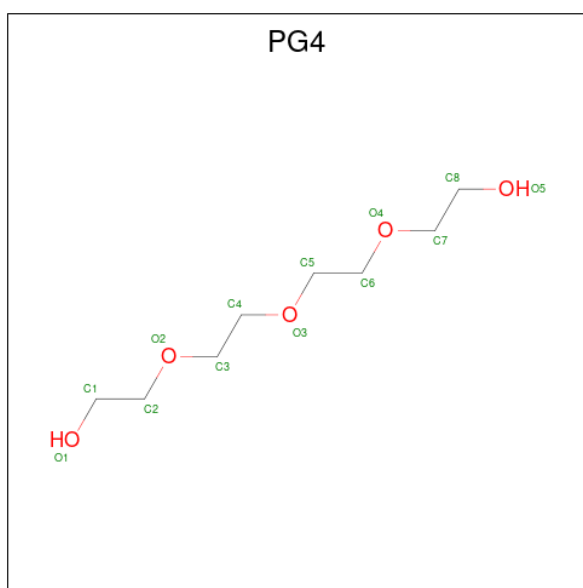
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

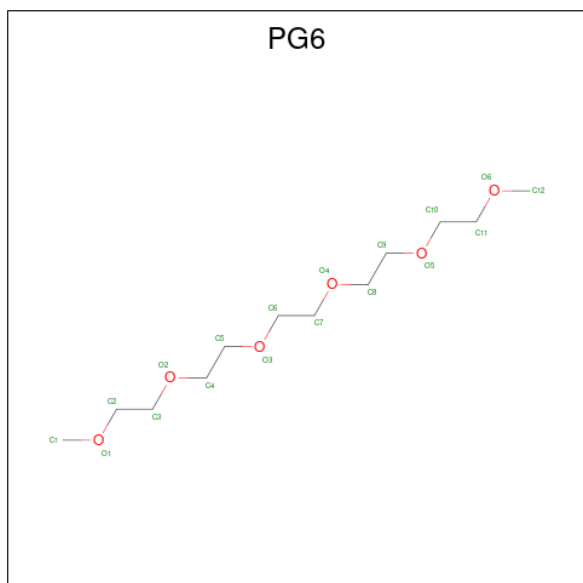
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
			7	4	3		
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
			9	6	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
			7	5	2		

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



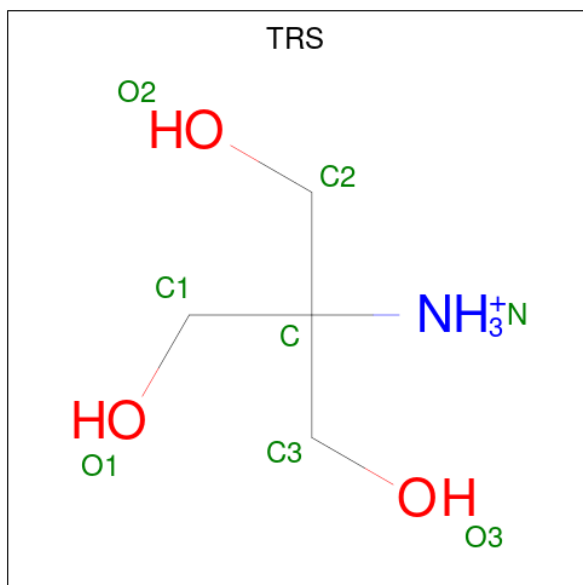
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			14	9	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			14	9	5		

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

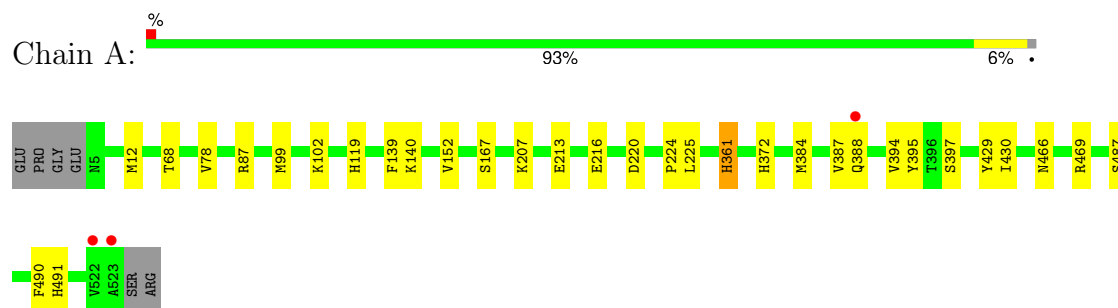
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	549	Total	O	0	0
			549	549		
9	B	575	Total	O	0	0
			575	575		

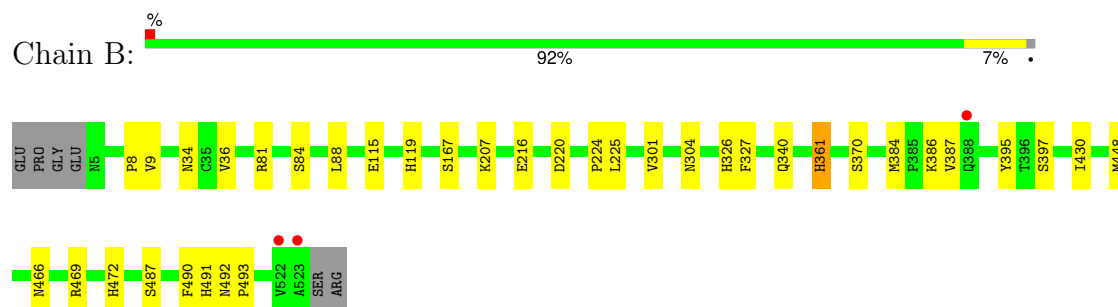
3 Residue-property plots [i](#)

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

- Molecule 1: 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	193.03Å 193.03Å 193.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 1.70 11.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (11.99-1.70) 98.4 (11.99-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.151 , 0.168 0.154 , 0.169	Depositor DCC
R_{free} test set	13645 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18499	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 2.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG6, TRS, PG4, AZI, HEC, NA, CA

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	0.76	0/4415	0.81	0/5986
1	B	0.80	0/4388	0.82	0/5949
All	All	0.78	0/8803	0.82	0/11935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4179	3850	3897	22	2
1	B	4180	3857	3906	33	0
2	A	348	242	218	8	0
2	B	348	242	218	8	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	45	0	49	18	0
7	A	14	0	14	1	0
7	B	14	0	14	1	0
8	A	8	0	12	1	0
8	B	8	0	9	0	0
9	A	549	0	0	7	0
9	B	575	0	0	7	1
All	All	10308	8191	8362	75	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLN:HE21	6:B:1015:PG4:C6	1.81	0.94
6:B:1014:PG4:H61	9:B:1397:HOH:O	1.68	0.92
1:B:361:HIS:NE2	3:B:526:AZI:N3	2.30	0.79
1:B:386:LYS:NZ	9:B:1183:HOH:O	2.15	0.78
1:B:9:VAL:HG13	1:B:36[B]:VAL:CG1	2.16	0.76
1:B:115:GLU:OE1	6:B:1014:PG4:H81	1.86	0.75
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.68	0.74
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.68	0.74
2:A:1008:HEC:HBC3	2:A:1008:HEC:HMC1	1.71	0.71
6:B:1009:PG4:H81	9:B:1396:HOH:O	1.92	0.68
6:B:1014:PG4:C6	9:B:1397:HOH:O	2.35	0.68
1:A:361:HIS:NE2	3:A:526:AZI:N3	2.40	0.68
1:B:370:SER:HA	6:B:1016:PG4:H61	1.75	0.68
1:A:68[B]:THR:HG21	9:A:1106:HOH:O	1.94	0.67
1:B:34:ASN:HD22	6:B:1009:PG4:H61	1.59	0.67
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.81	0.63
1:B:84:SER:HA	6:B:1014:PG4:H72	1.80	0.62
1:B:81:ARG:HH22	6:B:1014:PG4:C3	2.14	0.61
7:A:1010:PG6:C10	9:A:1252:HOH:O	2.49	0.59
2:B:1001:HEC:HBC3	2:B:1001:HEC:HMC1	1.83	0.59
2:A:1003:HEC:HMC1	2:A:1003:HEC:HBC3	1.84	0.59
6:B:1014:PG4:C8	9:B:1446:HOH:O	2.52	0.57
1:B:34:ASN:HD22	6:B:1009:PG4:C6	2.21	0.54
1:B:492:ASN:HA	6:B:1016:PG4:H62	1.90	0.53
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	1.91	0.53
1:A:139:PHE:HB2	6:A:1011:PG4:H22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:OE1	6:B:1014:PG4:C8	2.57	0.52
2:B:1003:HEC:HMC1	2:B:1003:HEC:HBC3	1.91	0.51
1:B:387[A]:VAL:HG21	1:B:395:TYR:CE1	2.46	0.50
1:A:466:ASN:HD22	1:A:469:ARG:HD2	1.79	0.47
1:A:394[B]:VAL:HG12	9:A:1549:HOH:O	2.14	0.47
2:A:1003:HEC:HMC3	9:A:1439:HOH:O	2.14	0.47
1:A:167:SER:HB2	1:A:216[B]:GLU:HG2	1.97	0.47
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.13	0.46
1:A:140:LYS:NZ	9:A:1516:HOH:O	2.45	0.45
1:A:207:LYS:NZ	1:A:220[B]:ASP:OD2	2.42	0.45
1:A:387[A]:VAL:HG21	1:A:395:TYR:CE1	2.51	0.45
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.15	0.44
1:B:119:HIS:CD2	2:B:1006:HEC:ND	2.86	0.44
1:A:102[B]:LYS:NZ	9:A:1415:HOH:O	2.50	0.44
1:A:119:HIS:CD2	2:A:1006:HEC:ND	2.86	0.44
1:A:384:MET:HB2	1:A:397:SER:O	2.17	0.44
1:B:224:PRO:O	1:B:225:LEU:C	2.60	0.44
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.83	0.44
1:B:493:PRO:HD2	6:B:1016:PG4:H62	2.00	0.44
6:B:1014:PG4:H82	9:B:1446:HOH:O	2.16	0.44
1:B:34:ASN:HB2	6:B:1009:PG4:H61	2.00	0.44
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.98	0.44
1:A:78[B]:VAL:HG23	1:A:152:VAL:HG21	2.00	0.43
1:B:81:ARG:HH12	6:B:1014:PG4:C5	2.31	0.43
1:A:99:MET:HE2	8:A:1012:TRS:H11	2.00	0.43
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.54	0.43
1:B:207:LYS:NZ	1:B:220[B]:ASP:OD2	2.43	0.43
2:A:1004:HEC:C4D	2:A:1006:HEC:HMD2	2.49	0.43
2:A:1008:HEC:HMB1	2:A:1008:HEC:HBB3	2.01	0.43
1:A:68[A]:THR:OG1	2:B:1003:HEC:HBD1	2.19	0.42
1:B:448:MET:HE1	1:B:472:HIS:CG	2.54	0.42
2:A:1008:HEC:HMC1	2:A:1008:HEC:CBC	2.45	0.42
1:A:12:MET:HE2	6:A:1013:PG4:H51	2.02	0.42
1:A:430:ILE:HG21	1:A:490:PHE:HA	2.02	0.41
1:A:224:PRO:O	1:A:225:LEU:C	2.62	0.41
1:B:448:MET:HE1	1:B:472:HIS:CD2	2.56	0.41
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.55	0.41
2:B:1008:HEC:HMC1	2:B:1008:HEC:CBC	2.45	0.41
1:A:372:HIS:HB2	9:A:1391:HOH:O	2.20	0.41
1:B:384:MET:HB2	1:B:397:SER:O	2.21	0.41
2:B:1002:HEC:HBC3	2:B:1002:HEC:CMC	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1013:PG4:H52	1:B:8:PRO:HG2	2.01	0.41
7:B:1011:PG6:O1	9:B:1368:HOH:O	2.22	0.41
1:B:34:ASN:OD1	1:B:36[B]:VAL:HG22	2.22	0.41
1:B:301:VAL:HG21	1:B:327:PHE:CE2	2.56	0.40
1:A:213[A]:GLU:OE1	1:A:216[A]:GLU:OE2	2.38	0.40
1:B:493:PRO:HD2	6:B:1016:PG4:C7	2.51	0.40
1:B:304:ASN:HB2	1:B:326:HIS:HB3	2.04	0.40
1:B:9:VAL:HG13	1:B:36[B]:VAL:HG11	1.97	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH12	1:A:429:TYR:HH[12_565]	1.32	0.28
1:A:388:GLN:OE1	9:B:1317:HOH:O[6_456]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/525 (103%)	520 (96%)	20 (4%)	1 (0%)	43	28
1	B	536/525 (102%)	514 (96%)	21 (4%)	1 (0%)	43	28
All	All	1077/1050 (103%)	1034 (96%)	41 (4%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS
1	B	361	HIS

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	459/443 (104%)	459 (100%)	0	100	100
1	B	456/443 (103%)	454 (100%)	2 (0%)	84	80
All	All	915/886 (103%)	913 (100%)	2 (0%)	88	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88[A]	LEU
1	B	88[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	175	GLN
1	A	466	ASN
1	A	521	GLN
1	B	138	GLN
1	B	222	ASN
1	B	267	GLN
1	B	340	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 6 are monoatomic - leaving 36 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$
6	PG4	B	1015	-	4,4,12	0.46	0	3,3,11	0.07	0
8	TRS	A	1012	-	7,7,7	0.16	0	9,9,9	0.91	0
2	HEC	A	1001	1	50,50,50	1.53	7 (14%)	68,82,82	1.43	12 (17%)
3	AZI	A	530	-	2,2,2	2.74	2 (100%)	0,1,1	-	-
2	HEC	A	1005	1	50,50,50	1.47	6 (12%)	68,82,82	1.20	6 (8%)
2	HEC	A	1008	1	50,50,50	1.52	6 (12%)	68,82,82	1.27	7 (10%)
2	HEC	A	1007[B]	4	50,50,50	1.54	8 (16%)	68,82,82	1.47	10 (14%)
2	HEC	B	1002	1	50,50,50	1.64	9 (18%)	68,82,82	1.32	6 (8%)
2	HEC	A	1003	1	50,50,50	1.36	4 (8%)	68,82,82	1.09	7 (10%)
2	HEC	B	1001	1	50,50,50	1.61	9 (18%)	68,82,82	1.46	14 (20%)
2	HEC	B	1007[B]	4	50,50,50	1.53	9 (18%)	68,82,82	1.39	8 (11%)
6	PG4	B	1014	4	8,8,12	0.45	0	7,7,11	0.76	0
8	TRS	B	1012	-	7,7,7	3.23	1 (14%)	9,9,9	2.61	3 (33%)
2	HEC	B	1003	1	50,50,50	1.43	4 (8%)	68,82,82	1.26	8 (11%)
2	HEC	A	1007[A]	-	50,50,50	1.55	8 (16%)	68,82,82	1.46	10 (14%)
6	PG4	B	1017	-	6,6,12	0.42	0	5,5,11	0.20	0
3	AZI	B	530	-	2,2,2	2.41	2 (100%)	0,1,1	-	-
2	HEC	B	1007[A]	-	50,50,50	1.53	9 (18%)	68,82,82	1.38	8 (11%)
2	HEC	A	1004	1,3,9	50,50,50	1.45	6 (12%)	68,82,82	1.12	6 (8%)
2	HEC	B	1006	4,1	50,50,50	1.54	7 (14%)	68,82,82	1.41	7 (10%)
3	AZI	B	526	2	2,2,2	2.85	2 (100%)	0,1,1	-	-
2	HEC	B	1008	1	50,50,50	1.53	6 (12%)	68,82,82	1.44	13 (19%)
6	PG4	A	1009	-	7,7,12	0.56	0	6,6,11	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	1002	1	50,50,50	1.59	10 (20%)	68,82,82	1.32	7 (10%)
7	PG6	B	1011	1	13,13,17	0.50	0	12,12,16	0.27	0
6	PG4	B	1009	-	6,6,12	0.53	0	5,5,11	0.62	0
6	PG4	B	1013	-	4,4,12	0.43	0	3,3,11	0.36	0
2	HEC	B	1005	1	50,50,50	1.47	7 (14%)	68,82,82	1.13	6 (8%)
2	HEC	B	1004	1,3,9	50,50,50	1.50	5 (10%)	68,82,82	1.23	7 (10%)
6	PG4	A	1011	-	5,5,12	0.56	0	4,4,11	0.71	0
6	PG4	B	1016	-	4,4,12	0.67	0	3,3,11	0.52	0
6	PG4	A	1013	-	7,7,12	0.45	0	6,6,11	0.27	0
7	PG6	A	1010	1	13,13,17	0.43	0	12,12,16	0.39	0
3	AZI	A	526	2	2,2,2	2.99	2 (100%)	0,1,1	-	-
2	HEC	A	1006	4,1	50,50,50	1.43	5 (10%)	68,82,82	1.23	6 (8%)
6	PG4	B	1010	-	6,6,12	0.38	0	5,5,11	0.70	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
6	PG4	B	1015	-	-	1/2/2/10	-
8	TRS	A	1012	-	-	7/9/9/9	-
2	HEC	A	1001	1	1/1/7/7	8/14/54/54	-
2	HEC	A	1005	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1008	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1007[B]	4	1/1/7/7	6/14/54/54	-
2	HEC	B	1002	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1003	1	1/1/7/7	6/14/54/54	-
2	HEC	B	1001	1	1/1/7/7	6/14/54/54	-
2	HEC	B	1007[B]	4	1/1/7/7	4/14/54/54	-
6	PG4	B	1014	4	-	3/6/6/10	-
8	TRS	B	1012	-	-	8/9/9/9	-
2	HEC	B	1003	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1007[A]	-	1/1/7/7	6/14/54/54	-
6	PG4	B	1017	-	-	1/4/4/10	-
2	HEC	B	1007[A]	-	1/1/7/7	6/14/54/54	-
2	HEC	A	1004	1,3,9	1/1/7/7	6/14/54/54	-
2	HEC	B	1006	4,1	1/1/7/7	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1008	1	-	6/14/54/54	-
6	PG4	A	1009	-	-	2/5/5/10	-
2	HEC	A	1002	1	1/1/7/7	6/14/54/54	-
7	PG6	B	1011	1	-	1/11/11/15	-
6	PG4	B	1009	-	-	4/4/4/10	-
2	HEC	B	1005	1	1/1/7/7	8/14/54/54	-
2	HEC	B	1004	1,3,9	1/1/7/7	6/14/54/54	-
6	PG4	A	1011	-	-	1/3/3/10	-
6	PG4	B	1016	-	-	2/2/2/10	-
6	PG4	A	1013	-	-	2/5/5/10	-
7	PG6	A	1010	1	-	3/11/11/15	-
6	PG4	B	1013	-	-	2/2/2/10	-
2	HEC	A	1006	4,1	1/1/7/7	4/14/54/54	-
6	PG4	B	1010	-	-	3/4/4/10	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1012	TRS	C-N	-8.40	1.22	1.49
2	A	1008	HEC	C3D-C2D	6.36	1.50	1.36
2	B	1002	HEC	C3D-C2D	6.09	1.49	1.36
2	B	1006	HEC	C3D-C2D	5.85	1.49	1.36
2	B	1003	HEC	C3D-C2D	5.77	1.49	1.36
2	B	1008	HEC	C3D-C2D	5.70	1.49	1.36
2	A	1001	HEC	C3D-C2D	5.62	1.48	1.36
2	B	1001	HEC	C3D-C2D	5.52	1.48	1.36
2	A	1005	HEC	C3D-C2D	5.48	1.48	1.36
2	A	1002	HEC	C3D-C2D	5.47	1.48	1.36
2	A	1007[A]	HEC	C3D-C2D	5.31	1.48	1.36
2	A	1007[B]	HEC	C3D-C2D	5.31	1.48	1.36
2	A	1003	HEC	C3D-C2D	5.28	1.48	1.36
2	A	1004	HEC	C3D-C2D	5.22	1.48	1.36
2	A	1006	HEC	C3D-C2D	5.13	1.47	1.36
2	B	1004	HEC	C3D-C2D	5.05	1.47	1.36
2	B	1007[A]	HEC	C3D-C2D	4.59	1.46	1.36
2	B	1007[B]	HEC	C3D-C2D	4.59	1.46	1.36
2	B	1005	HEC	C3D-C2D	4.56	1.46	1.36
2	B	1001	HEC	FE-NC	3.80	2.07	1.95
2	B	1004	HEC	CMB-C2B	3.36	1.57	1.50
2	B	1007[A]	HEC	FE-ND	3.25	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1007[B]	HEC	FE-ND	3.25	2.04	1.94
3	A	526	AZI	N1-N2	-3.17	1.16	1.23
2	A	1003	HEC	CMB-C2B	3.02	1.57	1.50
2	B	1006	HEC	FE-NC	3.02	2.05	1.95
2	B	1001	HEC	CMA-C3A	3.00	1.56	1.50
3	B	526	AZI	N1-N2	-2.99	1.17	1.23
2	B	1001	HEC	FE-NB	2.94	2.03	1.94
2	A	1002	HEC	FE-ND	2.92	2.03	1.94
2	B	1008	HEC	CMC-C2C	2.91	1.56	1.50
2	B	1007[A]	HEC	C4B-NB	-2.89	1.35	1.40
2	B	1007[B]	HEC	C4B-NB	-2.89	1.35	1.40
2	A	1007[A]	HEC	C4B-NB	-2.88	1.35	1.40
2	A	1007[B]	HEC	C4B-NB	-2.88	1.35	1.40
2	A	1001	HEC	CMC-C2C	2.84	1.56	1.50
3	A	530	AZI	N3-N2	-2.84	1.17	1.23
3	A	526	AZI	N3-N2	-2.79	1.17	1.23
2	A	1005	HEC	O2D-CGD	-2.76	1.21	1.30
2	B	1004	HEC	FE-NB	2.75	2.03	1.94
2	B	1003	HEC	CMA-C3A	2.72	1.56	1.50
2	A	1006	HEC	CMC-C2C	2.71	1.56	1.50
3	B	526	AZI	N3-N2	-2.70	1.17	1.23
2	B	1005	HEC	CMA-C3A	2.69	1.56	1.50
3	A	530	AZI	N1-N2	-2.64	1.17	1.23
2	B	1006	HEC	CMC-C2C	2.62	1.56	1.50
2	A	1002	HEC	CAB-C3B	2.60	1.57	1.51
2	B	1003	HEC	CMB-C2B	2.59	1.56	1.50
2	B	1005	HEC	CMB-C2B	2.57	1.56	1.50
2	B	1001	HEC	CAC-C3C	2.57	1.57	1.51
2	A	1005	HEC	CMD-C2D	2.56	1.56	1.50
2	A	1001	HEC	FE-NB	2.55	2.02	1.94
2	A	1004	HEC	CMC-C2C	2.51	1.55	1.50
2	A	1007[A]	HEC	FE-ND	2.51	2.02	1.94
2	A	1007[B]	HEC	FE-ND	2.51	2.02	1.94
2	B	1002	HEC	CMD-C2D	2.49	1.55	1.50
2	A	1002	HEC	CMA-C3A	2.48	1.55	1.50
2	A	1001	HEC	CAC-C3C	2.47	1.57	1.51
2	A	1004	HEC	FE-NB	2.47	2.02	1.94
2	A	1001	HEC	CMB-C2B	2.46	1.55	1.50
2	A	1002	HEC	CMB-C2B	2.46	1.55	1.50
2	A	1002	HEC	CMC-C2C	2.45	1.55	1.50
3	B	530	AZI	N1-N2	-2.44	1.18	1.23
2	B	1002	HEC	FE-NC	2.42	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1008	HEC	CMB-C2B	2.39	1.55	1.50
2	B	1005	HEC	O2D-CGD	-2.39	1.22	1.30
2	B	1001	HEC	FE-NA	2.38	2.03	1.95
3	B	530	AZI	N3-N2	-2.38	1.18	1.23
2	A	1007[A]	HEC	CMB-C2B	2.37	1.55	1.50
2	A	1007[B]	HEC	CMB-C2B	2.37	1.55	1.50
2	A	1004	HEC	CMB-C2B	2.37	1.55	1.50
2	A	1002	HEC	FE-NC	2.37	2.03	1.95
2	A	1006	HEC	CAC-C3C	2.36	1.57	1.51
2	B	1005	HEC	FE-NB	2.36	2.02	1.94
2	A	1007[A]	HEC	CMA-C3A	2.33	1.55	1.50
2	A	1007[B]	HEC	CMA-C3A	2.33	1.55	1.50
2	B	1007[A]	HEC	CHD-C1D	-2.33	1.33	1.38
2	B	1007[B]	HEC	CHD-C1D	-2.33	1.33	1.38
2	B	1007[A]	HEC	CMB-C2B	2.31	1.55	1.50
2	B	1007[B]	HEC	CMB-C2B	2.31	1.55	1.50
2	B	1002	HEC	CMA-C3A	2.31	1.55	1.50
2	B	1008	HEC	C3B-C2B	-2.30	1.31	1.36
2	A	1008	HEC	CMD-C2D	2.27	1.55	1.50
2	A	1003	HEC	CHA-C4D	-2.27	1.34	1.39
2	B	1001	HEC	CAB-C3B	2.25	1.56	1.51
2	B	1008	HEC	CAC-C3C	2.25	1.56	1.51
2	A	1005	HEC	FE-ND	2.23	2.01	1.94
2	A	1001	HEC	FE-NC	2.22	2.02	1.95
2	B	1004	HEC	CMA-C3A	2.21	1.55	1.50
2	A	1007[A]	HEC	CAB-C3B	2.21	1.56	1.51
2	A	1007[B]	HEC	CAB-C3B	2.21	1.56	1.51
2	A	1002	HEC	C4B-NB	-2.20	1.36	1.40
2	B	1001	HEC	CMD-C2D	2.19	1.55	1.50
2	B	1007[A]	HEC	CMA-C3A	2.18	1.55	1.50
2	B	1007[B]	HEC	CMA-C3A	2.18	1.55	1.50
2	B	1007[A]	HEC	FE-NB	2.18	2.01	1.94
2	B	1007[B]	HEC	FE-NB	2.18	2.01	1.94
2	B	1006	HEC	FE-NB	2.17	2.01	1.94
2	B	1002	HEC	C1C-NC	-2.16	1.35	1.39
2	A	1008	HEC	CMC-C2C	2.16	1.55	1.50
2	B	1003	HEC	CMD-C2D	2.16	1.55	1.50
2	B	1007[A]	HEC	C1D-ND	-2.15	1.36	1.40
2	B	1007[B]	HEC	C1D-ND	-2.15	1.36	1.40
2	A	1001	HEC	FE-NA	2.15	2.02	1.95
2	A	1005	HEC	CMB-C2B	2.14	1.55	1.50
2	A	1003	HEC	CMA-C3A	2.13	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1004	HEC	C1D-ND	-2.12	1.36	1.40
2	A	1005	HEC	C3C-C2C	-2.12	1.33	1.38
2	B	1006	HEC	FE-NA	2.12	2.02	1.95
2	B	1006	HEC	CMD-C2D	2.10	1.55	1.50
2	B	1001	HEC	C1A-NA	-2.10	1.35	1.39
2	B	1002	HEC	CAC-C3C	2.09	1.56	1.51
2	B	1002	HEC	CAB-C3B	2.09	1.56	1.51
2	B	1002	HEC	CHD-C4C	-2.08	1.34	1.39
2	A	1006	HEC	FE-NC	2.08	2.02	1.95
2	A	1007[A]	HEC	CMC-C2C	2.06	1.55	1.50
2	A	1007[B]	HEC	CMC-C2C	2.06	1.55	1.50
2	A	1007[A]	HEC	CHA-C4D	-2.06	1.34	1.39
2	A	1007[B]	HEC	CHA-C4D	-2.06	1.34	1.39
2	B	1008	HEC	FE-NA	2.05	2.01	1.95
2	B	1002	HEC	FE-NB	2.05	2.01	1.94
2	A	1008	HEC	CMA-C3A	2.05	1.55	1.50
2	B	1008	HEC	CMD-C2D	2.04	1.54	1.50
2	B	1005	HEC	C1C-NC	-2.04	1.35	1.39
2	A	1004	HEC	CAB-C3B	2.04	1.56	1.51
2	A	1006	HEC	O2A-CGA	-2.03	1.24	1.30
2	A	1008	HEC	FE-NA	2.03	2.01	1.95
2	B	1006	HEC	C2A-C3A	-2.02	1.32	1.36
2	B	1005	HEC	C3C-C2C	-2.02	1.33	1.38
2	A	1002	HEC	CAC-C3C	2.02	1.56	1.51
2	A	1004	HEC	CMA-C3A	2.01	1.54	1.50
2	A	1002	HEC	FE-NB	2.00	2.01	1.94
2	B	1007[A]	HEC	C3C-C2C	-2.00	1.33	1.38
2	B	1007[B]	HEC	C3C-C2C	-2.00	1.33	1.38

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1012	TRS	C3-C-N	-5.36	94.50	108.17
2	B	1007[A]	HEC	C1D-ND-C4D	5.01	111.14	105.21
2	B	1007[B]	HEC	C1D-ND-C4D	5.01	111.14	105.21
2	A	1007[A]	HEC	C1D-ND-C4D	4.71	110.78	105.21
2	A	1007[B]	HEC	C1D-ND-C4D	4.71	110.78	105.21
2	B	1004	HEC	C1D-C2D-C3D	-4.04	102.73	106.98
2	A	1008	HEC	C1D-ND-C4D	4.03	109.98	105.21
2	B	1008	HEC	CMC-C2C-C1C	-4.02	119.30	125.42
2	B	1006	HEC	CHB-C4A-NA	3.96	128.76	124.45
2	B	1008	HEC	C1D-ND-C4D	3.84	109.75	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1007[A]	HEC	CMB-C2B-C1B	-3.65	119.32	125.03
2	A	1007[B]	HEC	CMB-C2B-C1B	-3.65	119.32	125.03
2	B	1002	HEC	C1D-ND-C4D	3.62	109.49	105.21
8	B	1012	TRS	C1-C-N	-3.54	99.14	108.17
2	B	1006	HEC	C2A-C1A-NA	-3.46	106.99	110.32
8	B	1012	TRS	C3-C-C2	3.42	119.75	110.66
2	A	1001	HEC	CHD-C1D-ND	3.36	128.53	124.37
2	B	1001	HEC	CHB-C4A-NA	3.35	128.10	124.45
2	B	1006	HEC	CHA-C1A-NA	3.34	128.09	124.45
2	A	1001	HEC	CHB-C4A-NA	3.26	128.00	124.45
2	A	1002	HEC	CHB-C4A-NA	3.24	127.99	124.45
2	A	1002	HEC	CHD-C1D-ND	3.20	128.33	124.37
2	A	1004	HEC	C1D-C2D-C3D	-3.18	103.64	106.98
2	B	1004	HEC	CAD-C3D-C4D	3.16	130.20	124.70
2	A	1006	HEC	C2D-C1D-ND	3.15	113.46	109.84
2	A	1005	HEC	C1D-C2D-C3D	-3.15	103.67	106.98
2	B	1007[A]	HEC	C4B-NB-C1B	3.14	108.92	105.21
2	B	1007[B]	HEC	C4B-NB-C1B	3.14	108.92	105.21
2	B	1002	HEC	CHD-C1D-ND	3.13	128.24	124.37
2	A	1007[A]	HEC	CAD-C3D-C4D	3.04	130.00	124.70
2	A	1007[B]	HEC	CAD-C3D-C4D	3.04	130.00	124.70
2	B	1008	HEC	CBD-CAD-C3D	-3.04	104.12	112.53
2	A	1001	HEC	C2A-C1A-NA	-3.00	107.43	110.32
2	B	1001	HEC	CMC-C2C-C1C	-2.99	120.86	125.42
2	A	1006	HEC	C2A-C1A-NA	-2.99	107.44	110.32
2	B	1003	HEC	CAD-C3D-C4D	2.93	129.80	124.70
2	A	1001	HEC	CAD-C3D-C4D	2.92	129.79	124.70
2	B	1002	HEC	CAA-CBA-CGA	-2.92	105.92	113.67
2	A	1005	HEC	C1D-ND-C4D	2.92	108.66	105.21
2	B	1007[A]	HEC	C4C-NC-C1C	-2.91	101.07	105.82
2	B	1007[B]	HEC	C4C-NC-C1C	-2.91	101.07	105.82
2	B	1001	HEC	CHD-C1D-ND	2.90	127.95	124.37
2	B	1008	HEC	O1A-CGA-CBA	-2.89	113.92	123.09
2	B	1007[A]	HEC	CMB-C2B-C1B	-2.89	120.52	125.03
2	B	1007[B]	HEC	CMB-C2B-C1B	-2.89	120.52	125.03
2	B	1005	HEC	O1A-CGA-CBA	-2.86	114.03	123.09
2	A	1008	HEC	CHD-C1D-ND	2.85	127.90	124.37
2	B	1001	HEC	CHA-C1A-NA	2.81	127.52	124.45
2	A	1003	HEC	CAB-C3B-C4B	2.81	128.44	124.79
2	B	1006	HEC	CAD-C3D-C4D	2.80	129.58	124.70
2	B	1007[A]	HEC	C2B-C1B-NB	-2.80	106.67	109.90
2	B	1007[B]	HEC	C2B-C1B-NB	-2.80	106.67	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	HEC	C1D-ND-C4D	2.80	108.52	105.21
2	A	1002	HEC	C2A-C1A-NA	-2.80	107.62	110.32
2	B	1003	HEC	CMC-C2C-C1C	-2.77	121.20	125.42
2	B	1004	HEC	CAD-C3D-C2D	-2.76	122.70	127.87
2	B	1001	HEC	O1A-CGA-CBA	-2.73	114.45	123.09
2	A	1008	HEC	O1A-CGA-CBA	-2.70	114.53	123.09
2	B	1001	HEC	C1D-ND-C4D	2.68	108.38	105.21
2	A	1002	HEC	C1D-ND-C4D	2.66	108.35	105.21
2	B	1008	HEC	O2A-CGA-CBA	2.64	122.35	114.00
2	B	1002	HEC	CMD-C2D-C1D	2.60	129.10	125.03
2	B	1006	HEC	C4A-NA-C1A	2.58	110.03	105.82
2	B	1003	HEC	CMB-C2B-C1B	-2.57	121.01	125.03
2	B	1008	HEC	C1B-C2B-C3B	2.57	109.68	106.98
2	B	1008	HEC	CAD-CBD-CGD	-2.54	106.94	113.67
2	B	1003	HEC	O1A-CGA-CBA	-2.52	115.09	123.09
2	B	1005	HEC	CHC-C4B-NB	-2.52	121.26	124.37
2	A	1008	HEC	O2A-CGA-CBA	2.51	121.93	114.00
2	A	1008	HEC	CAD-C3D-C4D	2.49	129.04	124.70
2	B	1003	HEC	CMD-C2D-C1D	2.46	128.88	125.03
2	B	1003	HEC	CAB-C3B-C4B	2.46	127.98	124.79
2	A	1005	HEC	CAD-CBD-CGD	-2.45	107.17	113.67
2	B	1008	HEC	CHB-C1B-NB	2.44	127.05	124.42
2	B	1001	HEC	O2A-CGA-CBA	2.44	121.71	114.00
2	A	1002	HEC	CAA-CBA-CGA	-2.42	107.24	113.67
2	A	1003	HEC	CAD-CBD-CGD	-2.42	107.25	113.67
2	A	1002	HEC	CAD-C3D-C4D	2.41	128.90	124.70
2	A	1005	HEC	CMD-C2D-C1D	2.41	128.80	125.03
2	B	1002	HEC	C2A-C1A-NA	-2.39	108.02	110.32
2	B	1005	HEC	CMB-C2B-C1B	-2.39	121.31	125.03
2	B	1003	HEC	C3D-C4D-ND	2.38	112.66	110.35
2	A	1004	HEC	C1D-ND-C4D	2.38	108.03	105.21
2	A	1005	HEC	O1A-CGA-CBA	-2.38	115.56	123.09
2	A	1007[A]	HEC	C4C-NC-C1C	-2.37	101.95	105.82
2	A	1007[B]	HEC	C4C-NC-C1C	-2.37	101.95	105.82
2	A	1008	HEC	CMC-C2C-C1C	-2.36	121.82	125.42
2	A	1004	HEC	CAD-C3D-C4D	2.36	128.81	124.70
2	A	1004	HEC	CMC-C2C-C1C	-2.36	121.83	125.42
2	A	1006	HEC	C1D-C2D-C3D	-2.36	104.50	106.98
2	A	1006	HEC	CAD-C3D-C4D	2.35	128.80	124.70
2	B	1001	HEC	C2A-C1A-NA	-2.35	108.06	110.32
2	A	1007[A]	HEC	CMD-C2D-C1D	2.34	128.69	125.03
2	A	1007[B]	HEC	CMD-C2D-C1D	2.34	128.69	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	HEC	CMD-C2D-C1D	2.33	128.67	125.03
2	A	1001	HEC	O2A-CGA-CBA	2.32	121.33	114.00
2	B	1001	HEC	C4A-NA-C1A	2.32	109.61	105.82
2	B	1004	HEC	CAC-C3C-C4C	2.32	128.10	124.91
2	B	1001	HEC	CMD-C2D-C1D	2.32	128.66	125.03
2	A	1001	HEC	C1B-C2B-C3B	2.31	109.41	106.98
2	A	1005	HEC	CMB-C2B-C1B	-2.31	121.43	125.03
2	B	1007[A]	HEC	C3C-C4C-NC	2.30	112.71	110.15
2	B	1007[B]	HEC	C3C-C4C-NC	2.30	112.71	110.15
2	A	1001	HEC	CHA-C1A-NA	2.30	126.95	124.45
2	A	1001	HEC	C4A-NA-C1A	2.28	109.54	105.82
2	A	1007[A]	HEC	CBB-CAB-C3B	-2.28	106.23	112.42
2	A	1007[B]	HEC	CBB-CAB-C3B	-2.28	106.23	112.42
2	A	1004	HEC	CMD-C2D-C1D	2.27	128.59	125.03
2	A	1003	HEC	CAD-C3D-C4D	2.27	128.66	124.70
2	A	1001	HEC	CMD-C2D-C1D	2.26	128.56	125.03
2	A	1003	HEC	CMB-C2B-C1B	-2.24	121.53	125.03
2	B	1007[A]	HEC	CAD-C3D-C4D	2.24	128.59	124.70
2	B	1007[B]	HEC	CAD-C3D-C4D	2.24	128.59	124.70
2	A	1007[A]	HEC	CHB-C1B-C2B	2.23	128.56	125.03
2	A	1007[B]	HEC	CHB-C1B-C2B	2.23	128.56	125.03
2	A	1006	HEC	CHA-C1A-NA	2.21	126.86	124.45
2	A	1001	HEC	O1A-CGA-CBA	-2.20	116.10	123.09
2	B	1001	HEC	CAD-C3D-C4D	2.20	128.53	124.70
2	B	1002	HEC	CHA-C1A-NA	2.18	126.83	124.45
2	A	1007[A]	HEC	CBA-CAA-C2A	-2.17	106.54	112.53
2	B	1001	HEC	CAB-C3B-C4B	2.16	127.61	124.79
2	B	1005	HEC	CBB-CAB-C3B	-2.16	106.58	112.42
2	A	1003	HEC	CBD-CAD-C3D	-2.15	106.58	112.53
2	B	1001	HEC	C4D-C3D-C2D	-2.15	103.77	106.89
2	B	1006	HEC	CMC-C2C-C1C	-2.14	122.16	125.42
2	B	1005	HEC	CAD-CBD-CGD	-2.12	108.05	113.67
2	B	1008	HEC	O1D-CGD-CBD	-2.12	116.38	123.09
2	A	1004	HEC	C4B-NB-C1B	2.12	107.71	105.21
2	B	1008	HEC	CAD-C3D-C4D	2.11	128.38	124.70
2	B	1005	HEC	CAD-C3D-C4D	2.11	128.38	124.70
2	B	1004	HEC	C2D-C1D-ND	2.11	112.27	109.84
2	B	1004	HEC	CHD-C1D-C2D	-2.10	120.97	126.95
2	A	1007[A]	HEC	CHA-C4D-ND	2.10	126.69	124.42
2	A	1007[B]	HEC	CHA-C4D-ND	2.10	126.69	124.42
2	B	1008	HEC	CMC-C2C-C3C	2.09	130.06	125.62
2	A	1007[B]	HEC	O2A-CGA-CBA	2.09	120.60	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1007[A]	HEC	C2B-C1B-NB	-2.09	107.49	109.90
2	A	1007[B]	HEC	C2B-C1B-NB	-2.09	107.49	109.90
2	B	1008	HEC	CBA-CAA-C2A	-2.07	106.80	112.53
2	B	1004	HEC	CBC-CAC-C3C	2.07	118.03	112.42
2	B	1001	HEC	O1D-CGD-CBD	-2.06	116.56	123.09
2	A	1001	HEC	CMC-C2C-C1C	-2.05	122.30	125.42
2	B	1006	HEC	C2D-C1D-ND	2.04	112.19	109.84
2	A	1008	HEC	CBD-CAD-C3D	-2.04	106.90	112.53
2	A	1002	HEC	CAC-C3C-C2C	2.03	130.11	126.89
2	B	1008	HEC	C4B-NB-C1B	2.03	107.61	105.21
2	B	1007[A]	HEC	C3D-C4D-ND	-2.03	108.39	110.35
2	B	1007[B]	HEC	C3D-C4D-ND	-2.03	108.39	110.35
2	B	1003	HEC	CMC-C2C-C3C	2.02	129.92	125.62
2	A	1006	HEC	CBD-CAD-C3D	-2.02	106.94	112.53
2	A	1003	HEC	CBA-CAA-C2A	-2.01	106.97	112.53

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1004	HEC	NA
2	A	1005	HEC	NA
2	A	1006	HEC	NA
2	A	1007[A]	HEC	NA
2	A	1007[B]	HEC	NA
2	A	1008	HEC	NA
2	A	1002	HEC	NA
2	A	1003	HEC	NA
2	A	1001	HEC	NA
2	B	1004	HEC	NA
2	B	1005	HEC	NA
2	B	1006	HEC	NA
2	B	1007[A]	HEC	NA
2	B	1007[B]	HEC	NA
2	B	1002	HEC	NA
2	B	1003	HEC	NA
2	B	1001	HEC	NA

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1008	HEC	C2C-C3C-CAC-CBC
2	A	1002	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	1002	HEC	C2C-C3C-CAC-CBC
8	A	1012	TRS	C2-C-C1-O1
8	A	1012	TRS	C3-C-C1-O1
8	A	1012	TRS	N-C-C1-O1
8	A	1012	TRS	C1-C-C2-O2
8	A	1012	TRS	C3-C-C2-O2
8	B	1012	TRS	C1-C-C2-O2
8	B	1012	TRS	C3-C-C2-O2
8	B	1012	TRS	N-C-C2-O2
8	B	1012	TRS	C2-C-C3-O3
8	B	1012	TRS	N-C-C3-O3
2	B	1008	HEC	C2C-C3C-CAC-CBC
2	A	1008	HEC	C4C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	B	1008	HEC	C4C-C3C-CAC-CBC
2	B	1002	HEC	C4C-C3C-CAC-CBC
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C2B-C3B-CAB-CBB
2	A	1007[A]	HEC	C2B-C3B-CAB-CBB
2	A	1007[B]	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C2C-C3C-CAC-CBC
2	A	1003	HEC	C2C-C3C-CAC-CBC
2	B	1001	HEC	C2C-C3C-CAC-CBC
7	A	1010	PG6	O1-C2-C3-O2
2	B	1003	HEC	C4C-C3C-CAC-CBC
2	B	1007[A]	HEC	C2B-C3B-CAB-CBB
2	B	1007[B]	HEC	C2B-C3B-CAB-CBB
2	A	1001	HEC	C2B-C3B-CAB-CBB
2	A	1001	HEC	C2C-C3C-CAC-CBC
6	B	1017	PG4	O2-C3-C4-O3
2	A	1007[A]	HEC	C2C-C3C-CAC-CBC
2	A	1007[B]	HEC	C2C-C3C-CAC-CBC
2	B	1007[A]	HEC	C2C-C3C-CAC-CBC
2	B	1007[B]	HEC	C2C-C3C-CAC-CBC
2	A	1001	HEC	C4C-C3C-CAC-CBC
2	A	1008	HEC	C2B-C3B-CAB-CBB
2	B	1008	HEC	C2B-C3B-CAB-CBB
2	A	1003	HEC	C4C-C3C-CAC-CBC
2	A	1007[A]	HEC	C4C-C3C-CAC-CBC
2	A	1007[B]	HEC	C4C-C3C-CAC-CBC
6	A	1009	PG4	O2-C3-C4-O3
2	A	1004	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	B	1014	PG4	O3-C5-C6-O4
2	B	1007[A]	HEC	C4C-C3C-CAC-CBC
2	B	1007[B]	HEC	C4C-C3C-CAC-CBC
2	B	1004	HEC	C4B-C3B-CAB-CBB
2	B	1005	HEC	C2B-C3B-CAB-CBB
2	B	1001	HEC	C4C-C3C-CAC-CBC
2	A	1006	HEC	C2B-C3B-CAB-CBB
6	B	1015	PG4	C8-C7-O4-C6
6	B	1014	PG4	O4-C7-C8-O5
2	A	1005	HEC	C2B-C3B-CAB-CBB
2	A	1003	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C2B-C3B-CAB-CBB
6	B	1009	PG4	O3-C5-C6-O4
6	B	1010	PG4	O1-C1-C2-O2
2	B	1001	HEC	C2B-C3B-CAB-CBB
8	B	1012	TRS	C1-C-C3-O3
2	A	1002	HEC	C2B-C3B-CAB-CBB
2	B	1006	HEC	C2B-C3B-CAB-CBB
6	B	1010	PG4	O2-C3-C4-O3
2	A	1007[A]	HEC	C4B-C3B-CAB-CBB
2	A	1007[B]	HEC	C4B-C3B-CAB-CBB
7	B	1011	PG6	O4-C8-C9-O5
6	B	1013	PG4	C1-C2-O2-C3
2	B	1005	HEC	C4C-C3C-CAC-CBC
7	A	1010	PG6	O4-C8-C9-O5
2	A	1001	HEC	C4B-C3B-CAB-CBB
6	A	1009	PG4	O1-C1-C2-O2
6	B	1009	PG4	O4-C7-C8-O5
6	B	1013	PG4	O1-C1-C2-O2
2	A	1005	HEC	C2C-C3C-CAC-CBC
2	A	1005	HEC	C4C-C3C-CAC-CBC
2	A	1006	HEC	C4C-C3C-CAC-CBC
2	B	1007[A]	HEC	C4B-C3B-CAB-CBB
2	B	1007[B]	HEC	C4B-C3B-CAB-CBB
2	A	1006	HEC	C2C-C3C-CAC-CBC
2	B	1002	HEC	C2B-C3B-CAB-CBB
6	B	1010	PG4	C1-C2-O2-C3
8	A	1012	TRS	N-C-C2-O2
8	B	1012	TRS	N-C-C1-O1
2	B	1005	HEC	C2C-C3C-CAC-CBC
7	A	1010	PG6	C8-C9-O5-C10
2	B	1006	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	1005	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C2C-C3C-CAC-CBC
6	A	1011	PG4	O1-C1-C2-O2
6	B	1016	PG4	C5-C6-O4-C7
2	B	1001	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C4C-C3C-CAC-CBC
8	B	1012	TRS	C2-C-C1-O1
2	A	1006	HEC	C4B-C3B-CAB-CBB
6	B	1014	PG4	C3-C4-O3-C5
2	B	1008	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	C4B-C3B-CAB-CBB
2	A	1002	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	CAA-CBA-CGA-O2A
2	B	1002	HEC	CAA-CBA-CGA-O1A
2	B	1005	HEC	CAA-CBA-CGA-O2A
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	B	1004	HEC	C2C-C3C-CAC-CBC
2	A	1005	HEC	CAA-CBA-CGA-O1A
6	B	1009	PG4	C5-C6-O4-C7
2	A	1002	HEC	CAA-CBA-CGA-O1A
2	B	1006	HEC	C2C-C3C-CAC-CBC
2	B	1004	HEC	CAA-CBA-CGA-O2A
6	B	1009	PG4	C8-C7-O4-C6
2	A	1001	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAD-CBD-CGD-O1D
2	B	1004	HEC	C4C-C3C-CAC-CBC
2	A	1004	HEC	CAA-CBA-CGA-O1A
2	B	1005	HEC	CAA-CBA-CGA-O1A
2	B	1007[A]	HEC	CAA-CBA-CGA-O1A
2	A	1002	HEC	CAA-CBA-CGA-O2A
2	B	1002	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O1A
2	B	1007[A]	HEC	CAA-CBA-CGA-O2A
2	B	1004	HEC	CAA-CBA-CGA-O1A
2	B	1002	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	CAD-CBD-CGD-O2D
2	A	1001	HEC	CAD-CBD-CGD-O2D
6	A	1013	PG4	C5-C6-O4-C7
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	A	1003	HEC	CAD-CBD-CGD-O1D
2	A	1007[A]	HEC	CAA-CBA-CGA-O1A
2	B	1008	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	B	1003	HEC	CAD-CBD-CGD-O2D
2	B	1005	HEC	CAD-CBD-CGD-O2D
2	B	1001	HEC	CAD-CBD-CGD-O1D
2	B	1008	HEC	CAD-CBD-CGD-O1D
2	A	1003	HEC	C4B-C3B-CAB-CBB
8	A	1012	TRS	C2-C-C3-O3
2	B	1005	HEC	CAD-CBD-CGD-O1D
2	B	1003	HEC	CAD-CBD-CGD-O1D
6	B	1016	PG4	O3-C5-C6-O4
2	B	1006	HEC	C4B-C3B-CAB-CBB
2	A	1008	HEC	C4B-C3B-CAB-CBB
2	A	1008	HEC	CAD-CBD-CGD-O1D
2	A	1008	HEC	CAD-CBD-CGD-O2D
6	A	1013	PG4	O3-C5-C6-O4
2	A	1007[A]	HEC	CAA-CBA-CGA-O2A
2	B	1003	HEC	C4B-C3B-CAB-CBB
2	A	1007[B]	HEC	CAA-CBA-CGA-O2A
2	A	1007[B]	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

21 monomers are involved in 42 short contacts:

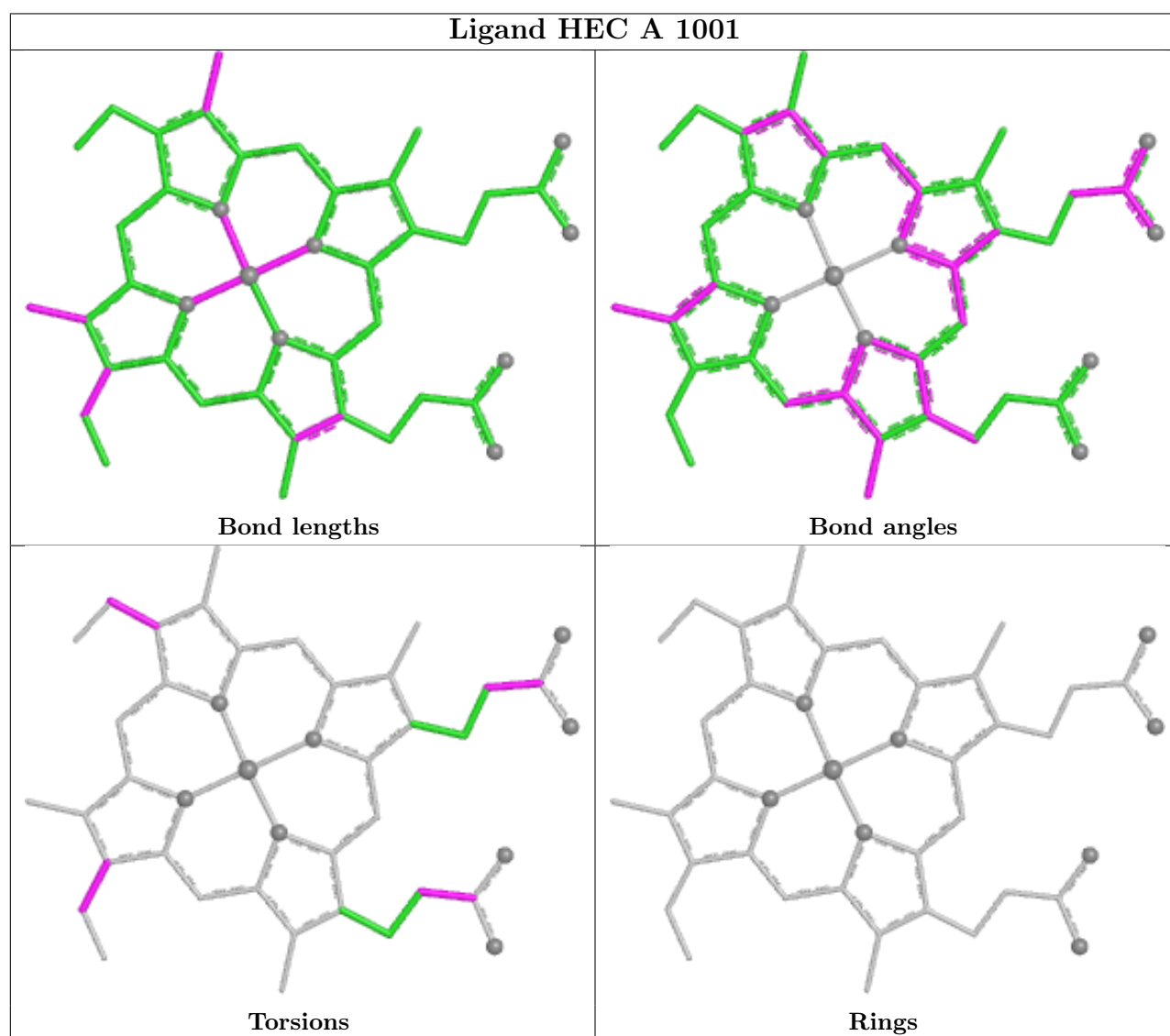
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1015	PG4	1	0
8	A	1012	TRS	1	0
2	A	1008	HEC	3	0
2	B	1002	HEC	2	0
2	A	1003	HEC	2	0
2	B	1001	HEC	1	0
6	B	1014	PG4	9	0
2	B	1003	HEC	2	0
2	A	1004	HEC	1	0
2	B	1006	HEC	1	0
3	B	526	AZI	1	0
2	B	1008	HEC	2	0
2	A	1002	HEC	1	0
7	B	1011	PG6	1	0
6	B	1009	PG4	4	0
6	A	1011	PG4	1	0
6	B	1016	PG4	4	0
6	A	1013	PG4	2	0
7	A	1010	PG6	1	0

Continued on next page...

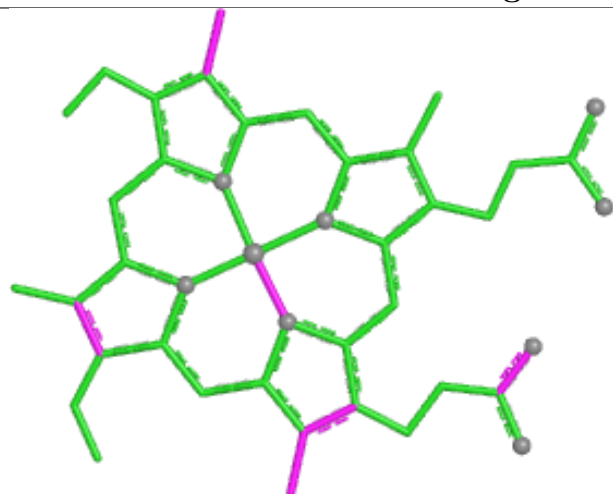
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	526	AZI	1	0
2	A	1006	HEC	2	0

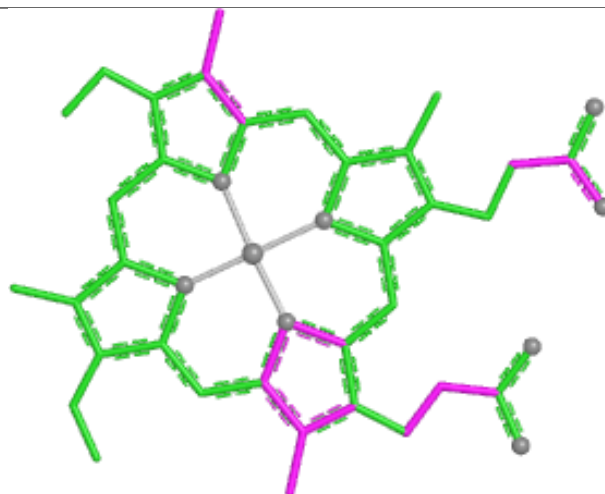
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



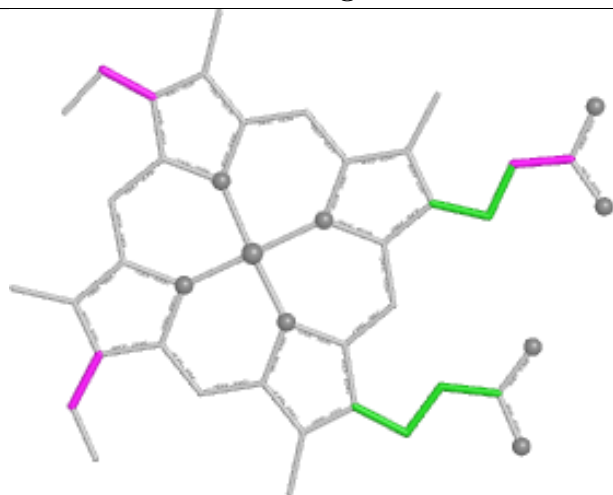
Ligand HEC A 1005



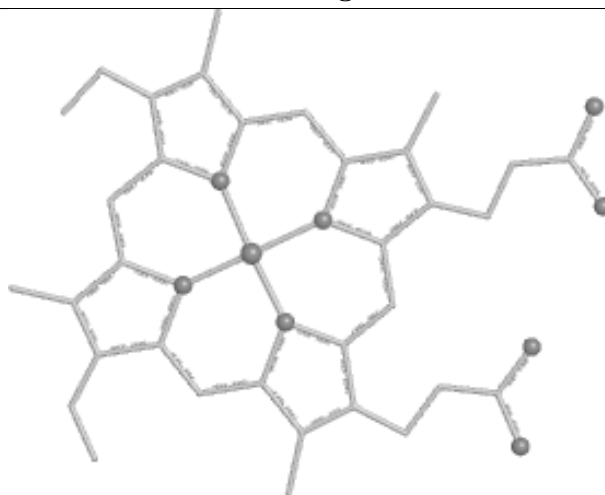
Bond lengths



Bond angles

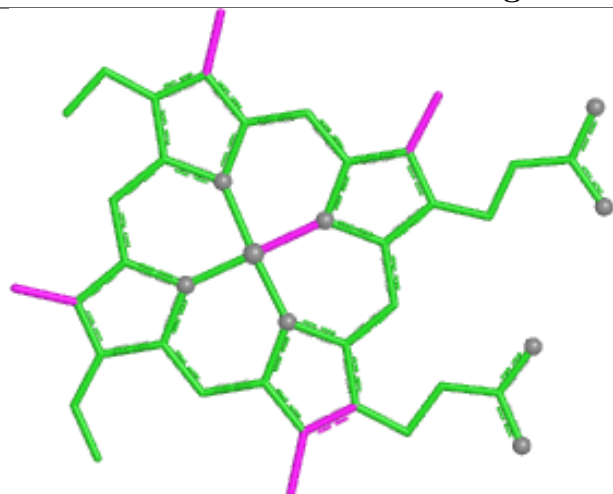


Torsions

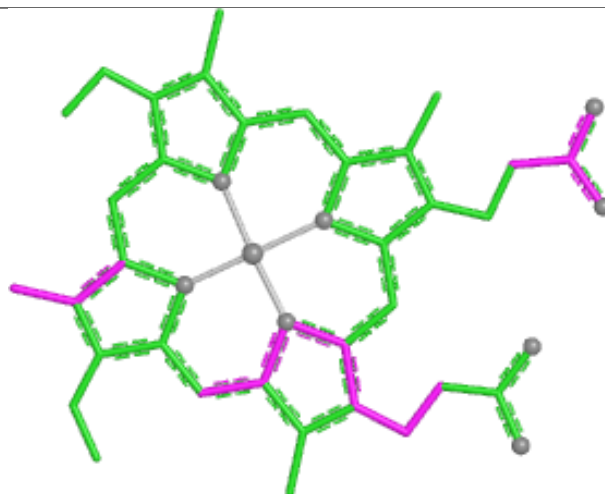


Rings

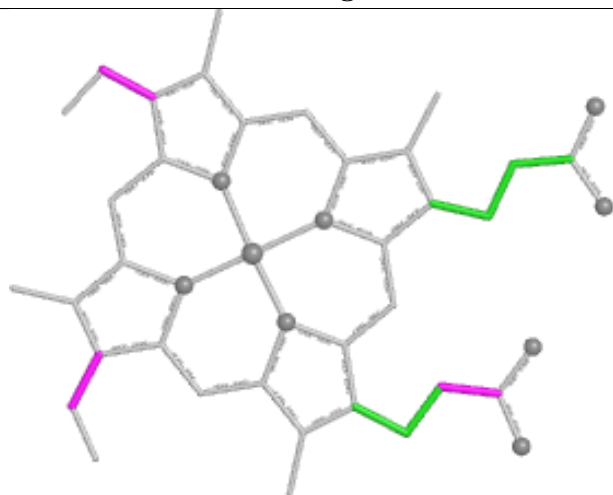
Ligand HEC A 1008



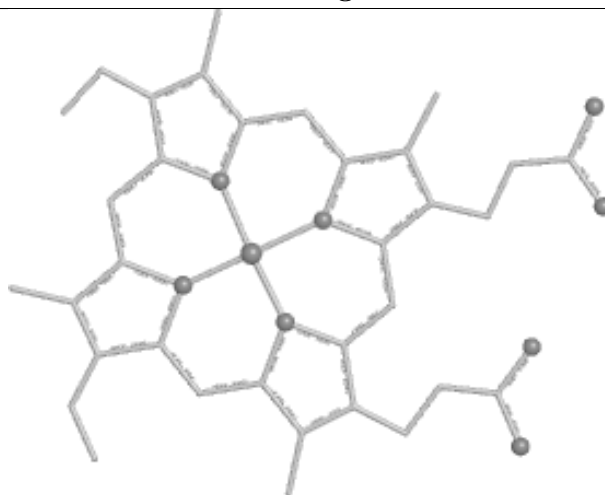
Bond lengths



Bond angles

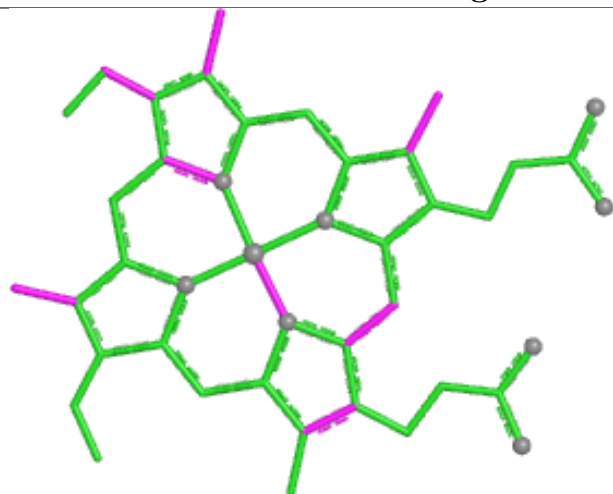


Torsions

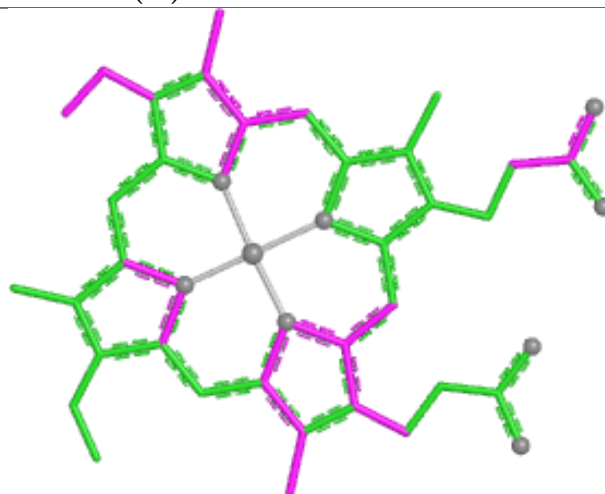


Rings

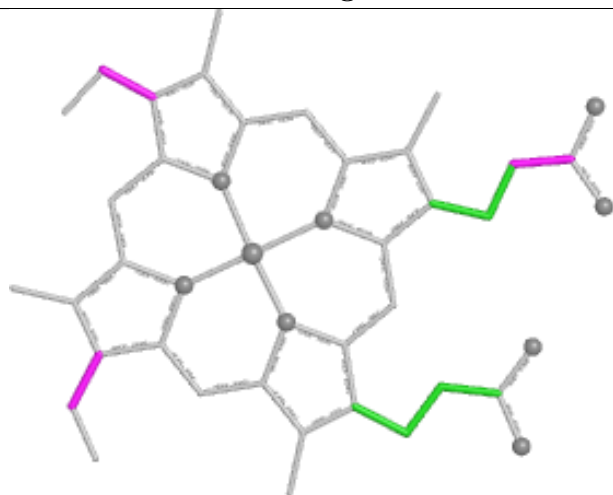
Ligand HEC A 1007 (B)



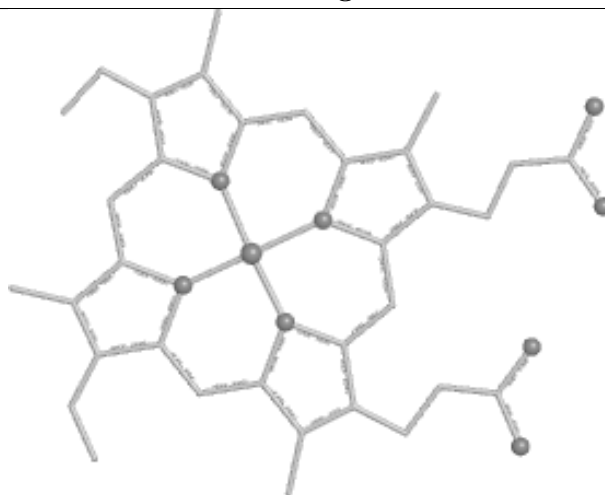
Bond lengths



Bond angles

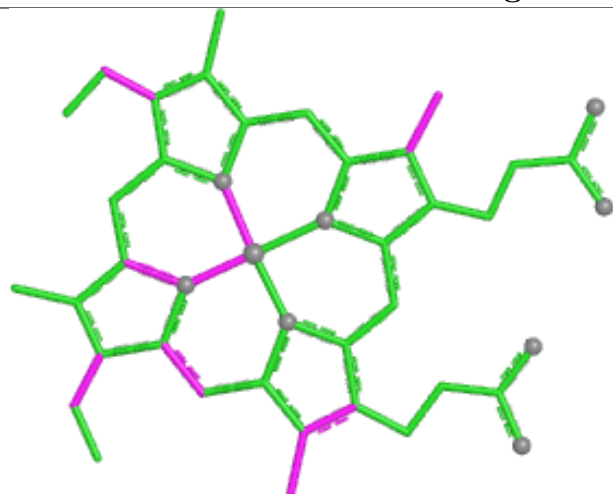


Torsions

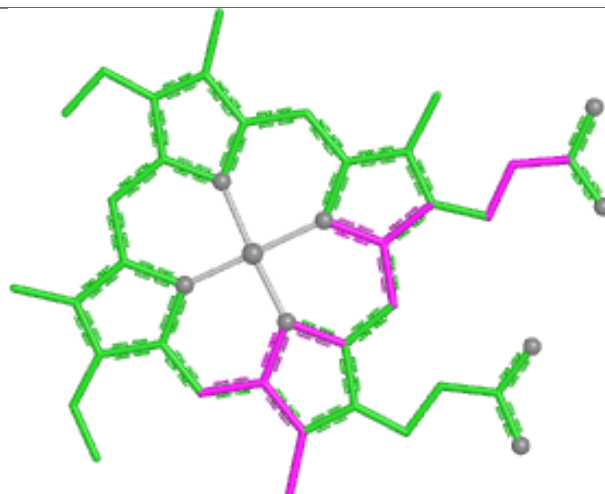


Rings

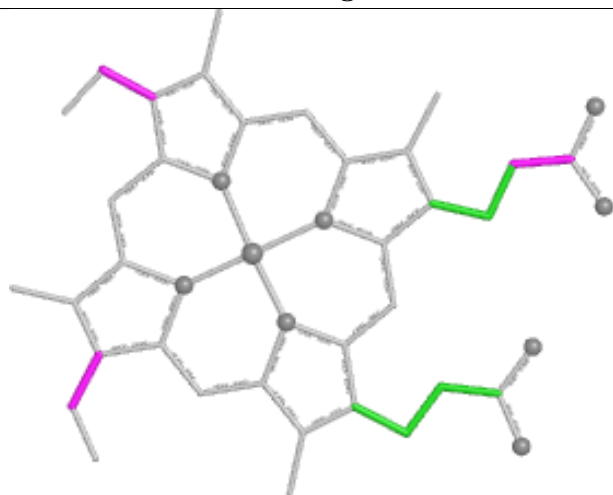
Ligand HEC B 1002



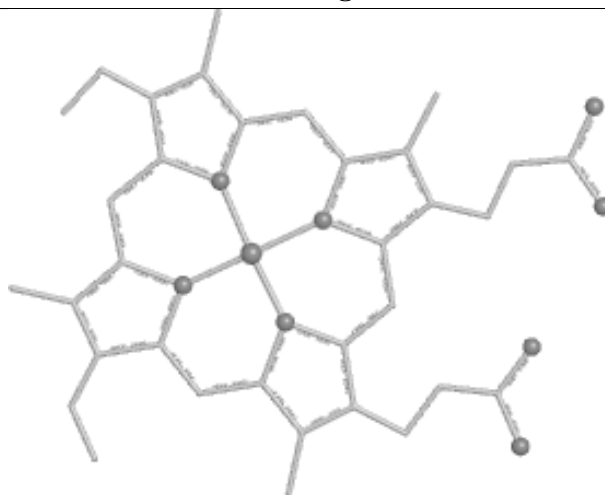
Bond lengths



Bond angles

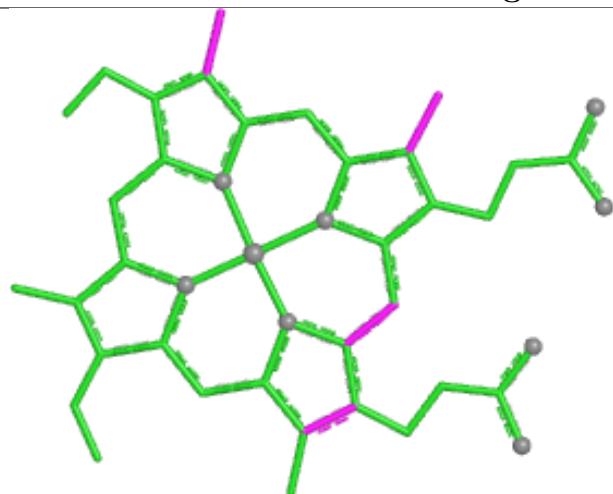


Torsions

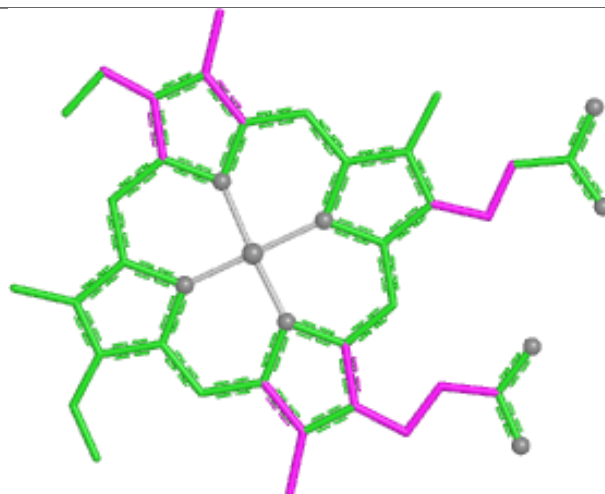


Rings

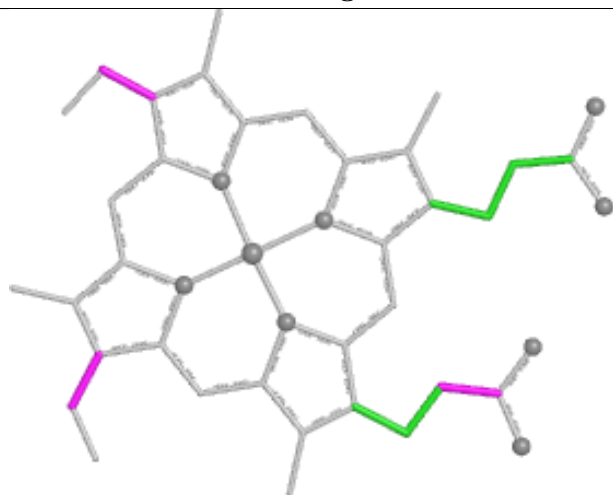
Ligand HEC A 1003



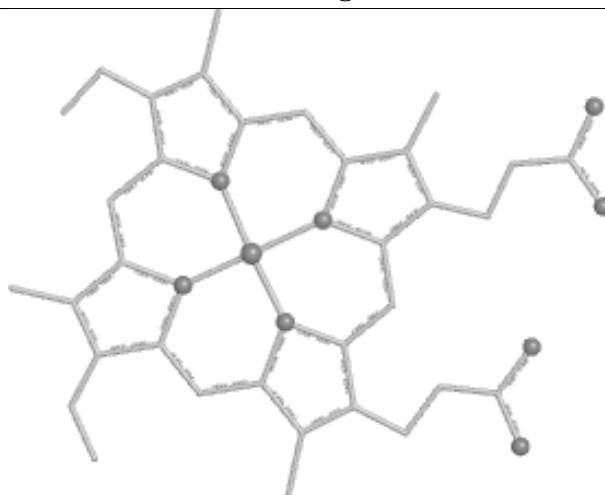
Bond lengths



Bond angles

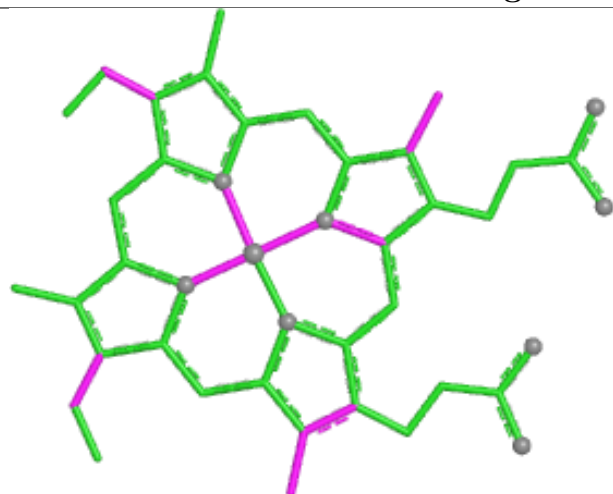


Torsions

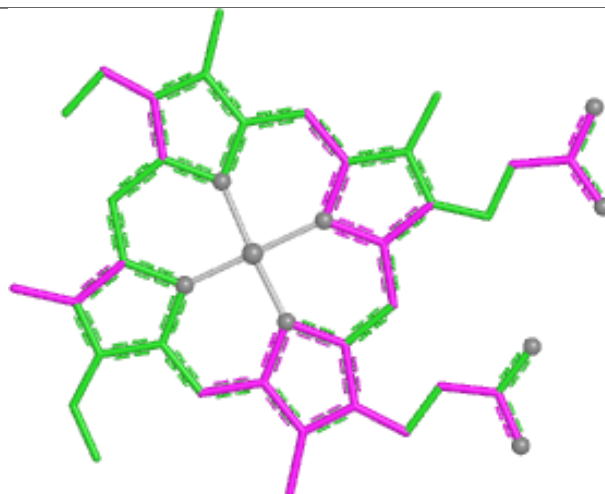


Rings

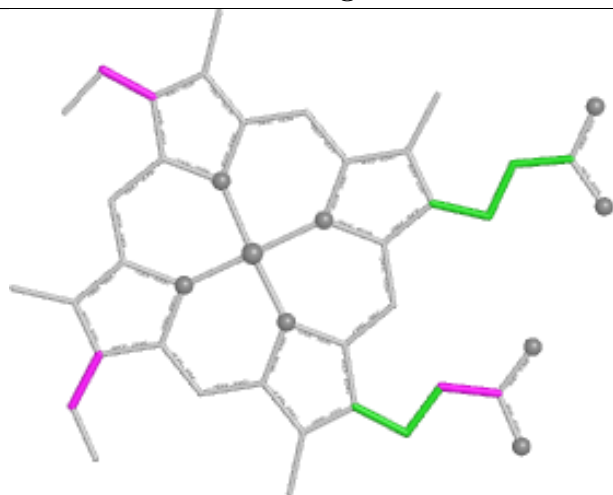
Ligand HEC B 1001



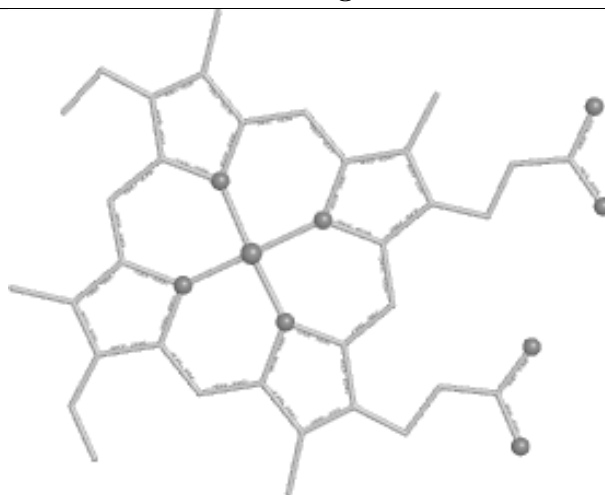
Bond lengths



Bond angles

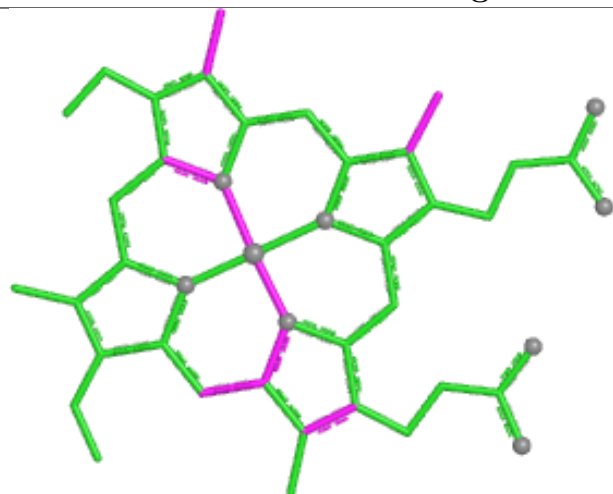


Torsions

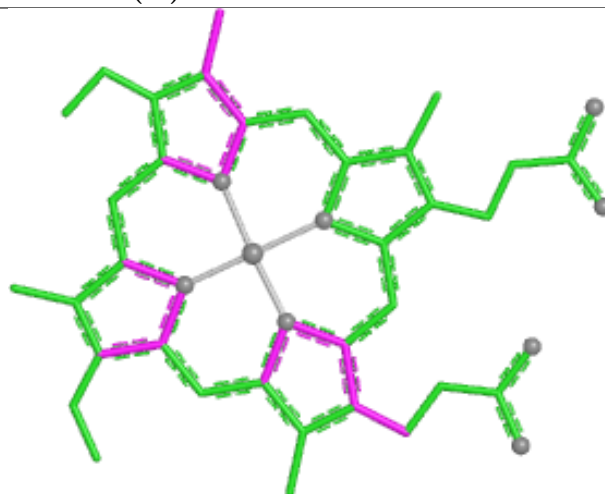


Rings

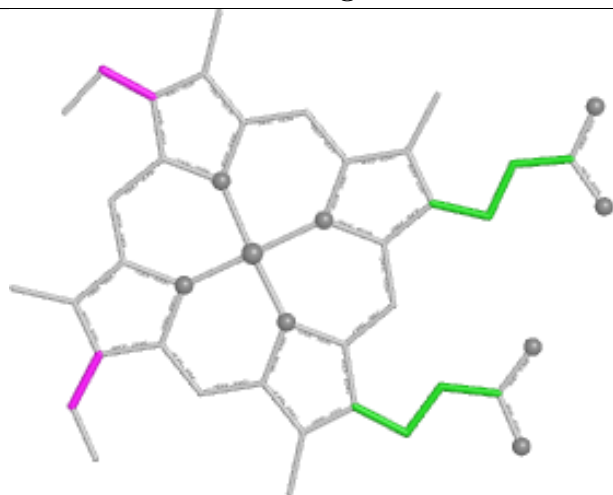
Ligand HEC B 1007 (B)



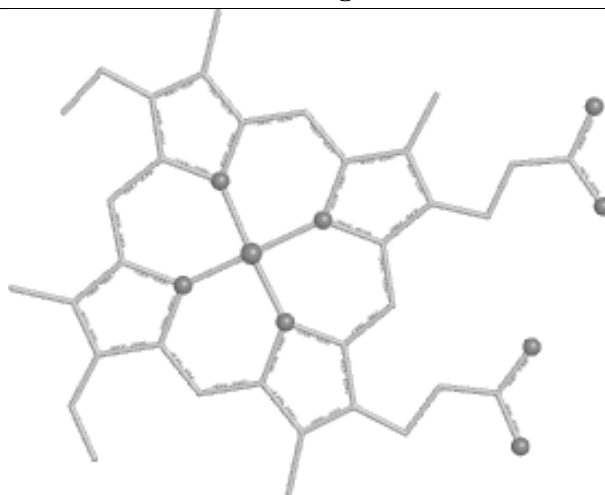
Bond lengths



Bond angles

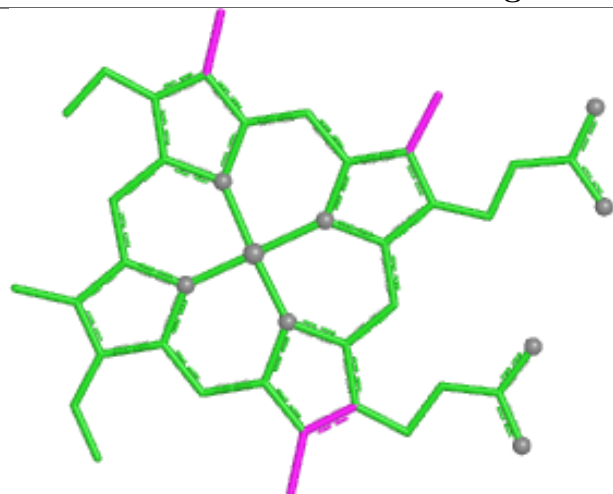


Torsions

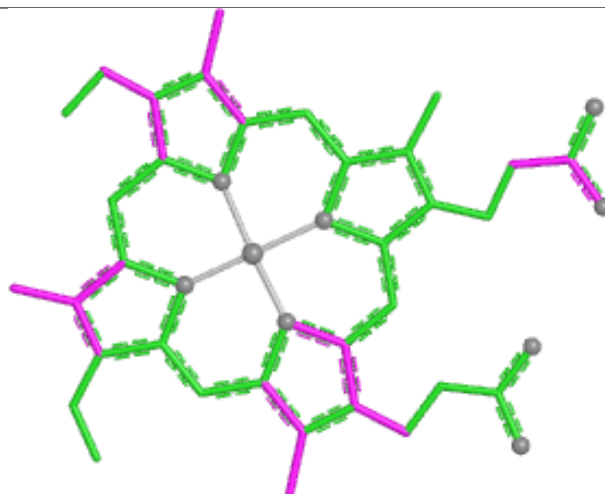


Rings

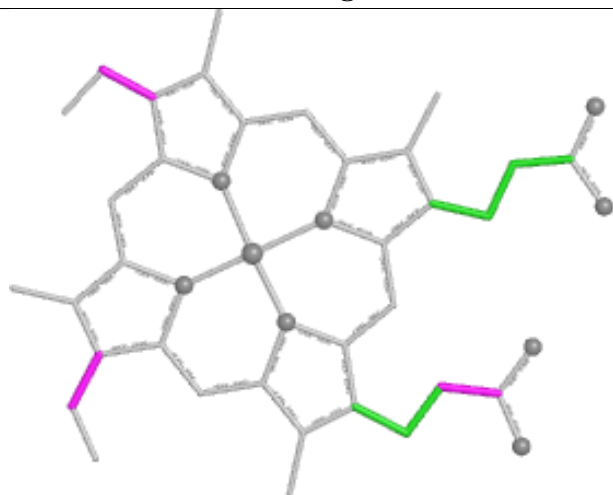
Ligand HEC B 1003



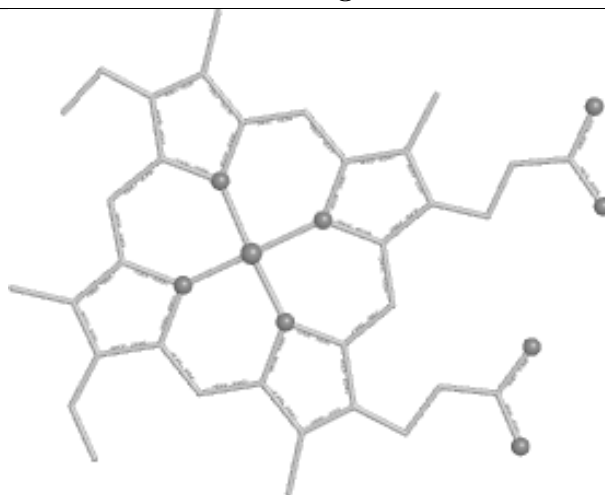
Bond lengths



Bond angles

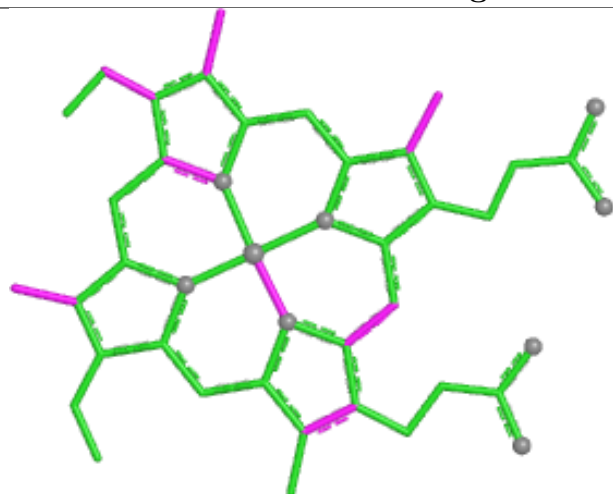


Torsions

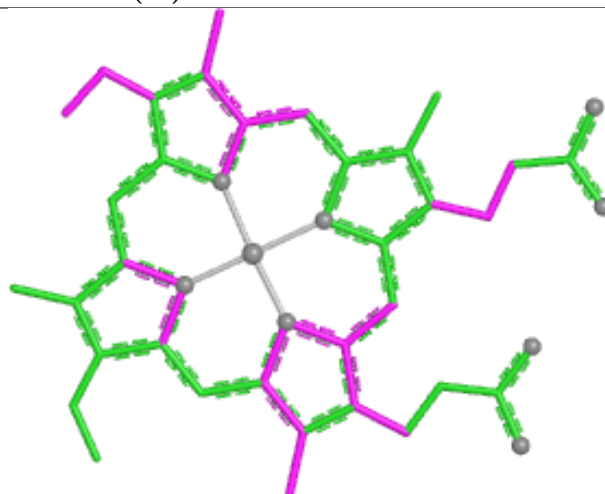


Rings

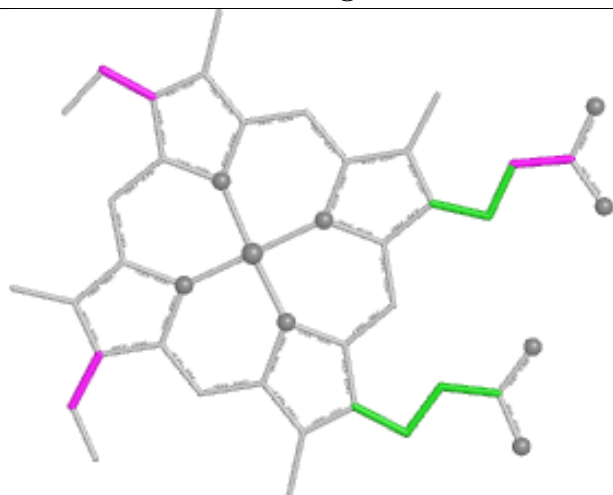
Ligand HEC A 1007 (A)



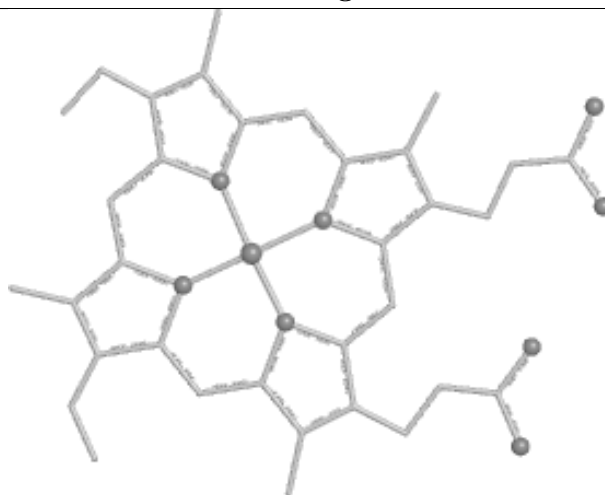
Bond lengths



Bond angles

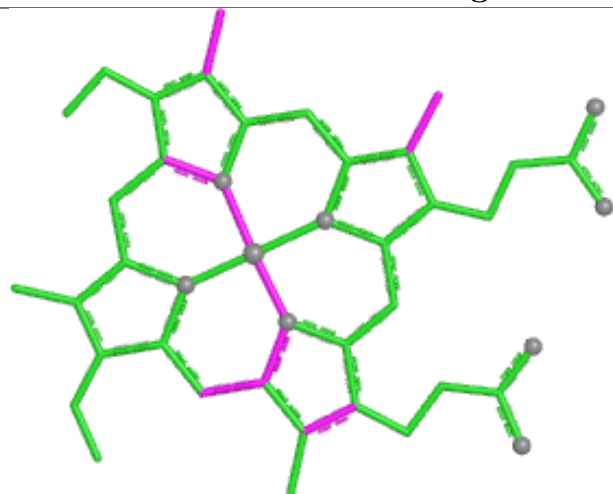


Torsions

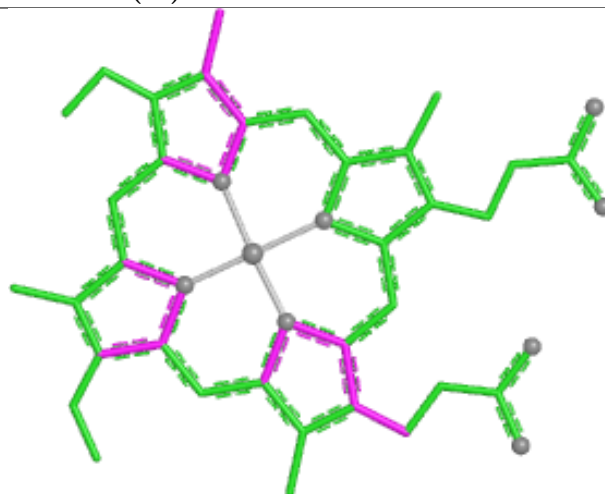


Rings

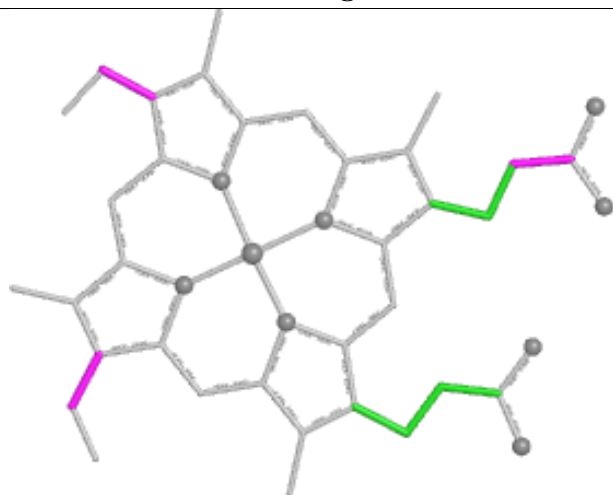
Ligand HEC B 1007 (A)



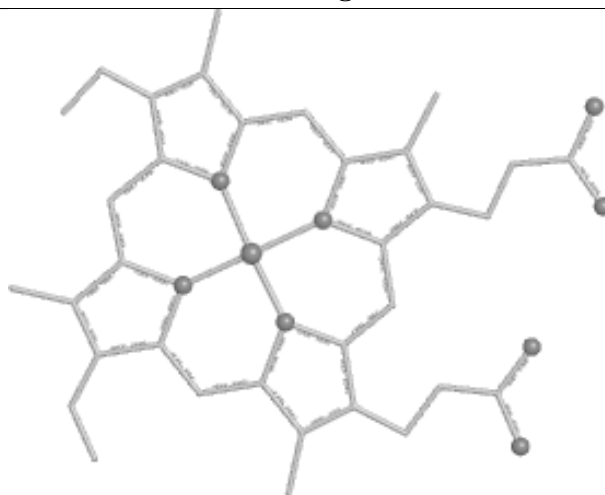
Bond lengths



Bond angles

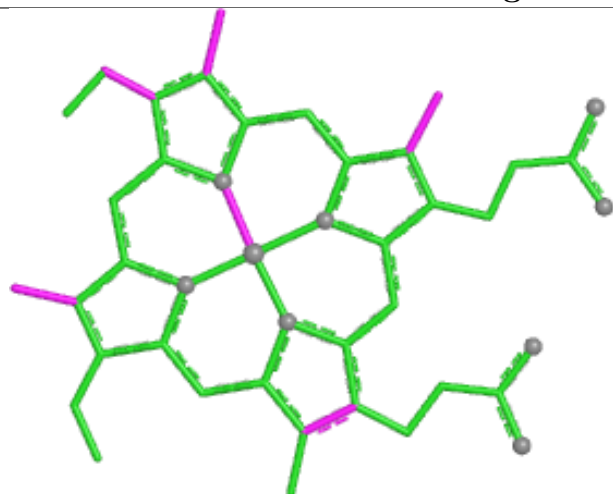


Torsions

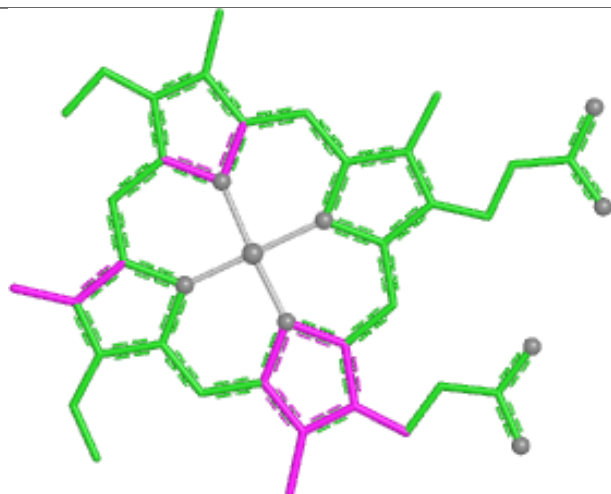


Rings

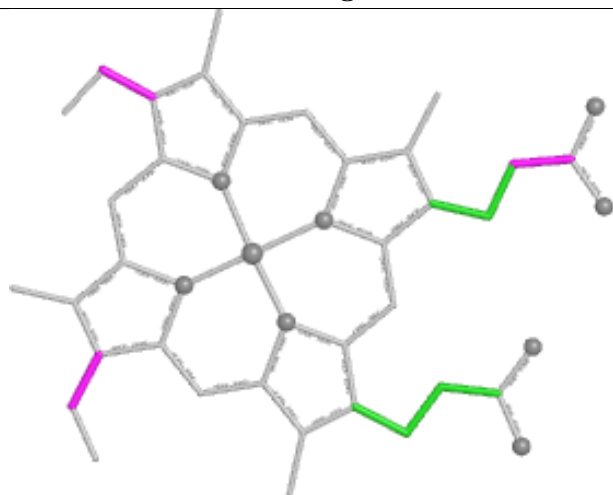
Ligand HEC A 1004



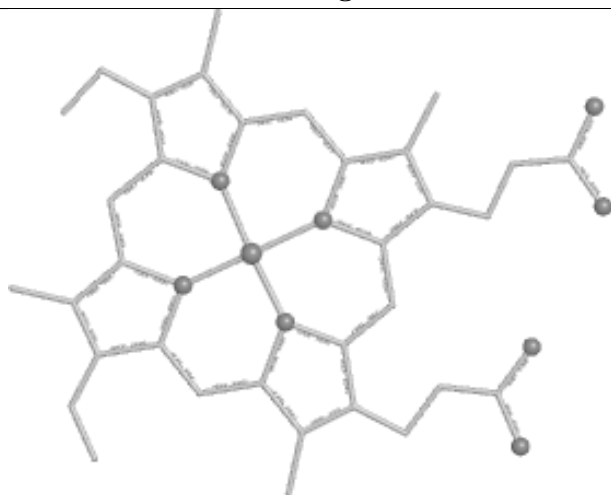
Bond lengths



Bond angles

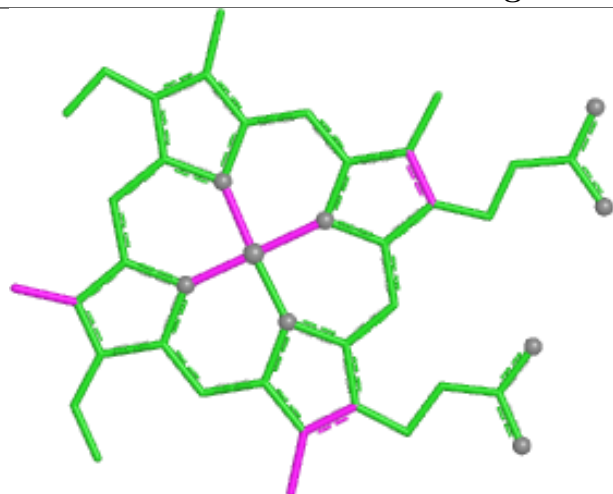


Torsions

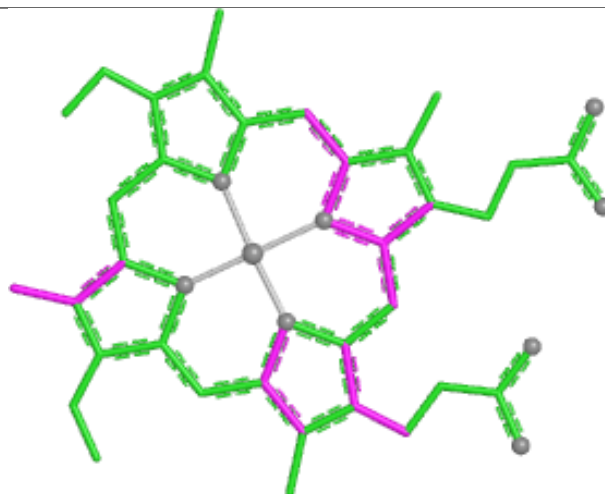


Rings

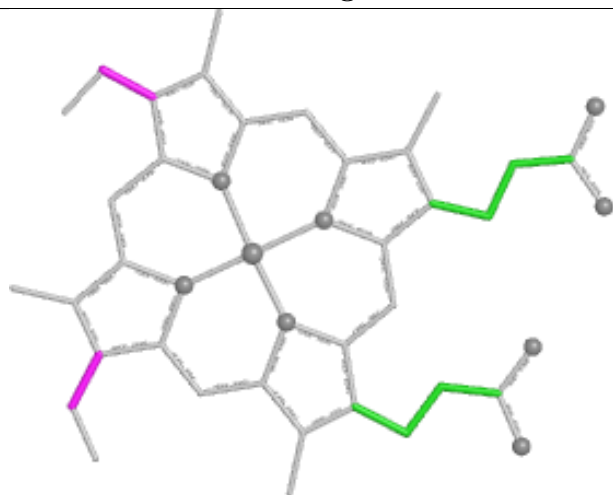
Ligand HEC B 1006



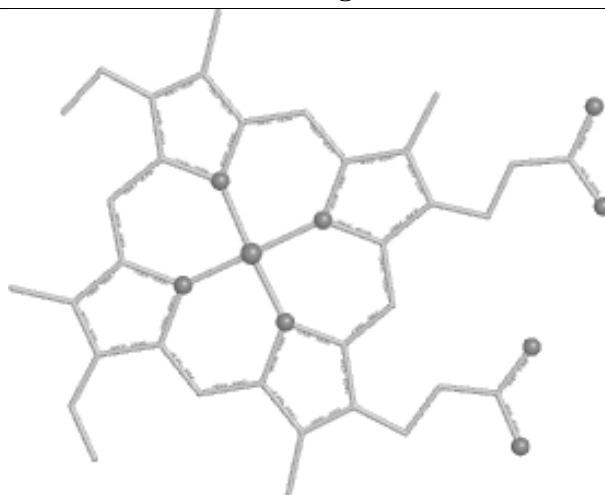
Bond lengths



Bond angles

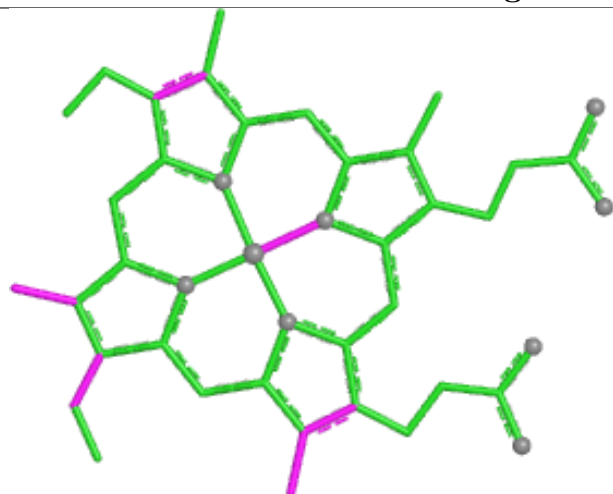


Torsions

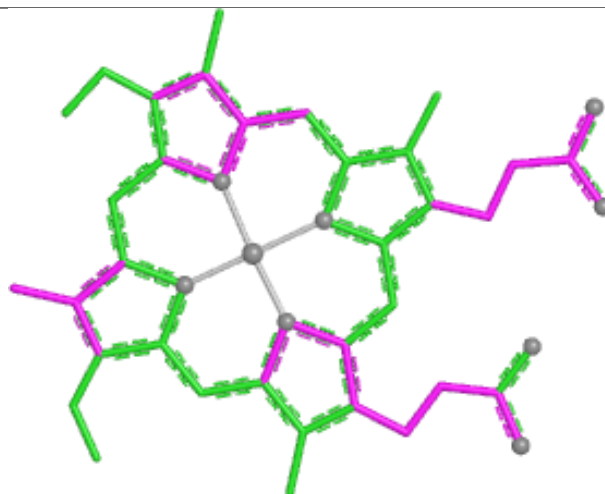


Rings

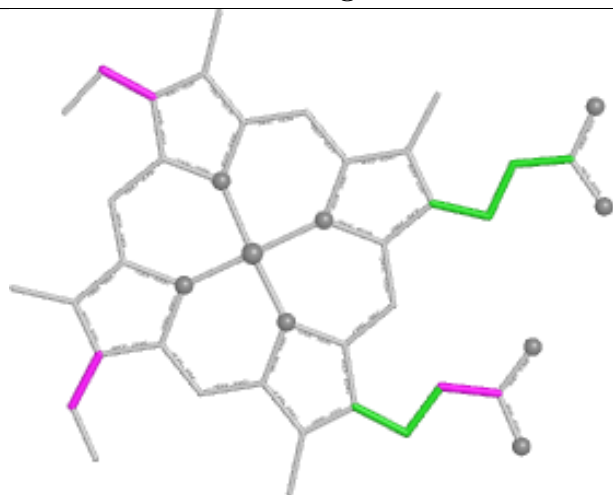
Ligand HEC B 1008



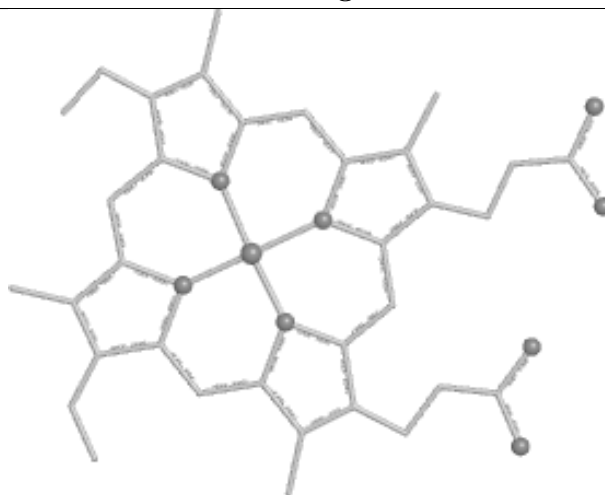
Bond lengths



Bond angles

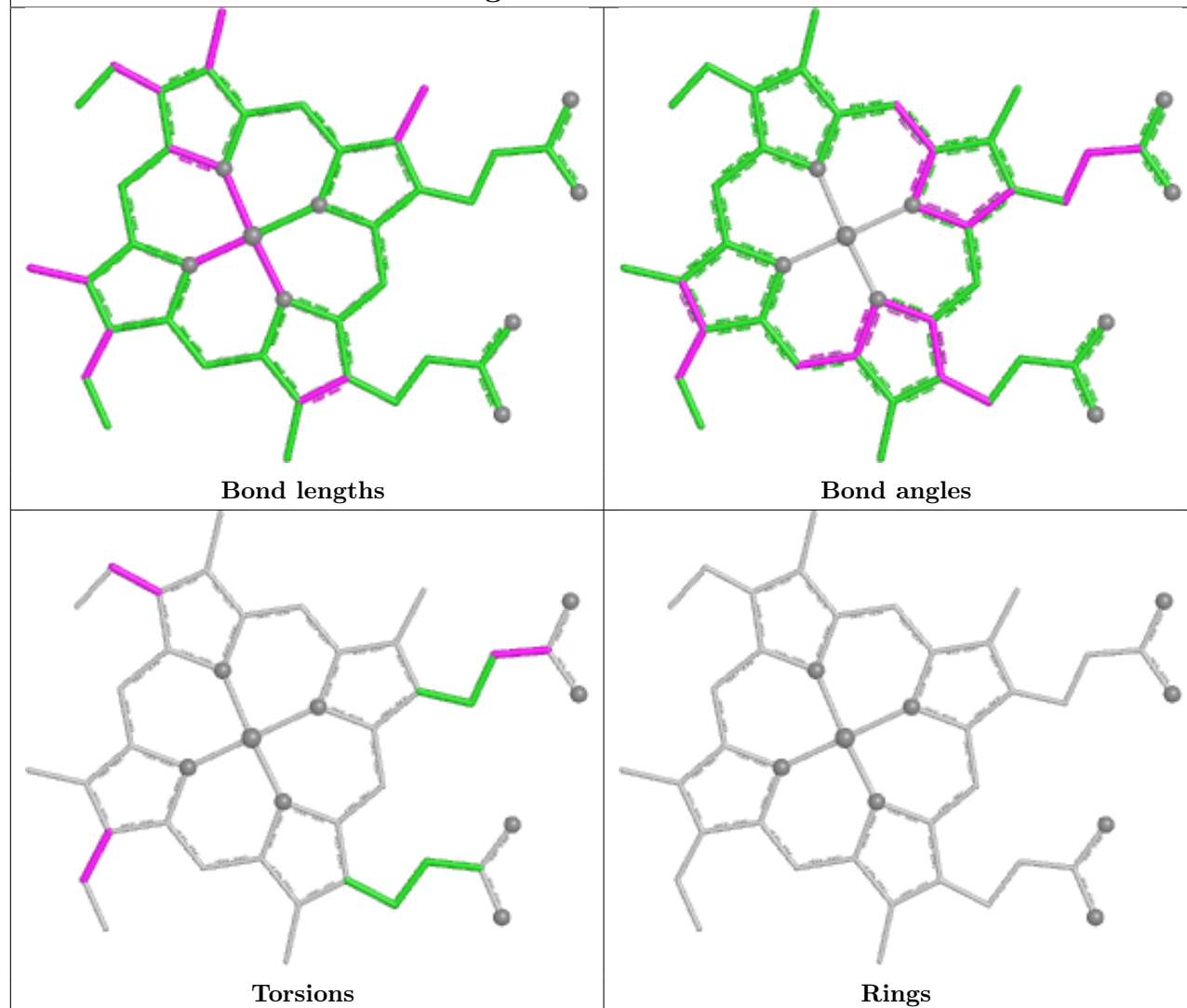


Torsions

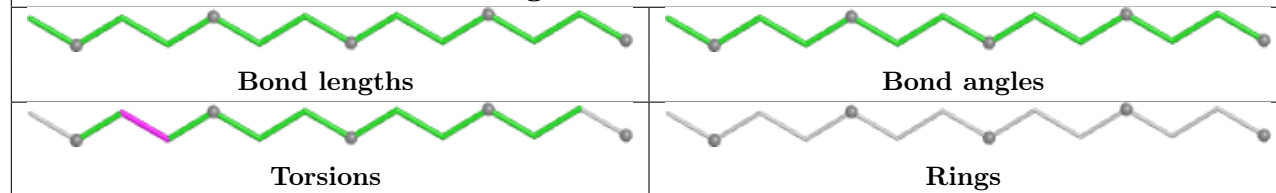


Rings

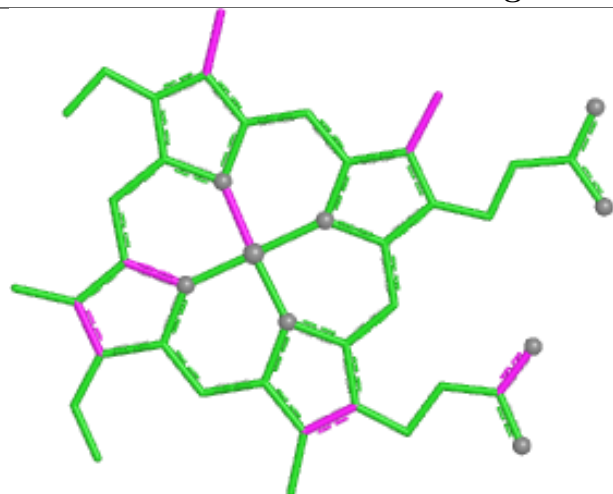
Ligand HEC A 1002



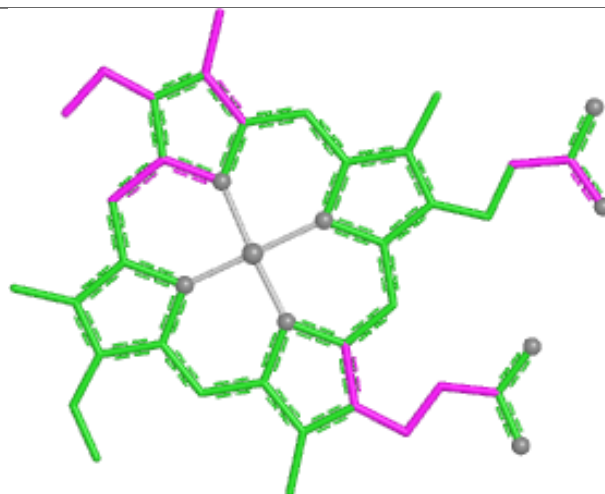
Ligand PG6 B 1011



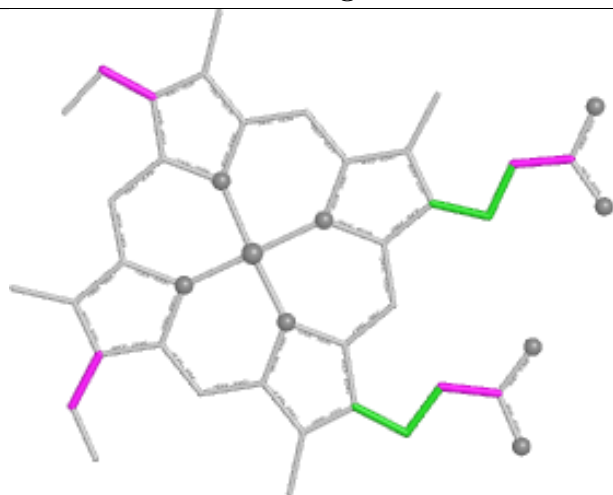
Ligand HEC B 1005



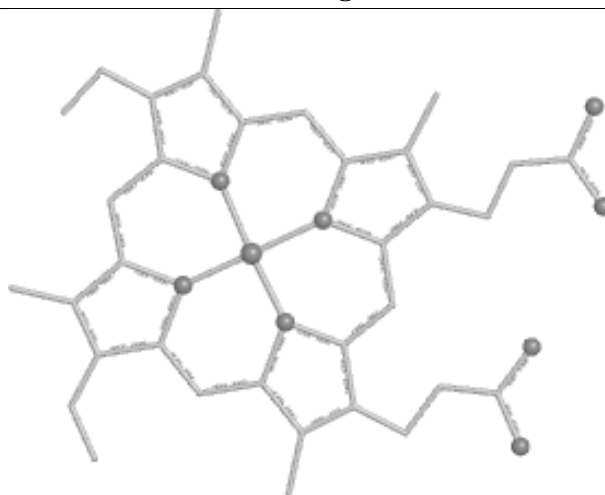
Bond lengths



Bond angles

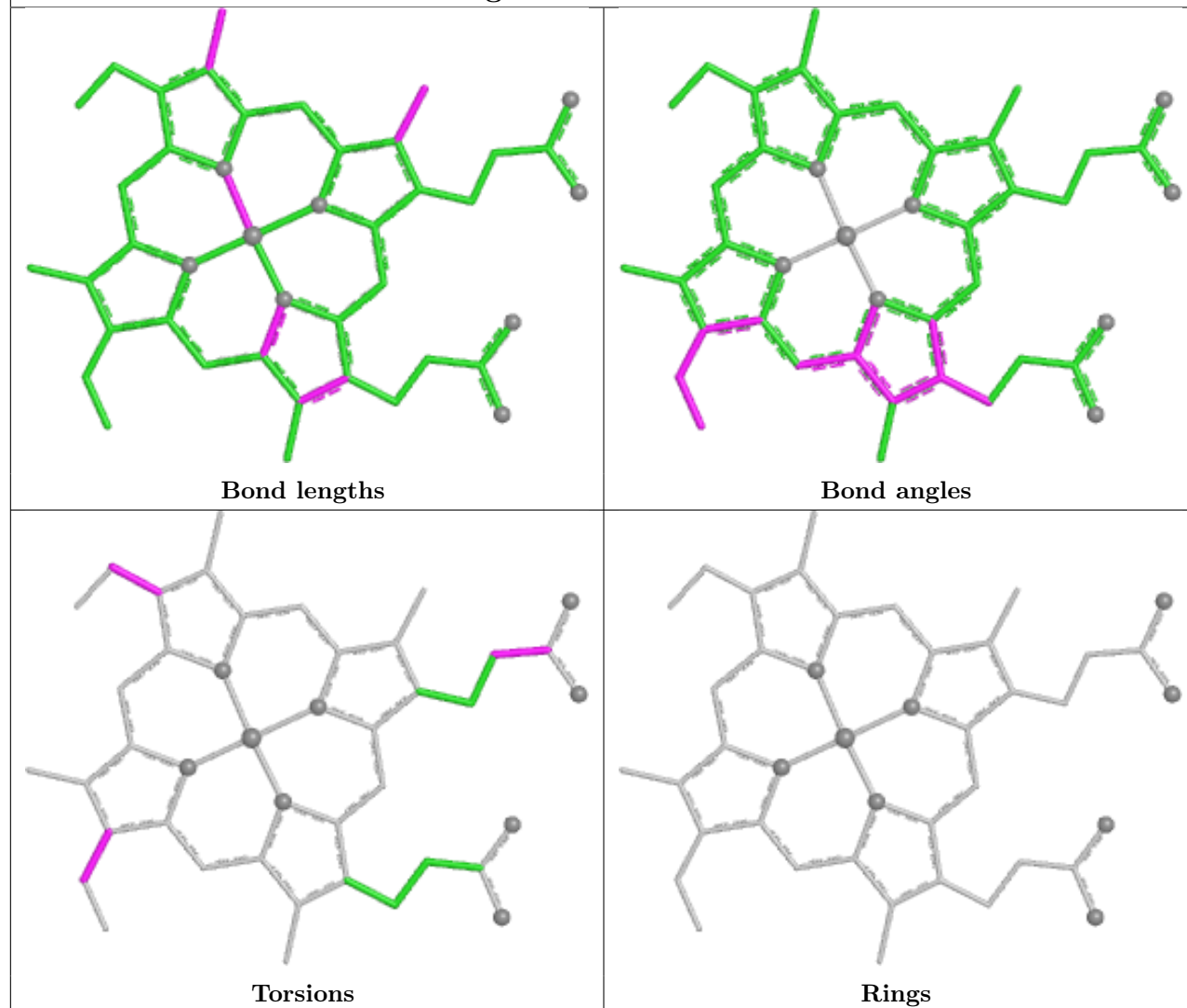


Torsions

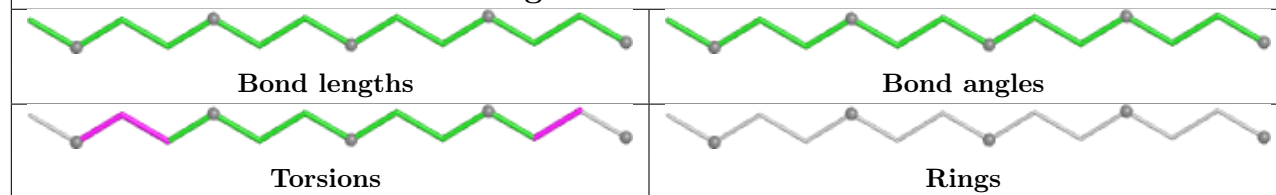


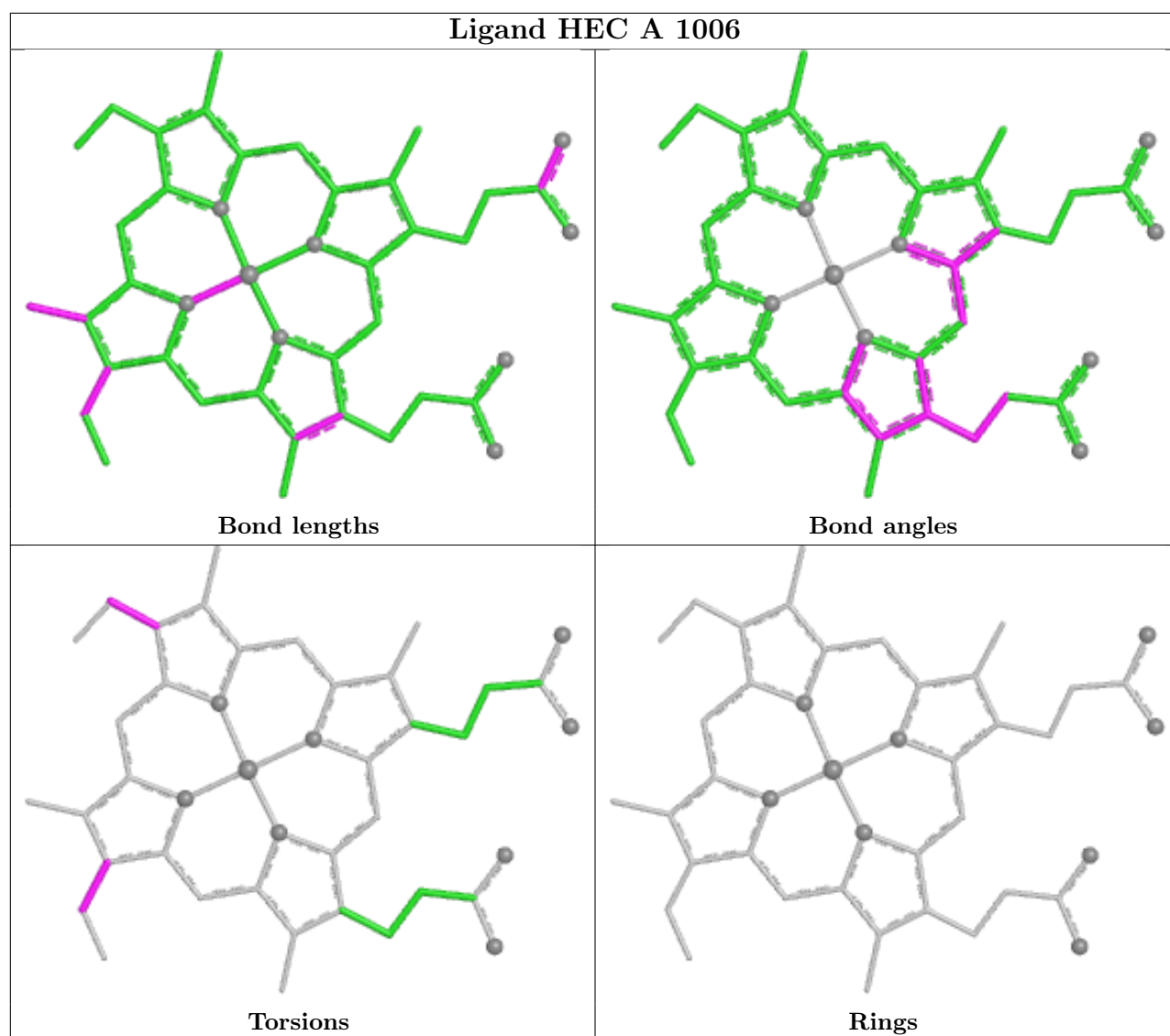
Rings

Ligand HEC B 1004



Ligand PG6 A 1010





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	519/525 (98%)	-0.75	3 (0%)	85 88	6, 16, 26, 37	22 (4%)
1	B	519/525 (98%)	-0.79	3 (0%)	85 88	6, 14, 25, 49	18 (3%)
All	All	1038/1050 (98%)	-0.77	6 (0%)	85 88	6, 15, 25, 49	40 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	5.1
1	A	523	ALA	5.0
1	A	522	VAL	4.5
1	B	522	VAL	4.4
1	B	388	GLN	2.8
1	A	388	GLN	2.2

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 oligosaccharides in this entry.

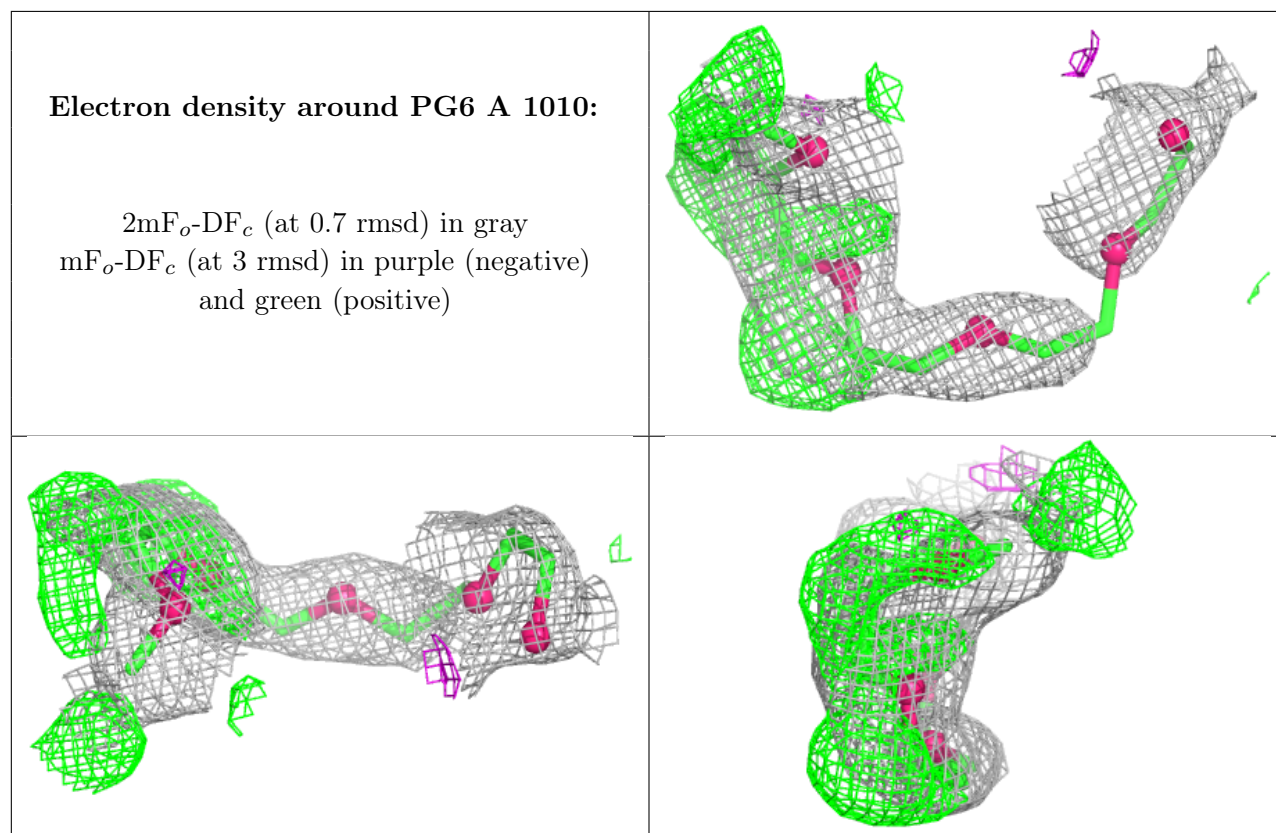
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
6	PG4	B	1013	5/13	0.72	0.36	26,26,28,28	5
6	PG4	B	1017	7/13	0.72	0.39	30,30,33,33	7
6	PG4	A	1009	8/13	0.73	0.22	29,33,34,35	8
6	PG4	B	1010	7/13	0.73	0.28	27,29,31,32	7
6	PG4	B	1016	5/13	0.76	0.21	17,18,22,23	5
8	TRS	A	1012	8/8	0.78	0.23	27,28,28,28	8
7	PG6	A	1010	14/18	0.80	0.18	21,27,31,32	14
6	PG4	B	1009	7/13	0.80	0.25	18,22,26,26	7
7	PG6	B	1011	14/18	0.82	0.18	27,31,33,35	14
6	PG4	B	1015	5/13	0.83	0.22	23,24,25,27	5
8	TRS	B	1012	8/8	0.85	0.20	22,25,26,27	8
6	PG4	A	1011	6/13	0.86	0.24	14,23,26,27	6
3	AZI	B	530	3/3	0.87	0.15	31,31,35,36	0
3	AZI	A	530	3/3	0.88	0.14	33,33,35,38	0
6	PG4	B	1014	9/13	0.89	0.17	15,19,24,25	9
6	PG4	A	1013	8/13	0.90	0.10	35,43,50,51	0
3	AZI	A	526	3/3	0.93	0.15	20,20,22,23	3
3	AZI	B	526	3/3	0.94	0.12	18,18,18,21	3
4	CA	A	528	1/1	0.94	0.08	19,19,19,19	1
4	CA	B	528	1/1	0.96	0.06	19,19,19,19	1
2	HEC	A	1003	43/43	0.98	0.05	12,14,23,34	18
2	HEC	B	1008	43/43	0.98	0.06	13,17,25,35	18
2	HEC	B	1003	43/43	0.98	0.06	11,14,25,34	18
2	HEC	B	1001	43/43	0.98	0.06	16,19,23,25	18
2	HEC	A	1008	43/43	0.98	0.07	15,20,31,40	18
5	NA	A	529	1/1	0.98	0.13	25,25,25,25	1
5	NA	B	529	1/1	0.98	0.09	18,18,18,18	1
2	HEC	B	1007[A]	43/43	0.99	0.05	11,12,14,15	24
2	HEC	B	1007[B]	43/43	0.99	0.05	11,12,14,19	24
2	HEC	A	1006	43/43	0.99	0.04	11,13,15,16	18
2	HEC	B	1002	43/43	0.99	0.04	13,16,17,19	18
2	HEC	A	1007[A]	43/43	0.99	0.05	12,14,15,15	24
2	HEC	A	1007[B]	43/43	0.99	0.05	12,14,16,19	24
2	HEC	A	1004	43/43	0.99	0.05	13,15,20,21	18
2	HEC	A	1002	43/43	0.99	0.05	13,15,17,19	18
2	HEC	A	1005	43/43	0.99	0.05	11,14,21,27	18
2	HEC	A	1001	43/43	0.99	0.05	14,17,19,23	18
4	CA	A	527	1/1	0.99	0.03	16,16,16,16	0
2	HEC	B	1004	43/43	0.99	0.04	12,14,18,18	18
4	CA	B	527	1/1	0.99	0.02	14,14,14,14	0
2	HEC	B	1005	43/43	0.99	0.05	10,13,21,27	18
2	HEC	B	1006	43/43	0.99	0.04	9,12,13,14	18

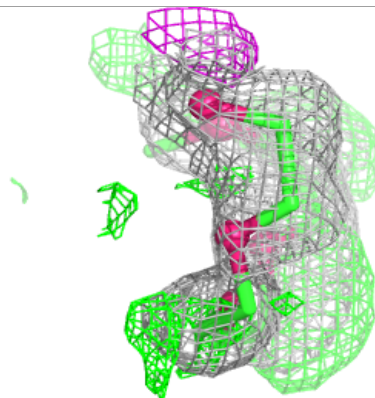
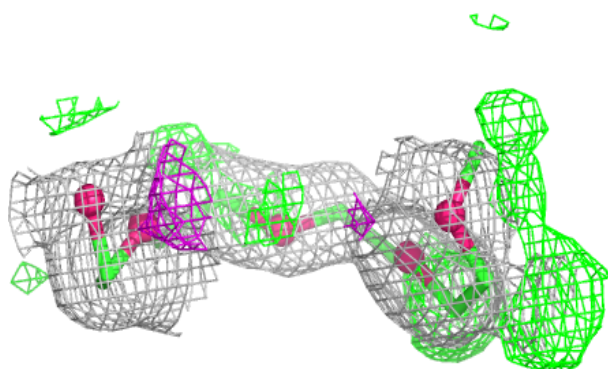
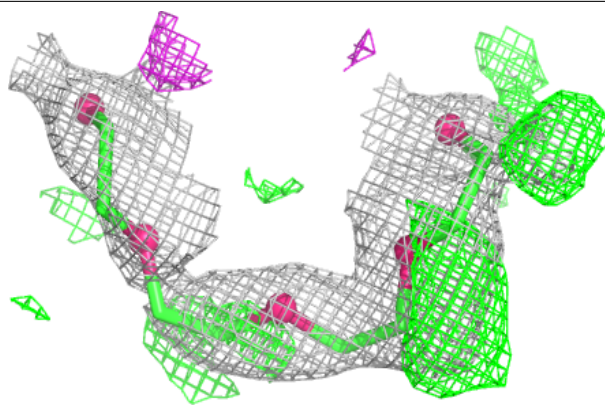
The following is a graphical depiction of the model fit to experimental electron density of all

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.



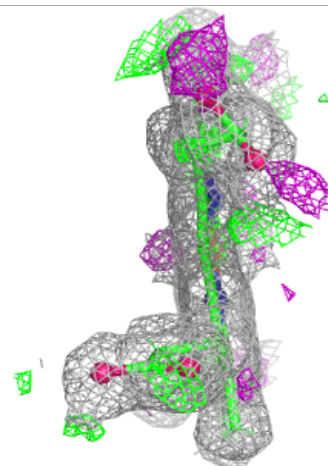
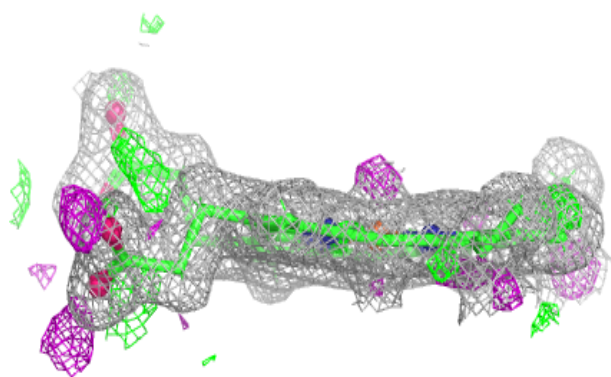
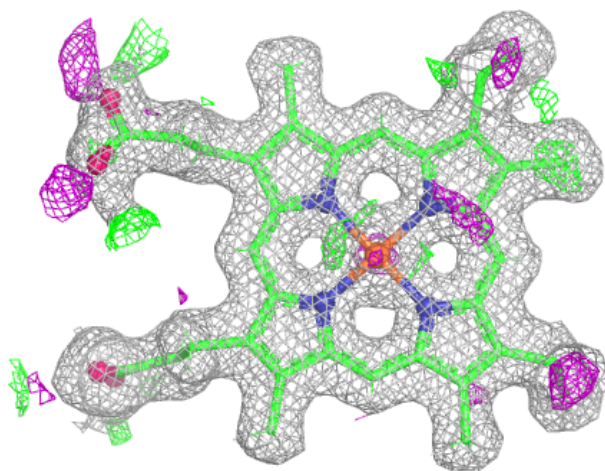
Electron density around PG6 B 1011:

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



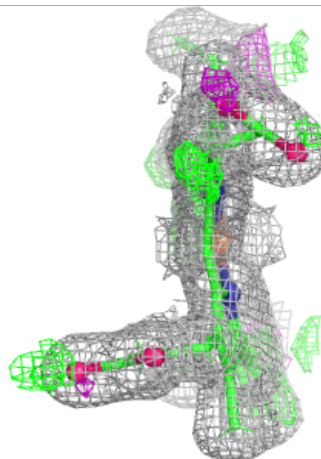
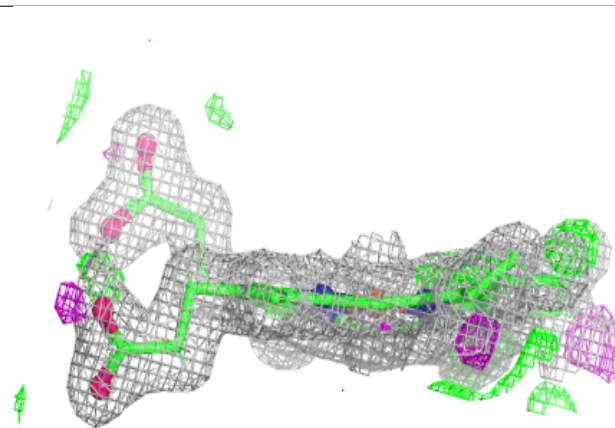
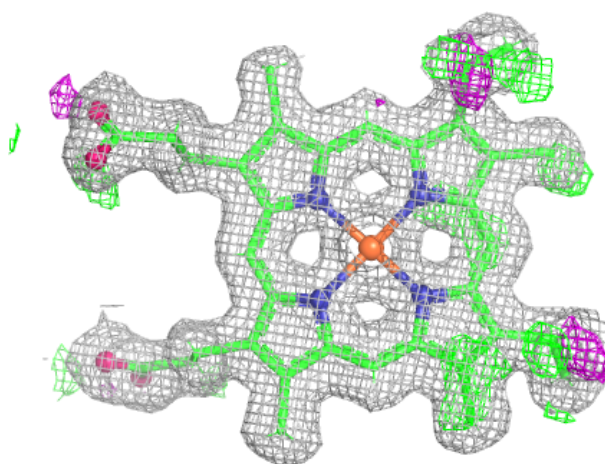
Electron density around HEC A 1003:

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



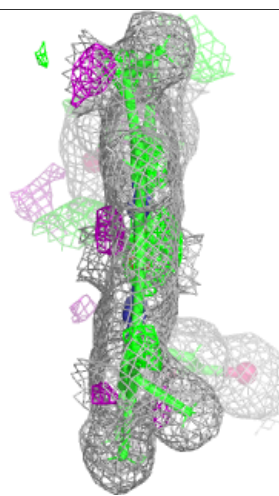
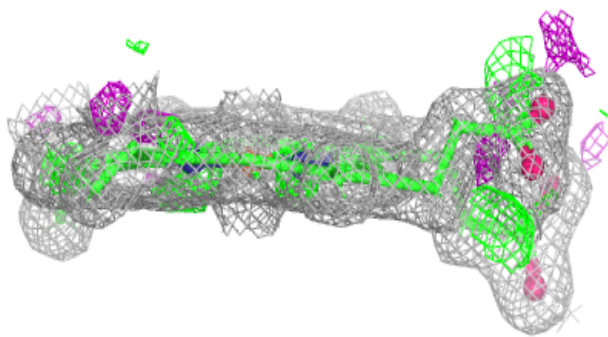
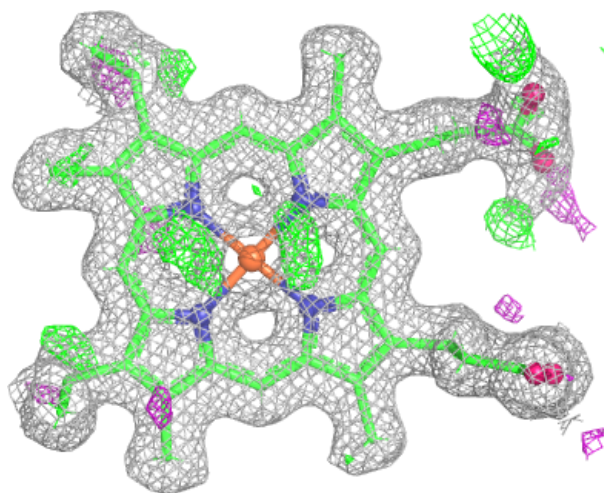
Electron density around HEC B 1008:

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



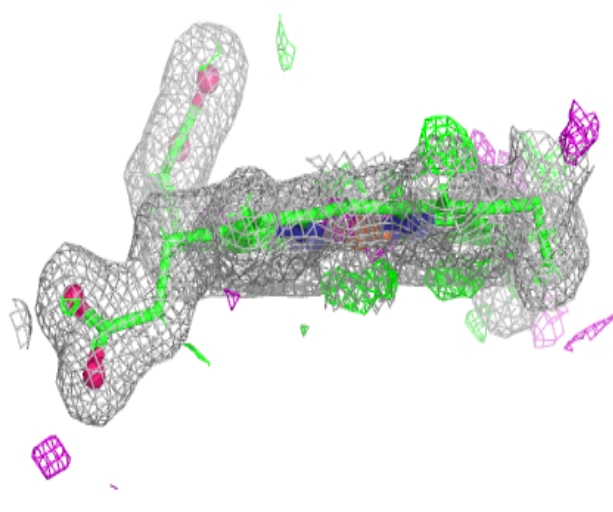
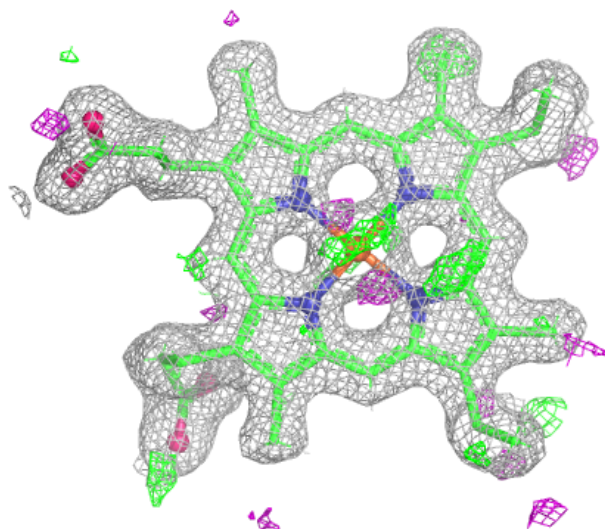
Electron density around HEC B 1003:

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



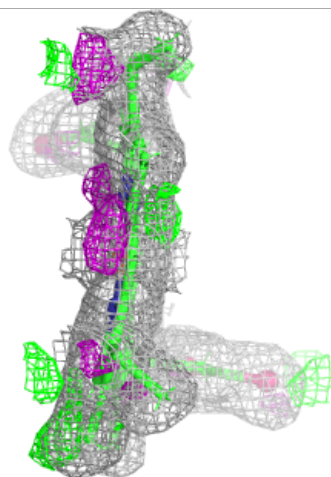
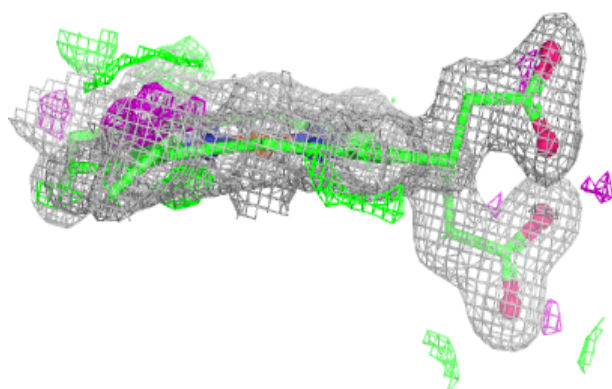
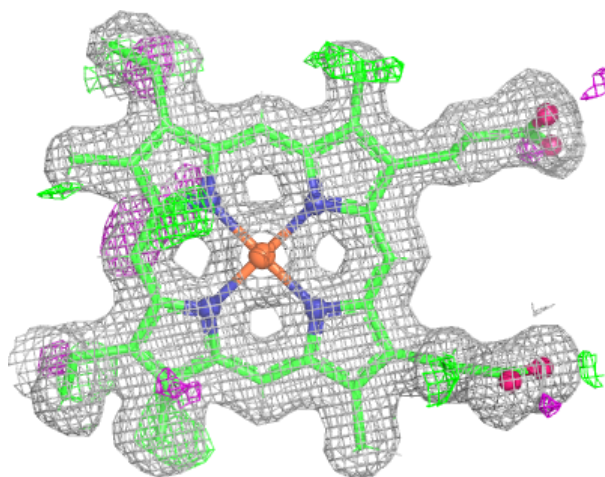
Electron density around HEC B 1001:

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



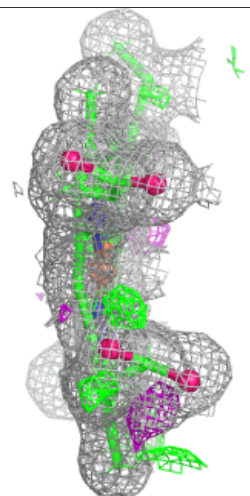
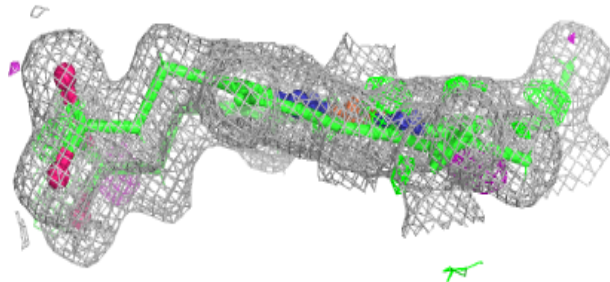
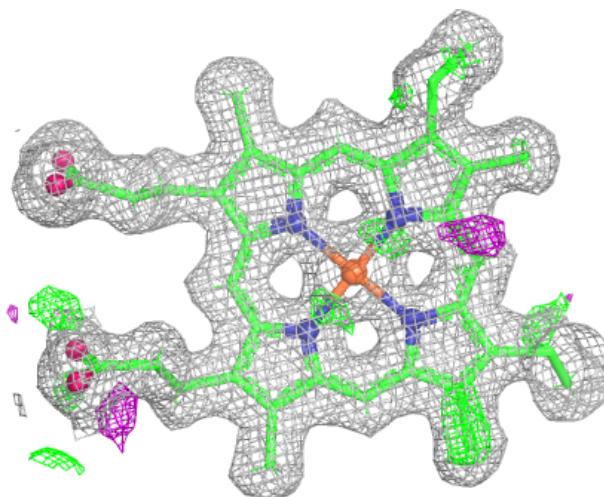
Electron density around HEC A 1008:

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



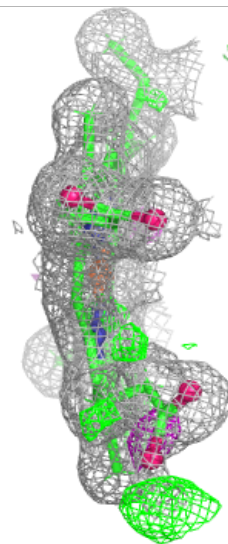
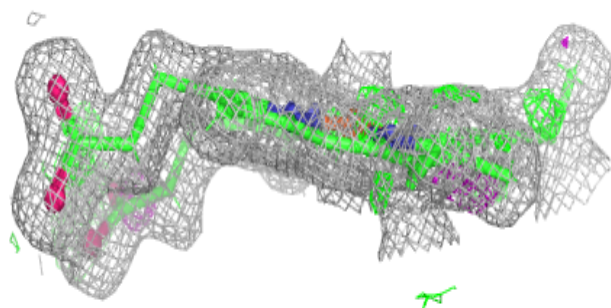
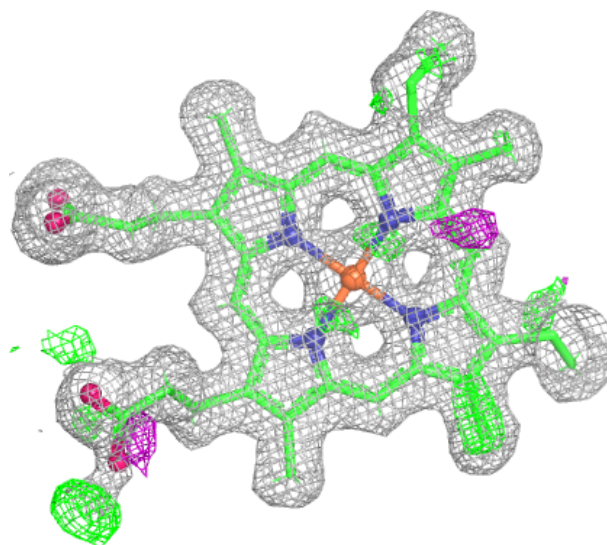
Electron density around HEC B 1007 (A):

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



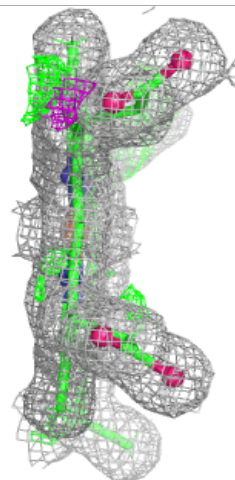
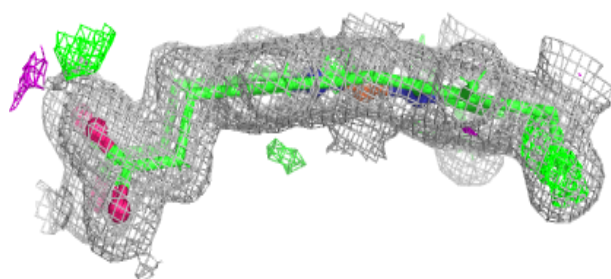
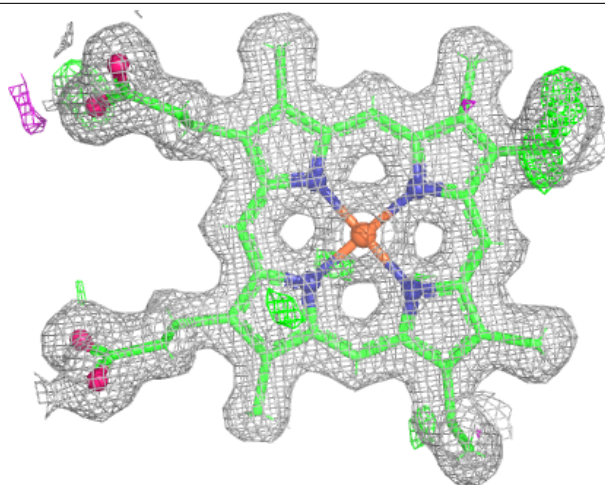
Electron density around HEC B 1007 (B):

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



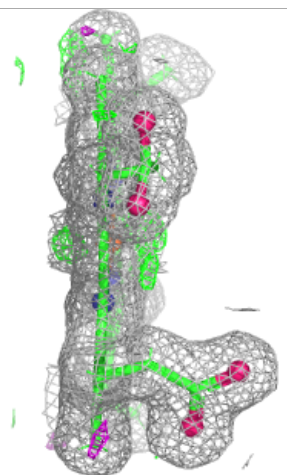
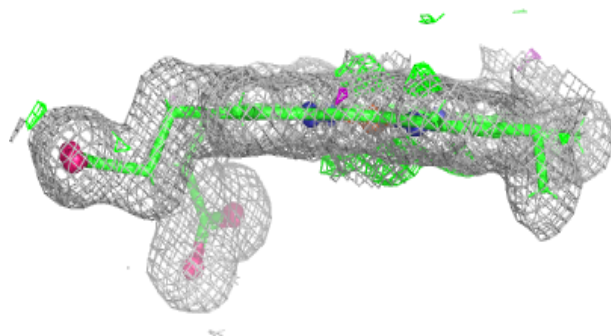
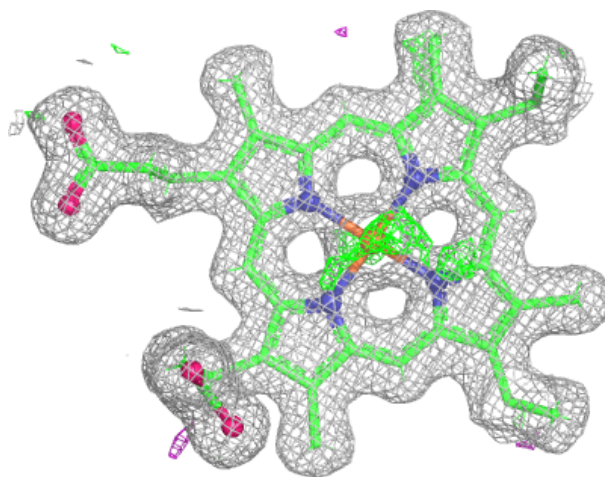
Electron density around HEC A 1006:

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



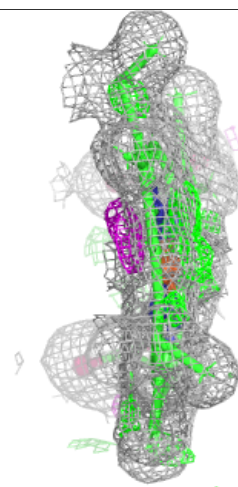
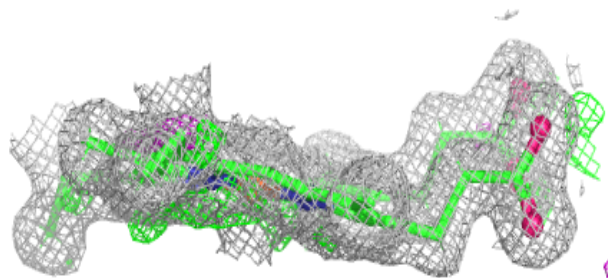
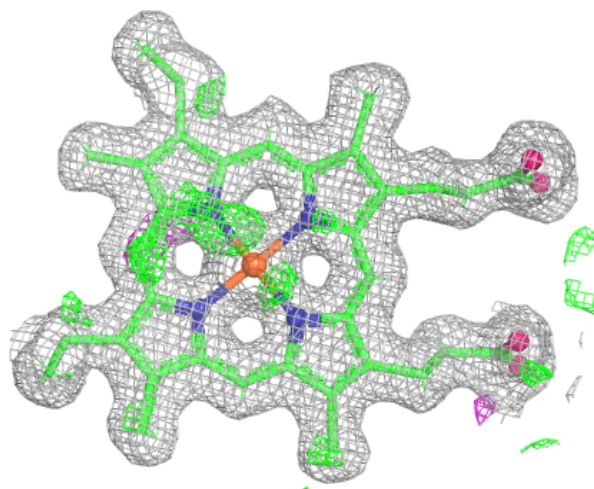
Electron density around HEC B 1002:

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



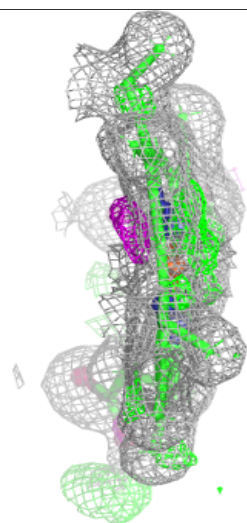
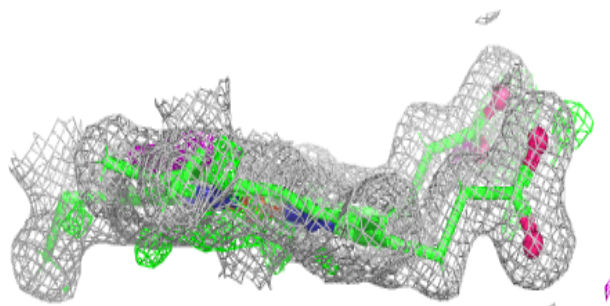
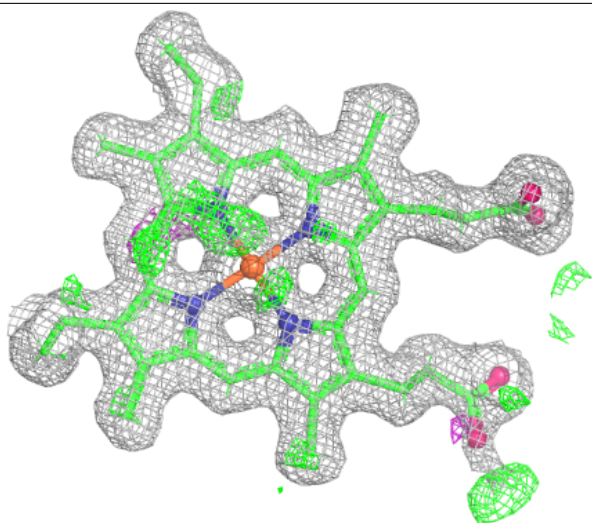
Electron density around HEC A 1007 (A):

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



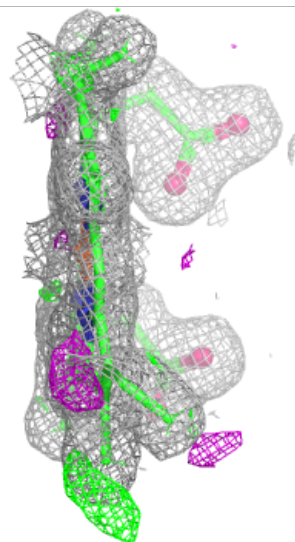
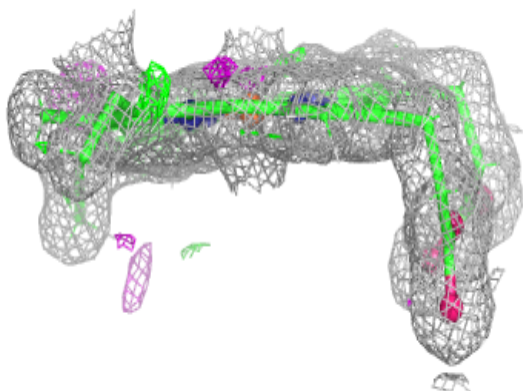
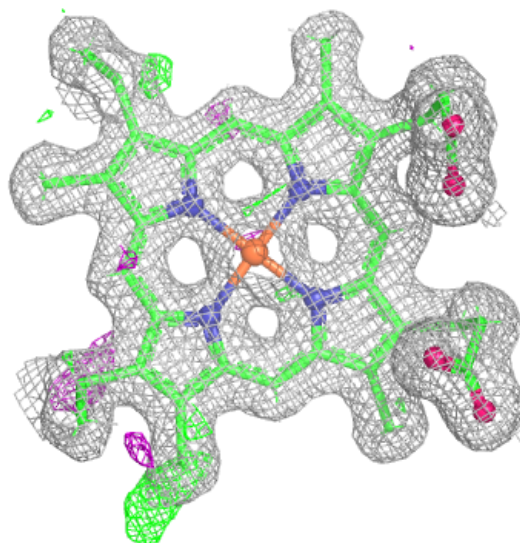
Electron density around HEC A 1007 (B):

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



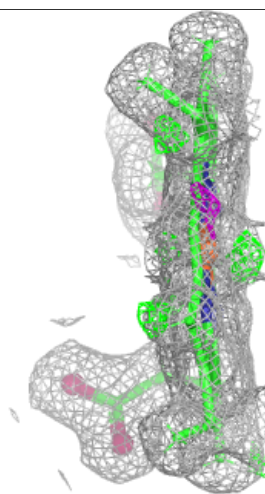
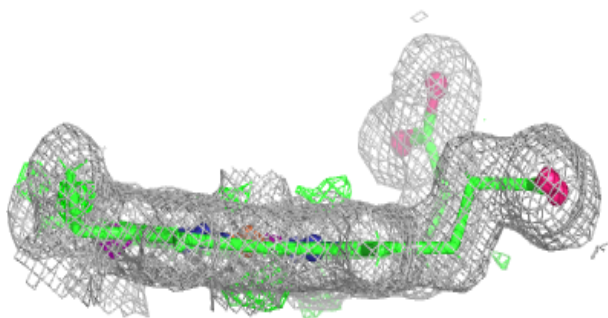
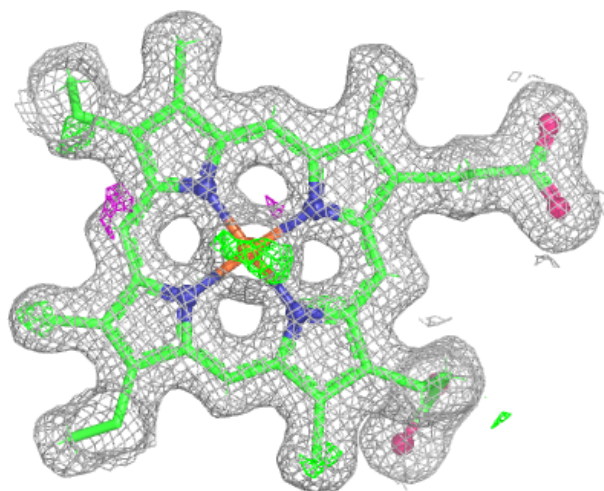
Electron density around HEC A 1004:

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



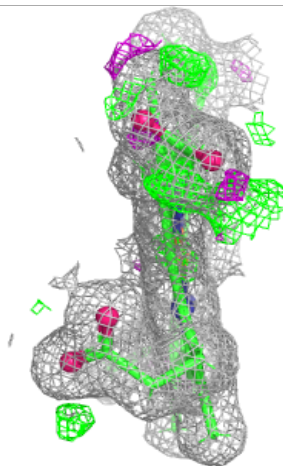
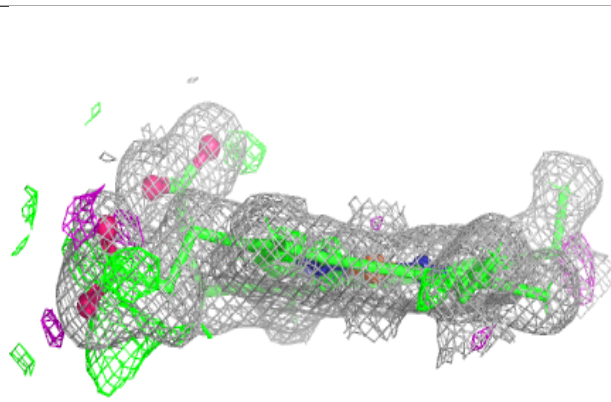
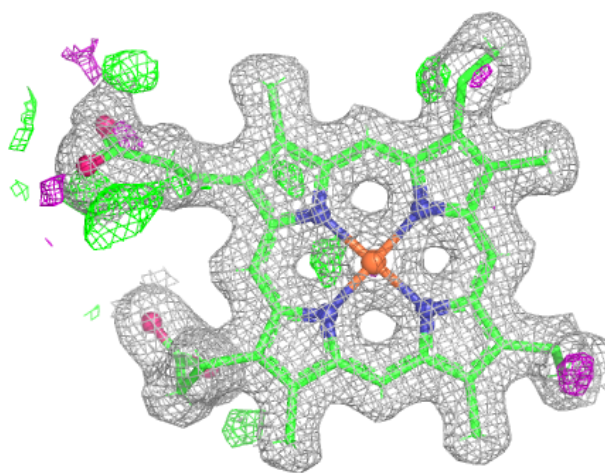
Electron density around HEC A 1002:

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



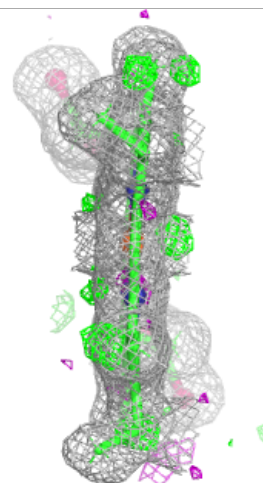
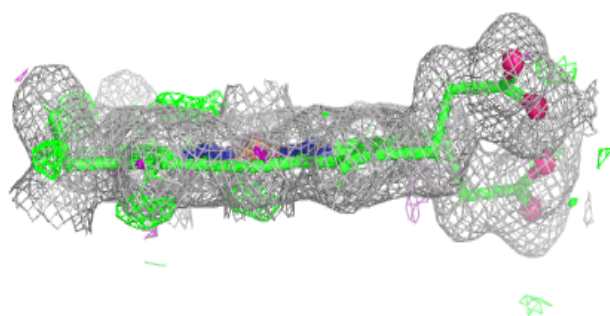
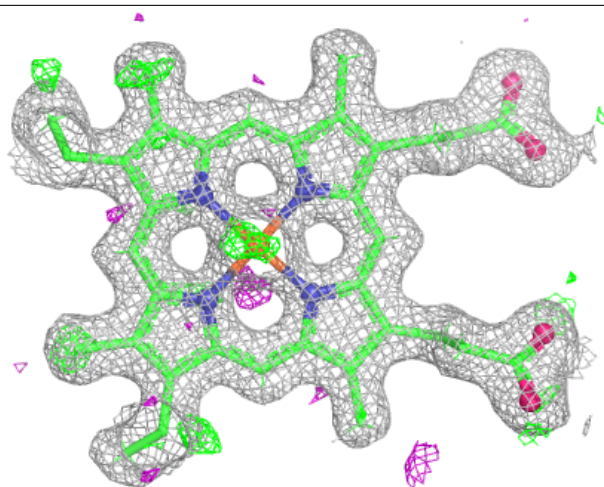
Electron density around HEC A 1005:

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



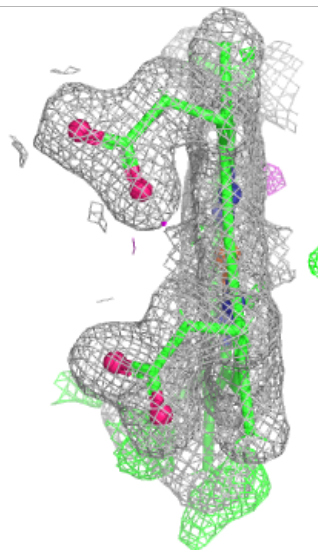
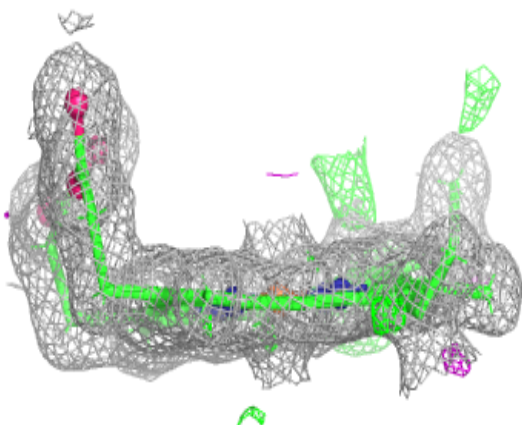
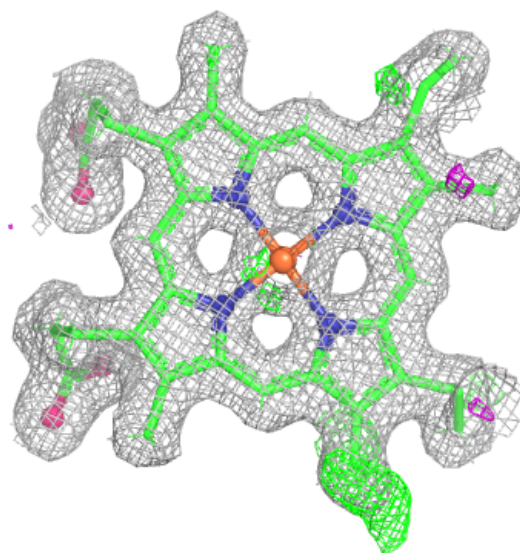
Electron density around HEC A 1001:

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



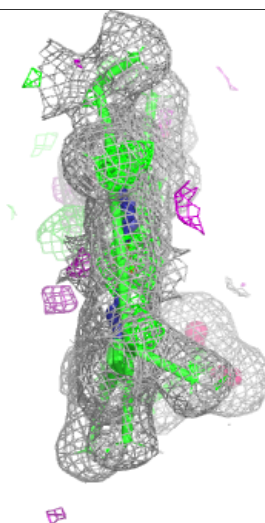
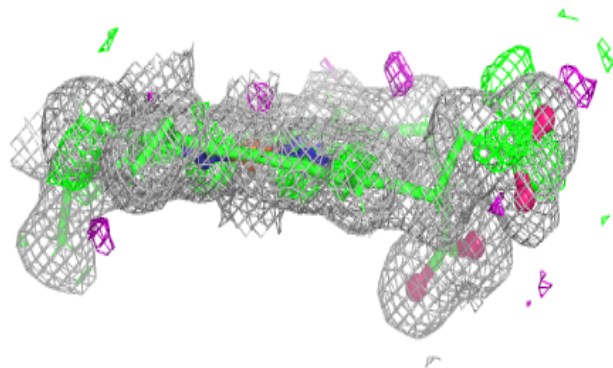
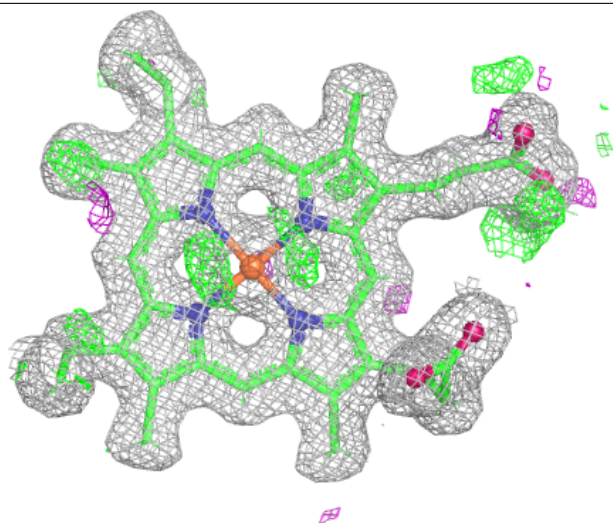
Electron density around HEC B 1004:

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



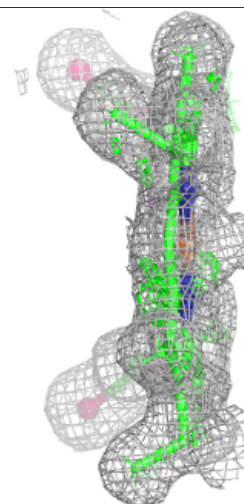
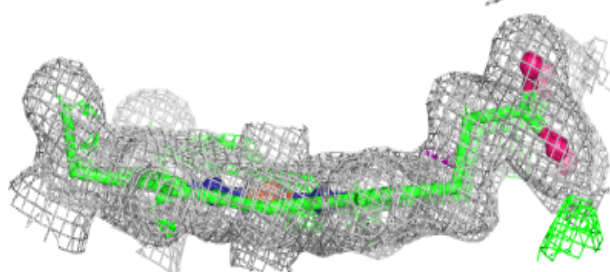
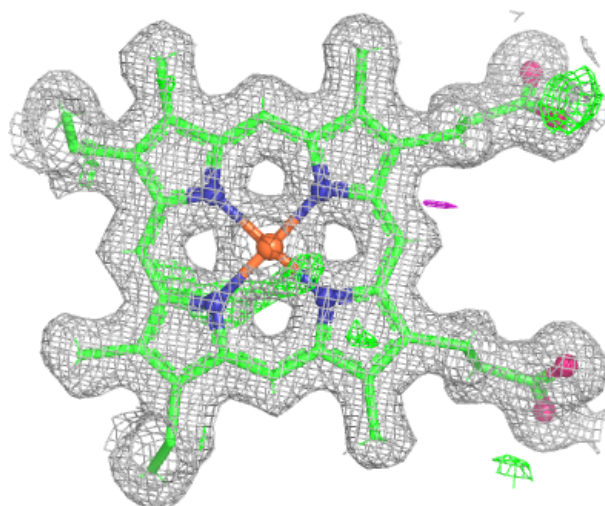
Electron density around HEC B 1005:

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



Electron density around HEC B 1006:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.