



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:14 PM EDT

PDB ID : 1J0P / pdb_00001j0p
Title : Three dimensional Structure of the Y43L mutant of Tetraheme Cytochrome c3 from Desulfovibrio vulgaris Miyazaki F
Authors : Ozawa, K.; Yasukawa, F.; Kumagai, J.; Ohmura, T.; Cusanvich, M.A.; Tomimoto, Y.; Ogata, H.; Higuchi, Y.; Akutsu, H.
Deposited on : 2002-11-19
Resolution : 0.91 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

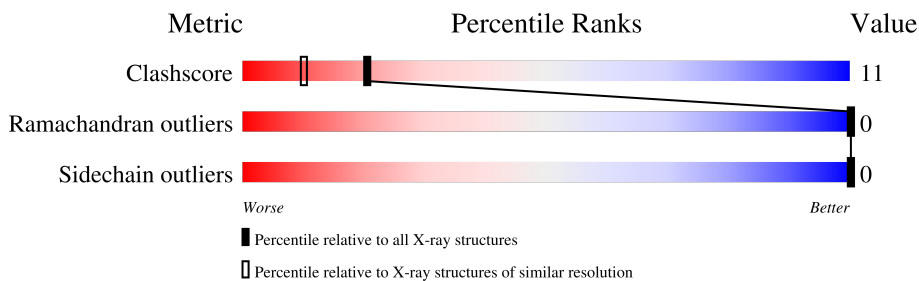
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.91 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))
Clashscore	190562	1358 (1.00-0.84)
Ramachandran outliers	187476	1283 (1.00-0.84)
Sidechain outliers	187428	1284 (1.00-0.84)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	 89% 8%

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
3	HEC	A	1001[A]	X	-	-	-
3	HEC	A	1001[B]	X	-	-	-
3	HEC	A	1002[A]	X	-	-	-
3	HEC	A	1002[B]	X	-	-	-
3	HEC	A	1003	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	A	1004	X	-	-	-
4	EOH	A	2002	-	-	X	-
4	EOH	A	2009	-	-	X	-
4	EOH	A	2014	-	-	X	-
4	EOH	A	2015	-	-	X	-
4	EOH	A	2017	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1412 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			802	489	151	151	11			

There is a discrepancy between the modelled and reference sequences:

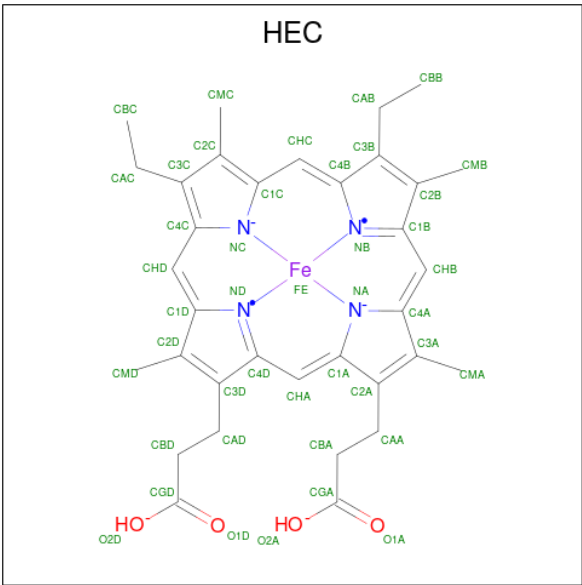
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	LEU	TYR	engineered mutation	UNP P00132

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



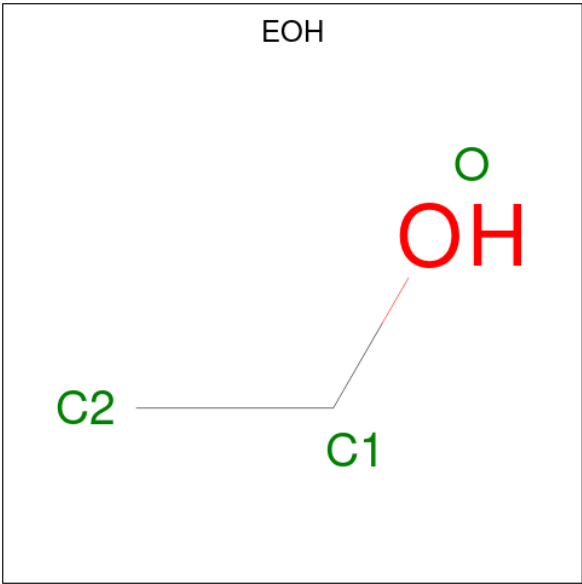
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 46	C 35	Fe 1	N 4	O 6	0	1
3	A	1	Total 46	C 35	Fe 1	N 4	O 6	0	1
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	371	Total O 371 371	0	0

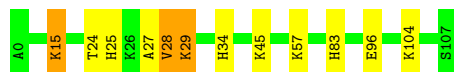
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: Cytochrome c3

Chain A:  89% 8% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.87Å 67.31Å 34.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 0.91	Depositor
% Data completeness (in resolution range)	88.7 (10.00-0.91)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.099 , 0.136	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1412	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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: HEC, SO4, EOH

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	1.02	0/818	1.37	8/1089 (0.7%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LYS	CA-CB-CG	13.22	140.55	114.10
1	A	29	LYS	CB-CG-CD	10.49	135.43	111.30
1	A	15	LYS	CA-C-N	7.39	132.01	123.21
1	A	15	LYS	C-N-CA	7.39	132.01	123.21
1	A	28	VAL	O-C-N	-6.59	114.27	122.97
1	A	83	HIS	CE1-NE2-CD2	-5.30	103.69	109.00
1	A	29	LYS	CG-CD-CE	5.25	123.37	111.30
1	A	34	HIS	CE1-NE2-CD2	-5.20	103.81	109.00

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	802	0	787	10	0
2	A	10	0	0	0	0
3	A	178	0	68	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	101	17	0
5	A	371	0	0	14	0
All	All	1412	0	956	23	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 11.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:O	4:A:2015:EOH:H12	1.98	0.63
4:A:2017:EOH:H21	5:A:3213:HOH:O	2.00	0.62
4:A:2014:EOH:H22	5:A:3255:HOH:O	2.04	0.57
1:A:28:VAL:HG23	4:A:2015:EOH:C2	2.35	0.57
4:A:2002:EOH:H22	5:A:3165:HOH:O	2.05	0.55
4:A:2002:EOH:H23	5:A:3292:HOH:O	2.09	0.52
1:A:29:LYS:HB3	5:A:3191:HOH:O	2.10	0.52
4:A:2014:EOH:H23	5:A:3186:HOH:O	2.09	0.51
4:A:2009:EOH:H22	4:A:2015:EOH:O	2.12	0.50
1:A:57:LYS:HB3	5:A:3212:HOH:O	2.11	0.50
4:A:2017:EOH:H22	5:A:3012:HOH:O	2.12	0.50
1:A:45:LYS:NZ	5:A:3326:HOH:O	2.47	0.48
3:A:1001[B]:HEC:O1D	4:A:2017:EOH:H23	2.14	0.47
1:A:25:HIS:HA	4:A:2015:EOH:C2	2.44	0.47
1:A:15:LYS:CE	4:A:2004:EOH:H21	2.45	0.47
4:A:2009:EOH:H23	5:A:3310:HOH:O	2.15	0.46
3:A:1003:HEC:HBC3	3:A:1003:HEC:HMC3	1.98	0.45
1:A:15:LYS:HG2	5:A:3342:HOH:O	2.15	0.45
4:A:2017:EOH:H11	5:A:3287:HOH:O	2.17	0.44
4:A:2014:EOH:H12	5:A:3352:HOH:O	2.17	0.43
1:A:27:ALA:HB3	4:A:2015:EOH:H22	2.01	0.42
4:A:2011:EOH:H11	5:A:3153:HOH:O	2.20	0.41
1:A:96:GLU:OE1	1:A:104:LYS:HE3	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	106/108 (98%)	105 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/85 (100%)	85 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEC	A	1002[A]	-	50,50,50	1.38	10 (20%)	68,82,82	1.10	5 (7%)
2	SO4	A	2502	-	4,4,4	0.47	0	6,6,6	0.58	0
4	EOH	A	2007	-	2,2,2	0.49	0	1,1,1	0.17	0
4	EOH	A	2009	-	2,2,2	0.48	0	1,1,1	0.36	0
4	EOH	A	2008	-	2,2,2	0.52	0	1,1,1	0.82	0
4	EOH	A	2015	-	2,2,2	0.30	0	1,1,1	1.70	0
4	EOH	A	2006	-	2,2,2	0.51	0	1,1,1	0.33	0
4	EOH	A	2011	-	2,2,2	0.52	0	1,1,1	0.06	0
3	HEC	A	1001[B]	-	50,50,50	1.29	9 (18%)	68,82,82	0.98	2 (2%)
4	EOH	A	2003	-	2,2,2	0.55	0	1,1,1	0.57	0
3	HEC	A	1002[B]	-	50,50,50	1.38	10 (20%)	68,82,82	1.13	6 (8%)
2	SO4	A	2501	-	4,4,4	0.41	0	6,6,6	0.54	0
3	HEC	A	1004	1	50,50,50	1.19	4 (8%)	68,82,82	0.95	1 (1%)
4	EOH	A	2001	-	2,2,2	1.02	0	1,1,1	0.09	0
4	EOH	A	2005	-	2,2,2	0.50	0	1,1,1	0.16	0
4	EOH	A	2004	-	2,2,2	0.62	0	1,1,1	1.14	0
4	EOH	A	2002	-	2,2,2	0.62	0	1,1,1	1.20	0
4	EOH	A	2016	-	2,2,2	0.53	0	1,1,1	0.34	0
4	EOH	A	2013	-	2,2,2	0.47	0	1,1,1	0.02	0
4	EOH	A	2012	-	2,2,2	0.13	0	1,1,1	0.10	0
4	EOH	A	2014	-	2,2,2	0.66	0	1,1,1	0.45	0
3	HEC	A	1003	1	50,50,50	1.24	8 (16%)	68,82,82	1.16	6 (8%)
4	EOH	A	2017	-	2,2,2	0.40	0	1,1,1	0.44	0
3	HEC	A	1001[A]	-	50,50,50	1.29	9 (18%)	68,82,82	0.96	2 (2%)
4	EOH	A	2010	-	2,2,2	0.46	0	1,1,1	0.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	1002[A]	-	1/1/3/7	6/14/54/54	-
3	HEC	A	1001[B]	-	1/1/3/7	6/14/54/54	-
3	HEC	A	1002[B]	-	1/1/3/7	6/14/54/54	-
3	HEC	A	1003	1	1/1/3/7	6/14/54/54	-
3	HEC	A	1001[A]	-	1/1/3/7	7/14/54/54	-
3	HEC	A	1004	1	1/1/3/7	6/14/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	HEC	FE-NC	3.24	2.05	1.95
3	A	1002[A]	HEC	FE-ND	3.08	2.04	1.94
3	A	1002[B]	HEC	FE-ND	3.08	2.04	1.94
3	A	1002[A]	HEC	C1B-NB	-2.93	1.33	1.38
3	A	1002[B]	HEC	C1B-NB	-2.93	1.33	1.38
3	A	1002[A]	HEC	C1D-ND	-2.92	1.35	1.40
3	A	1002[B]	HEC	C1D-ND	-2.92	1.35	1.40
3	A	1001[A]	HEC	C1D-ND	-2.85	1.35	1.40
3	A	1001[B]	HEC	C1D-ND	-2.85	1.35	1.40
3	A	1001[A]	HEC	C4C-NC	-2.66	1.34	1.39
3	A	1001[B]	HEC	C4C-NC	-2.66	1.34	1.39
3	A	1004	HEC	C1D-ND	-2.63	1.35	1.40
3	A	1004	HEC	FE-ND	2.59	2.02	1.94
3	A	1002[A]	HEC	C4C-NC	-2.58	1.34	1.39
3	A	1002[B]	HEC	C4C-NC	-2.58	1.34	1.39
3	A	1001[A]	HEC	O2A-CGA	-2.50	1.22	1.30
3	A	1001[B]	HEC	O2A-CGA	-2.50	1.22	1.30
3	A	1003	HEC	C1C-NC	-2.47	1.35	1.39
3	A	1002[A]	HEC	C1C-NC	-2.45	1.35	1.39
3	A	1002[B]	HEC	C1C-NC	-2.45	1.35	1.39
3	A	1002[A]	HEC	FE-NB	2.42	2.02	1.94
3	A	1002[B]	HEC	FE-NB	2.42	2.02	1.94
3	A	1003	HEC	FE-ND	2.38	2.02	1.94
3	A	1003	HEC	FE-NA	2.35	2.02	1.95
3	A	1003	HEC	C4D-ND	-2.34	1.34	1.38
3	A	1001[A]	HEC	C1C-NC	-2.32	1.35	1.39
3	A	1001[B]	HEC	C1C-NC	-2.32	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002[A]	HEC	C1A-NA	-2.31	1.35	1.39
3	A	1002[B]	HEC	C1A-NA	-2.31	1.35	1.39
3	A	1003	HEC	FE-NB	2.31	2.02	1.94
3	A	1002[A]	HEC	C4A-NA	-2.28	1.35	1.39
3	A	1002[B]	HEC	C4A-NA	-2.28	1.35	1.39
3	A	1001[A]	HEC	C1A-NA	-2.28	1.35	1.39
3	A	1001[B]	HEC	C1A-NA	-2.28	1.35	1.39
3	A	1004	HEC	FE-NB	2.24	2.01	1.94
3	A	1001[A]	HEC	FE-NC	2.22	2.02	1.95
3	A	1001[B]	HEC	FE-NC	2.22	2.02	1.95
3	A	1001[A]	HEC	FE-NA	2.21	2.02	1.95
3	A	1001[B]	HEC	FE-NA	2.21	2.02	1.95
3	A	1004	HEC	C4B-NB	-2.15	1.36	1.40
3	A	1003	HEC	O2A-CGA	-2.14	1.23	1.30
3	A	1002[A]	HEC	FE-NC	2.10	2.02	1.95
3	A	1002[B]	HEC	FE-NC	2.10	2.02	1.95
3	A	1002[A]	HEC	C4B-NB	-2.08	1.36	1.40
3	A	1002[B]	HEC	C4B-NB	-2.08	1.36	1.40
3	A	1001[A]	HEC	CAB-C3B	-2.07	1.45	1.51
3	A	1001[B]	HEC	CAB-C3B	-2.07	1.45	1.51
3	A	1003	HEC	C4B-NB	-2.07	1.36	1.40
3	A	1001[A]	HEC	CBA-CGA	2.02	1.55	1.50
3	A	1001[B]	HEC	CBA-CGA	2.02	1.55	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	HEC	C1D-ND-C4D	3.08	108.85	105.21
3	A	1003	HEC	O1A-CGA-CBA	-2.71	114.51	123.09
3	A	1001[A]	HEC	CMC-C2C-C3C	2.69	131.33	125.62
3	A	1001[B]	HEC	CMC-C2C-C3C	2.69	131.33	125.62
3	A	1003	HEC	CHD-C1D-ND	2.59	127.58	124.37
3	A	1002[A]	HEC	C1B-C2B-C3B	-2.59	104.25	106.98
3	A	1002[B]	HEC	C1B-C2B-C3B	-2.59	104.25	106.98
3	A	1002[A]	HEC	CHB-C4A-NA	2.57	127.25	124.45
3	A	1002[B]	HEC	CHB-C4A-NA	2.57	127.25	124.45
3	A	1002[A]	HEC	C2B-C1B-NB	2.49	112.78	109.90
3	A	1002[B]	HEC	C2B-C1B-NB	2.49	112.78	109.90
3	A	1003	HEC	CMC-C2C-C3C	2.40	130.71	125.62
3	A	1002[A]	HEC	CHA-C1A-NA	2.36	127.02	124.45
3	A	1002[B]	HEC	CHA-C1A-NA	2.36	127.02	124.45
3	A	1002[B]	HEC	O1D-CGD-CBD	-2.31	115.75	123.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001[A]	HEC	C3B-C4B-NB	2.21	112.60	110.17
3	A	1001[B]	HEC	C3B-C4B-NB	2.21	112.60	110.17
3	A	1002[A]	HEC	C4C-NC-C1C	2.17	109.35	105.82
3	A	1002[B]	HEC	C4C-NC-C1C	2.17	109.35	105.82
3	A	1003	HEC	CAC-C3C-C2C	2.14	130.27	126.89
3	A	1003	HEC	C3D-C4D-ND	-2.04	108.38	110.35
3	A	1004	HEC	CMA-C3A-C4A	-2.03	121.15	124.73

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1004	HEC	NA
3	A	1002[A]	HEC	NA
3	A	1002[B]	HEC	NA
3	A	1001[A]	HEC	NA
3	A	1001[B]	HEC	NA
3	A	1003	HEC	NA

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	HEC	C2C-C3C-CAC-CBC
3	A	1003	HEC	C4C-C3C-CAC-CBC
3	A	1001[A]	HEC	C2C-C3C-CAC-CBC
3	A	1001[B]	HEC	C2C-C3C-CAC-CBC
3	A	1003	HEC	C2B-C3B-CAB-CBB
3	A	1001[A]	HEC	C4C-C3C-CAC-CBC
3	A	1001[B]	HEC	C4C-C3C-CAC-CBC
3	A	1002[A]	HEC	C2B-C3B-CAB-CBB
3	A	1002[B]	HEC	C2B-C3B-CAB-CBB
3	A	1004	HEC	C2C-C3C-CAC-CBC
3	A	1003	HEC	C4B-C3B-CAB-CBB
3	A	1004	HEC	C4C-C3C-CAC-CBC
3	A	1002[A]	HEC	C4C-C3C-CAC-CBC
3	A	1002[B]	HEC	C4C-C3C-CAC-CBC
3	A	1001[A]	HEC	C2B-C3B-CAB-CBB
3	A	1001[B]	HEC	C2B-C3B-CAB-CBB
3	A	1002[A]	HEC	C2C-C3C-CAC-CBC
3	A	1002[B]	HEC	C2C-C3C-CAC-CBC
3	A	1002[A]	HEC	C4B-C3B-CAB-CBB
3	A	1002[B]	HEC	C4B-C3B-CAB-CBB
3	A	1001[A]	HEC	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1001[B]	HEC	C4B-C3B-CAB-CBB
3	A	1003	HEC	CAA-CBA-CGA-O1A
3	A	1002[A]	HEC	CAD-CBD-CGD-O2D
3	A	1003	HEC	CAA-CBA-CGA-O2A
3	A	1004	HEC	CAD-CBD-CGD-O2D
3	A	1002[B]	HEC	CAD-CBD-CGD-O2D
3	A	1001[A]	HEC	CAA-CBA-CGA-O2A
3	A	1001[B]	HEC	CAA-CBA-CGA-O2A
3	A	1002[B]	HEC	CAD-CBD-CGD-O1D
3	A	1004	HEC	CAA-CBA-CGA-O2A
3	A	1002[A]	HEC	CAD-CBD-CGD-O1D
3	A	1004	HEC	CAD-CBD-CGD-O1D
3	A	1001[A]	HEC	CAA-CBA-CGA-O1A
3	A	1001[B]	HEC	CAA-CBA-CGA-O1A
3	A	1001[A]	HEC	C3D-CAD-CBD-CGD
3	A	1004	HEC	CAA-CBA-CGA-O1A

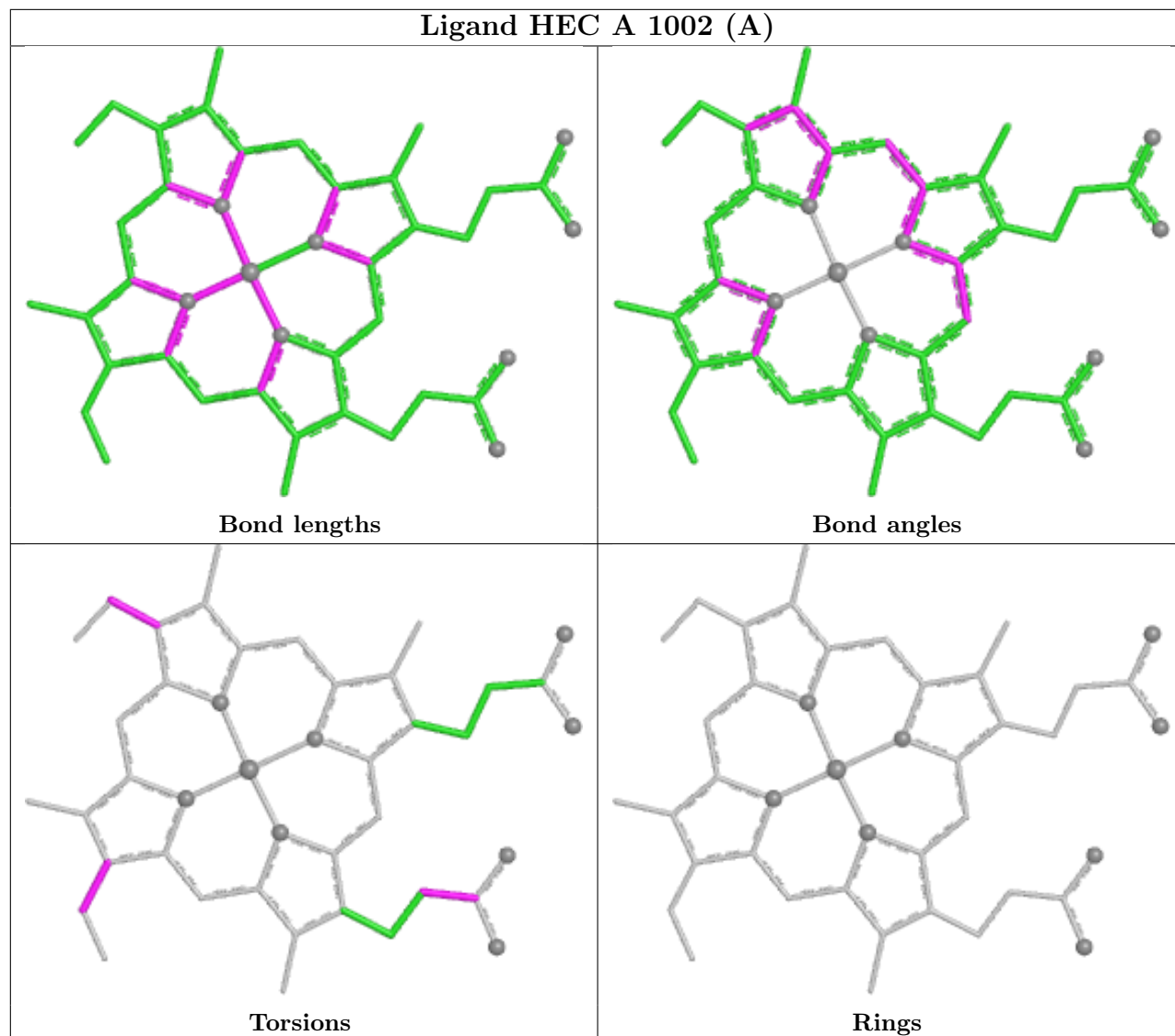
There are no ring outliers.

9 monomers are involved in 18 short contacts:

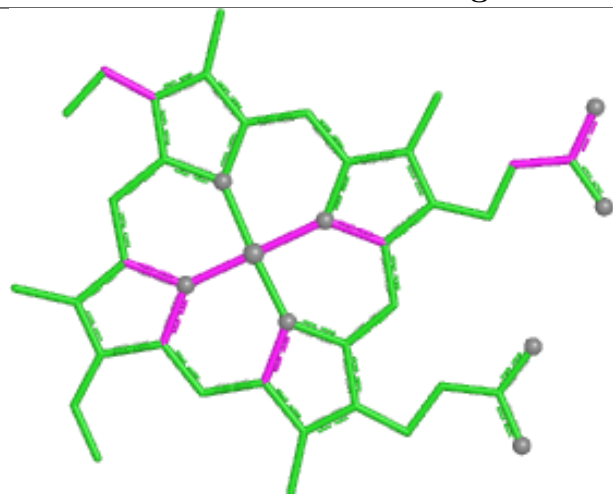
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2009	EOH	2	0
4	A	2015	EOH	5	0
4	A	2011	EOH	1	0
3	A	1001[B]	HEC	1	0
4	A	2004	EOH	1	0
4	A	2002	EOH	2	0
4	A	2014	EOH	3	0
3	A	1003	HEC	1	0
4	A	2017	EOH	4	0

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

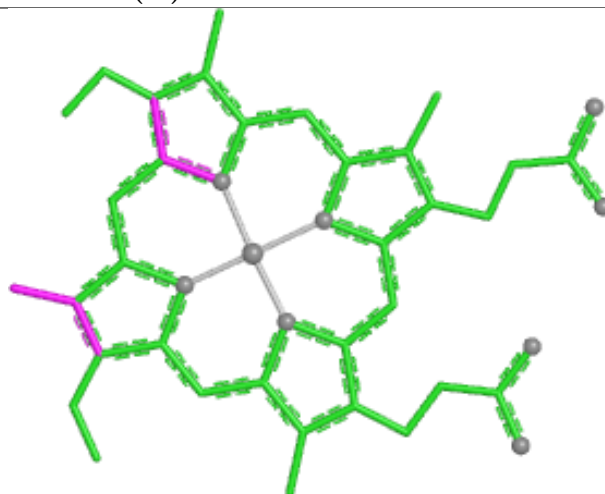
equivalents in the CSD to analyse the geometry.



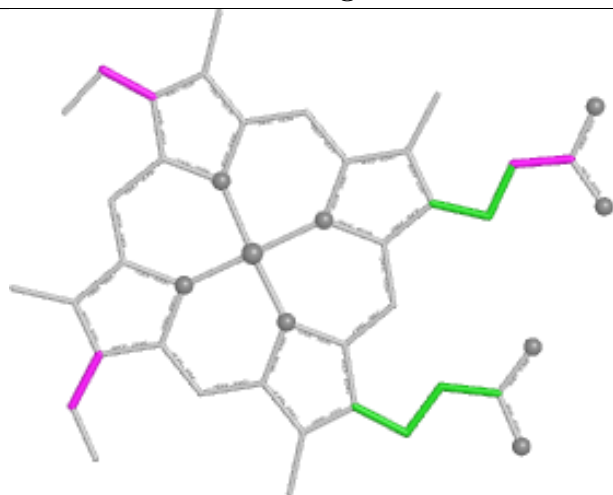
Ligand HEC A 1001 (B)



Bond lengths



Bond angles

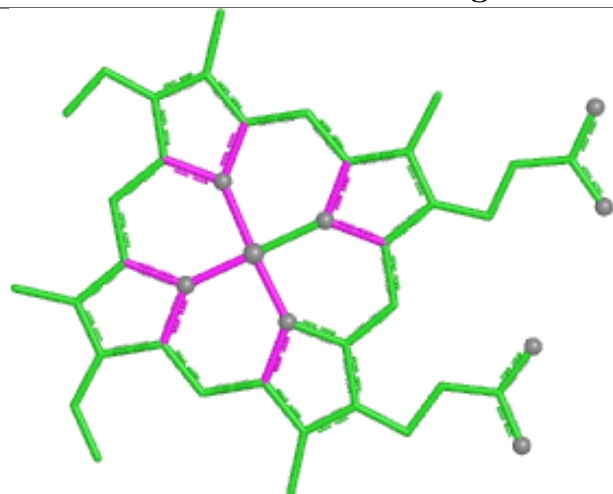


Torsions

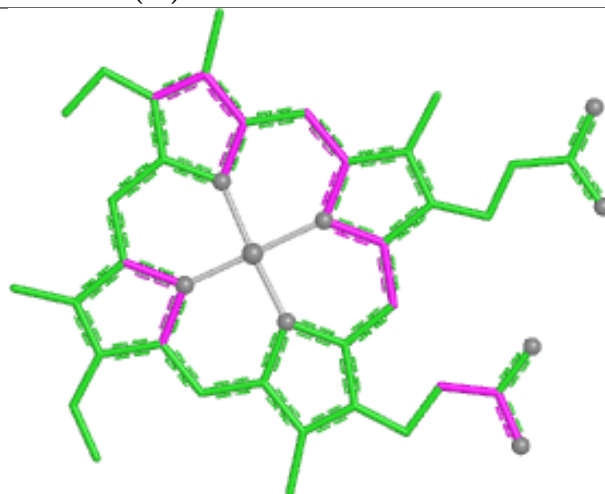


Rings

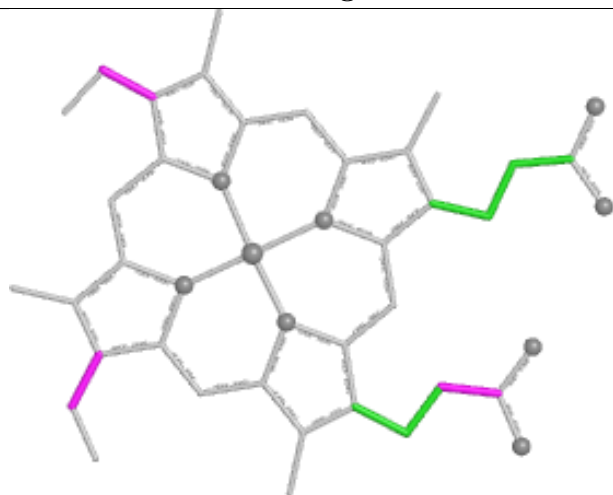
Ligand HEC A 1002 (B)



Bond lengths



Bond angles

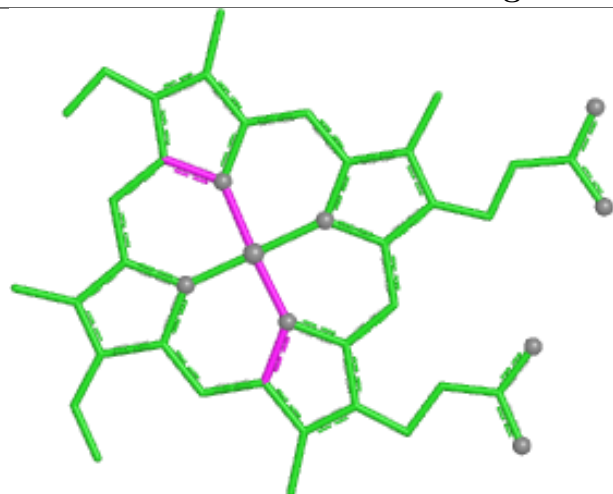


Torsions

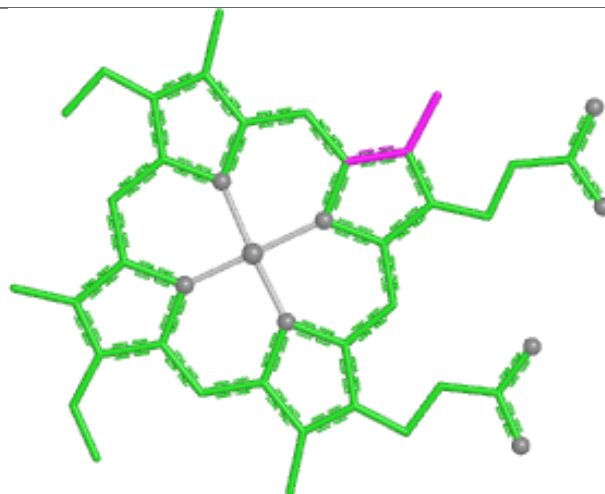


Rings

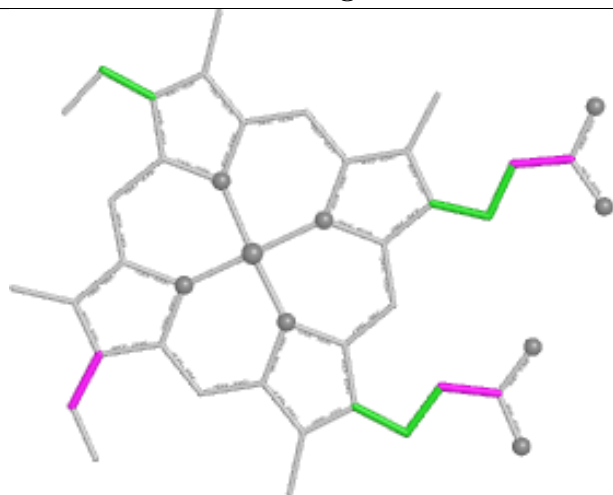
Ligand HEC A 1004



Bond lengths



Bond angles

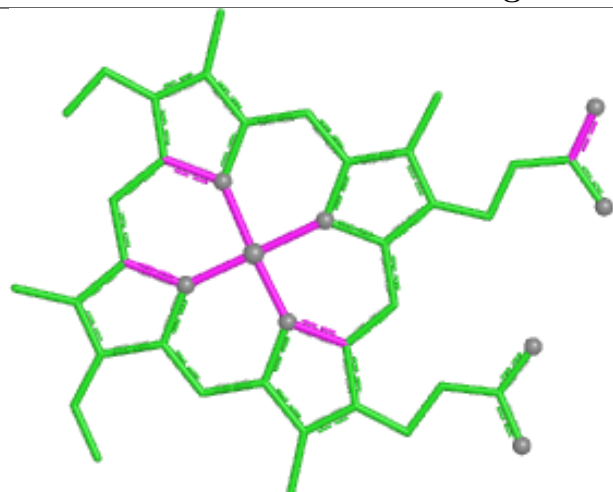


Torsions

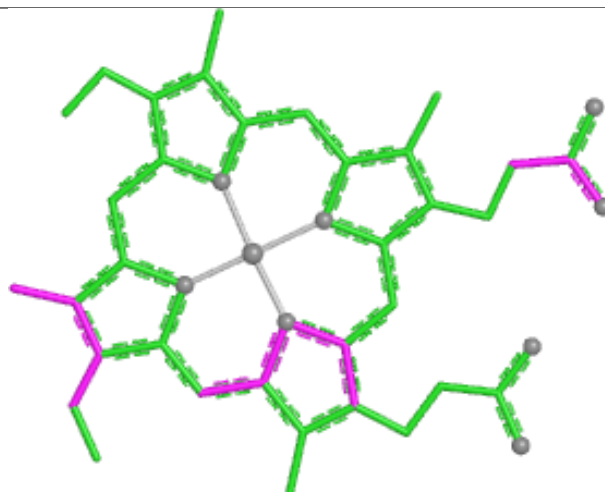


Rings

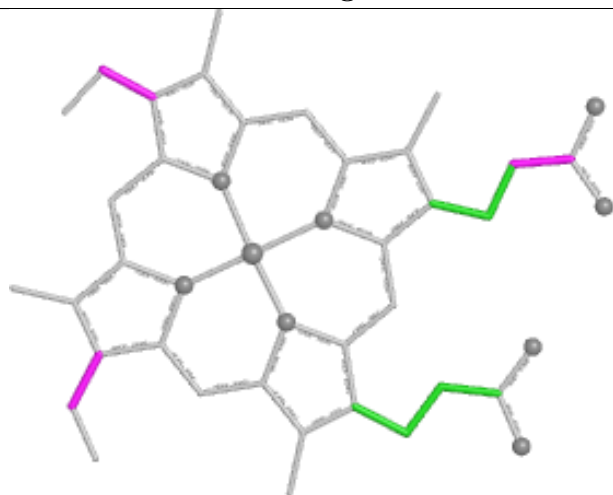
Ligand HEC A 1003



Bond lengths



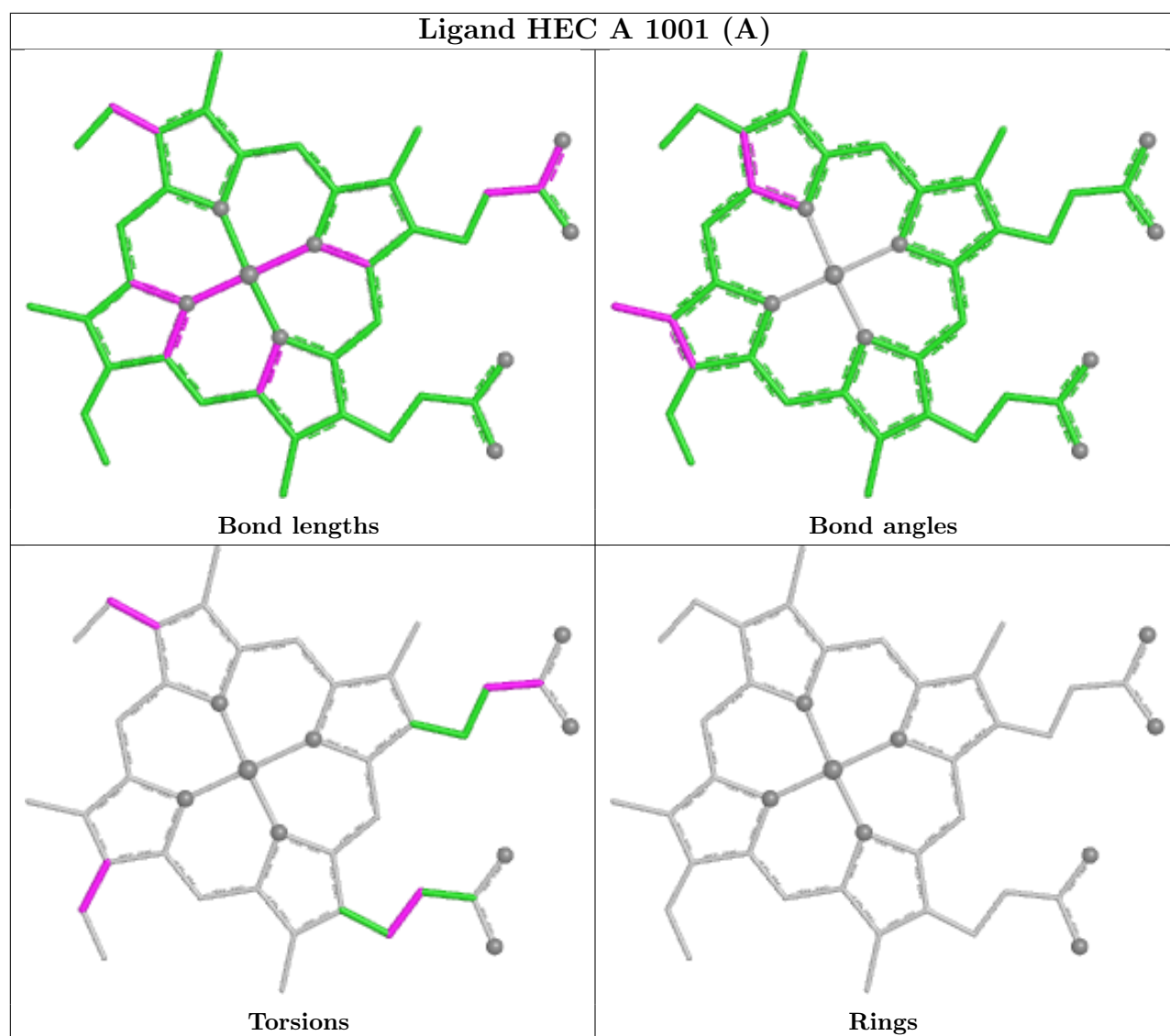
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.