Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 05:49 am BST

PDB ID	:	1E39 / pdb_00001e39
Title	:	Flavocytochrome C3 from Shewanella frigidimarina histidine 365 mutated to alanine
Authors	:	Doherty, M.K.; Pealing, S.L.; Miles, C.S.; Moysey, R.; Taylor, P.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on	:	2000-06-07
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

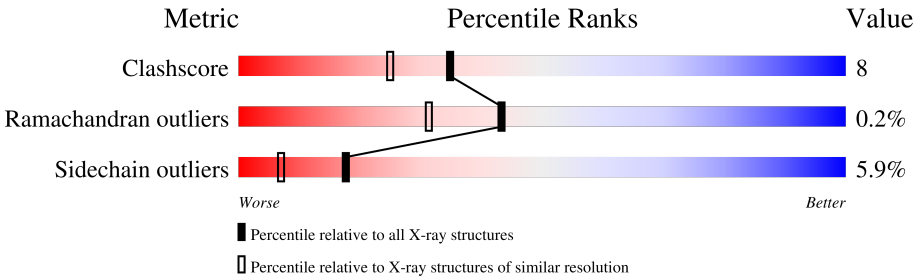
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	83% 14%

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	801	X	-	-	-
2	HEC	A	802	X	-	-	-
2	HEC	A	803	X	-	-	-
2	HEC	A	804	X	-	-	-
4	FUM	A	806	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5057 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.

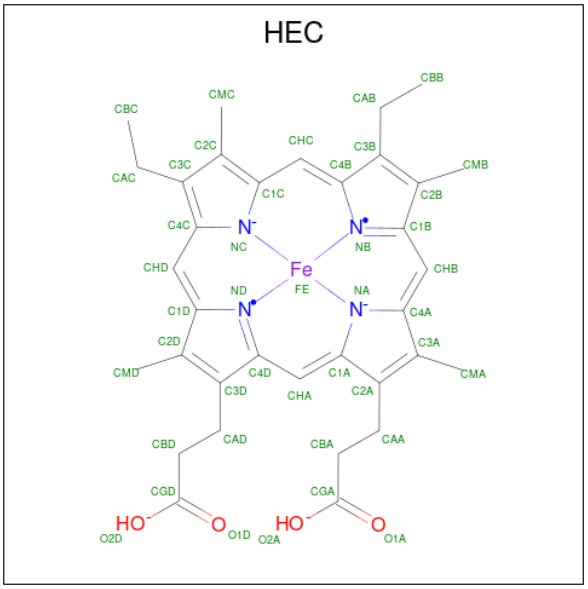
- Molecule 1 is a protein called FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4212	2612	742	833	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	ALA	HIS	engineered mutation	UNP Q07WU7

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



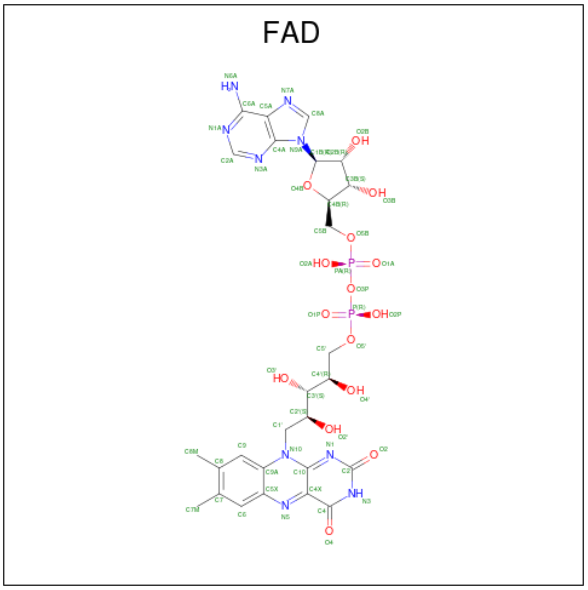
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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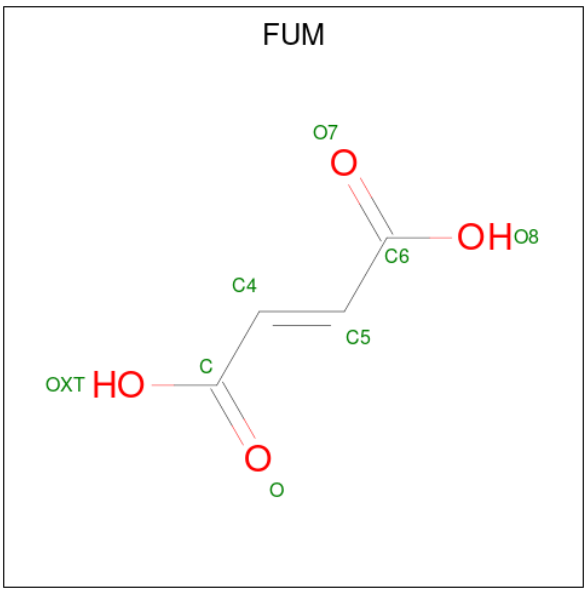
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).

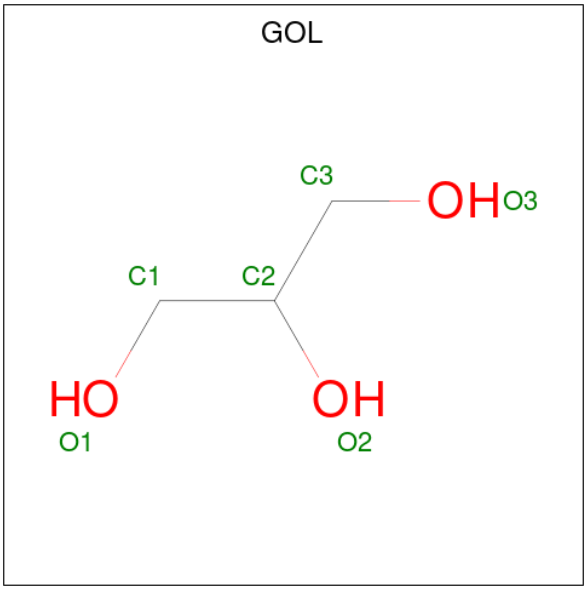


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0

- 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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	605	Total O 605 605	0	0

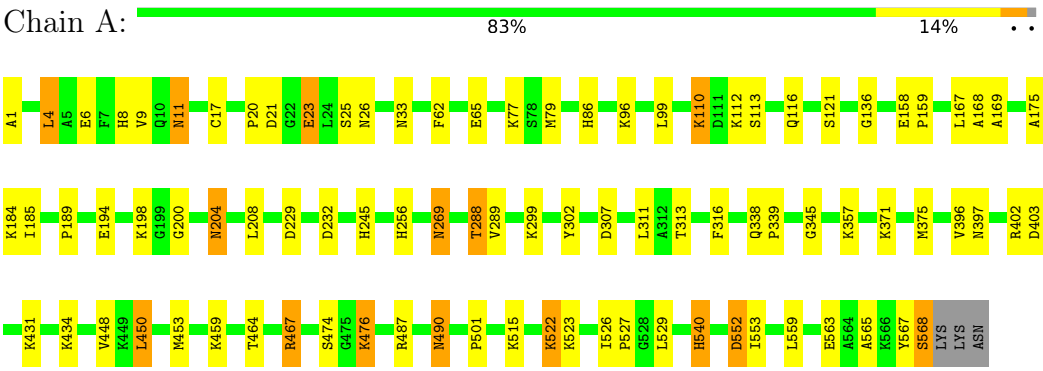
3 Residue-property plots (i)

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: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.57Å 92.17Å 78.49Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	18.00 – 1.80	Depositor
% Data completeness (in resolution range)	86.0 (18.00-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.181 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5057	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FUM, GOL, FAD, NA

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	0.46	0/4281	1.32	18/5787 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	HIS	CA-CB-CG	12.87	126.67	113.80
1	A	526	ILE	CA-C-O	7.78	123.47	119.12
1	A	552	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	567	TYR	CA-C-N	6.99	134.28	121.70
1	A	567	TYR	C-N-CA	6.99	134.28	121.70
1	A	316	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	540	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	62	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	288	THR	CA-C-N	-5.76	112.33	120.75
1	A	288	THR	C-N-CA	-5.76	112.33	120.75
1	A	490	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	232	ASP	CA-C-N	-5.18	115.96	123.11
1	A	232	ASP	C-N-CA	-5.18	115.96	123.11
1	A	175	ALA	CA-C-N	5.13	130.94	121.70
1	A	175	ALA	C-N-CA	5.13	130.94	121.70
1	A	33	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	526	ILE	O-C-N	-5.06	117.96	121.55
1	A	269	ASN	CA-CB-CG	-5.01	107.58	112.60

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	4212	0	4150	66	0
2	A	172	0	120	2	0
3	A	53	0	31	1	0
4	A	8	0	1	2	0
5	A	1	0	0	0	0
6	A	6	0	8	1	0
7	A	605	0	0	18	0
All	All	5057	0	4310	66	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 8.

All (66) 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:431:LYS:HD3	1:A:434:LYS:HD3	1.48	0.95
1:A:204:ASN:HD22	1:A:204:ASN:H	1.29	0.79
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.47	0.77
1:A:229:ASP:H	1:A:256:HIS:HE1	1.33	0.77
1:A:112:LYS:HD2	7:A:2207:HOH:O	1.84	0.75
1:A:450:LEU:HD23	1:A:453:MET:HE2	1.69	0.74
1:A:9:VAL:HG13	7:A:2020:HOH:O	1.89	0.73
1:A:65:GLU:HG2	7:A:2108:HOH:O	1.92	0.67
1:A:431:LYS:HA	1:A:434:LYS:HD2	1.77	0.67
1:A:1:ALA:HA	1:A:6:GLU:OE2	1.99	0.63
1:A:21:ASP:OD1	1:A:23:GLU:HB3	1.99	0.63
1:A:229:ASP:H	1:A:256:HIS:CE1	2.15	0.62
1:A:189:PRO:HG2	7:A:2284:HOH:O	1.99	0.62
1:A:396:VAL:HG22	7:A:2465:HOH:O	2.01	0.61
1:A:371:LYS:HD2	6:A:850:GOL:H11	1.83	0.60
1:A:11:ASN:HB3	7:A:2017:HOH:O	2.01	0.60
1:A:17:CYS:HB3	7:A:2025:HOH:O	2.02	0.58
1:A:20:PRO:HD3	7:A:2052:HOH:O	2.04	0.57
1:A:375:MET:HE3	4:A:806:FUM:O8	2.05	0.56
1:A:565:ALA:O	1:A:568:SER:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:HA	7:A:2390:HOH:O	2.06	0.56
1:A:515:LYS:HE3	1:A:563:GLU:OE1	2.06	0.55
1:A:112:LYS:O	1:A:116:GLN:HG3	2.08	0.54
1:A:450:LEU:HD23	1:A:453:MET:CE	2.38	0.53
1:A:4:LEU:HD22	1:A:8:HIS:CE1	2.44	0.53
1:A:476:LYS:HG2	1:A:476:LYS:O	2.08	0.52
1:A:23:GLU:O	1:A:23:GLU:HG2	2.06	0.51
1:A:110:LYS:N	1:A:110:LYS:HD2	2.22	0.51
1:A:540:HIS:HD2	7:A:2573:HOH:O	1.93	0.51
1:A:77:LYS:HG2	7:A:2128:HOH:O	2.10	0.51
1:A:501:PRO:HD2	7:A:2548:HOH:O	2.11	0.51
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.93	0.50
1:A:136:GLY:HA3	1:A:553:ILE:HD12	1.95	0.49
1:A:20:PRO:HD2	7:A:2032:HOH:O	2.13	0.48
1:A:183:LYS:O	1:A:185:ILE:HD12	2.13	0.48
1:A:302:TYR:HA	7:A:2384:HOH:O	2.13	0.48
1:A:431:LYS:HD3	1:A:434:LYS:CD	2.34	0.48
1:A:523:LYS:HE3	7:A:2562:HOH:O	2.14	0.47
1:A:204:ASN:H	1:A:204:ASN:ND2	2.03	0.47
1:A:168:ALA:HA	3:A:805:FAD:N5	2.29	0.47
1:A:540:HIS:HE1	1:A:552:ASP:OD2	1.98	0.46
1:A:4:LEU:HD22	1:A:8:HIS:HE1	1.81	0.46
1:A:397:ASN:HB3	7:A:2465:HOH:O	2.16	0.46
1:A:357:LYS:HE3	1:A:357:LYS:HB2	1.78	0.45
1:A:169:ALA:HB1	1:A:431:LYS:HE3	1.97	0.45
1:A:522:LYS:O	1:A:523:LYS:HB2	2.16	0.45
1:A:77:LYS:NZ	7:A:2129:HOH:O	2.50	0.45
1:A:79:MET:HE2	1:A:96:LYS:HE3	1.99	0.45
1:A:403:ASP:N	1:A:403:ASP:OD1	2.50	0.44
1:A:422:ASP:CG	1:A:424:SER:H	2.27	0.43
1:A:553:ILE:HD13	1:A:553:ILE:HG21	1.80	0.43
1:A:169:ALA:CB	1:A:431:LYS:HE3	2.48	0.43
1:A:79:MET:CE	1:A:96:LYS:HE3	2.49	0.43
1:A:229:ASP:N	1:A:256:HIS:HE1	2.09	0.42
1:A:402:ARG:HH22	4:A:806:FUM:C6	2.31	0.42
1:A:467:ARG:NE	7:A:2522:HOH:O	2.52	0.42
1:A:158:GLU:HB3	1:A:159:PRO:HD2	2.01	0.42
1:A:313:THR:OG1	1:A:345:GLY:HA3	2.20	0.42
1:A:338:GLN:HB2	1:A:339:PRO:HD2	2.01	0.42
1:A:167:LEU:HD11	2:A:804:HEC:HBC2	2.02	0.42
1:A:474:SER:O	1:A:476:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HB	1:A:527:PRO:HB2	2.02	0.41
1:A:311:LEU:HD21	1:A:529:LEU:HD11	2.01	0.41
1:A:474:SER:OG	1:A:476:LYS:NZ	2.52	0.41
1:A:25:SER:O	1:A:26:ASN:HB3	2.20	0.41
1:A:167:LEU:CD1	2:A:804:HEC:HBC2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	566/571 (99%)	551 (97%)	14 (2%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER

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	441/444 (99%)	415 (94%)	26 (6%)	18 7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	ASN
1	A	23	GLU
1	A	99	LEU
1	A	110	LYS
1	A	121	SER
1	A	183	LYS
1	A	184	LYS
1	A	194	GLU
1	A	198	LYS
1	A	204	ASN
1	A	208	LEU
1	A	269	ASN
1	A	289	VAL
1	A	299	LYS
1	A	448	VAL
1	A	450	LEU
1	A	459	LYS
1	A	464	THR
1	A	467	ARG
1	A	476	LYS
1	A	487	ARG
1	A	490	ASN
1	A	522	LYS
1	A	559	LEU
1	A	568	SER

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	35	GLN
1	A	56	ASN
1	A	91	ASN
1	A	116	GLN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	275	ASN
1	A	490	ASN
1	A	540	HIS

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)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	A	802	1	50,50,50	1.40	4 (8%)	68,82,82	1.31	8 (11%)
3	FAD	A	805	-	56,58,58	1.29	6 (10%)	81,89,89	1.14	7 (8%)
2	HEC	A	804	1	50,50,50	1.21	3 (6%)	68,82,82	0.77	0
4	FUM	A	806	-	7,7,7	2.74	4 (57%)	8,8,8	1.53	1 (12%)
2	HEC	A	803	1	50,50,50	1.39	5 (10%)	68,82,82	1.37	9 (13%)
6	GOL	A	850	-	5,5,5	0.35	0	5,5,5	0.57	0
2	HEC	A	801	1	50,50,50	1.23	4 (8%)	68,82,82	1.15	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	802	1	1/1/3/7	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	805	-	-	7/34/50/50	0/6/6/6
2	HEC	A	804	1	1/1/3/7	7/14/54/54	-
4	FUM	A	806	-	-	3/5/5/5	-
2	HEC	A	803	1	1/1/3/7	8/14/54/54	-
6	GOL	A	850	-	-	3/4/4/4	-
2	HEC	A	801	1	1/1/3/7	6/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	HEC	CAB-C3B	-4.61	1.39	1.51
2	A	802	HEC	CAC-C3C	-4.48	1.39	1.51
2	A	802	HEC	FE-NB	4.41	2.08	1.94
2	A	803	HEC	CAC-C3C	-4.32	1.40	1.51
2	A	801	HEC	CAB-C3B	-4.30	1.40	1.51
4	A	806	FUM	O-C	4.30	1.34	1.23
2	A	802	HEC	CAB-C3B	-4.26	1.40	1.51
2	A	804	HEC	CAB-C3B	-4.23	1.40	1.51
2	A	804	HEC	CAC-C3C	-4.01	1.40	1.51
2	A	801	HEC	CAC-C3C	-3.91	1.41	1.51
4	A	806	FUM	O7-C6	3.67	1.32	1.23
3	A	805	FAD	C9-C8	3.61	1.44	1.39
3	A	805	FAD	C2'-C3'	3.45	1.60	1.53
3	A	805	FAD	C6-C5X	3.36	1.45	1.40
4	A	806	FUM	OXT-C	-3.34	1.21	1.30
2	A	801	HEC	FE-NB	3.12	2.04	1.94
2	A	803	HEC	FE-NC	3.06	2.05	1.95
4	A	806	FUM	O8-C6	-2.97	1.22	1.30
3	A	805	FAD	C1'-C2'	-2.88	1.48	1.52
3	A	805	FAD	O4-C4	-2.76	1.18	1.23
2	A	802	HEC	FE-NC	-2.72	1.85	1.95
2	A	803	HEC	FE-NA	2.52	2.03	1.95
2	A	804	HEC	FE-NB	2.47	2.02	1.94
2	A	803	HEC	FE-ND	-2.37	1.87	1.94
3	A	805	FAD	C5'-C4'	2.09	1.54	1.51
2	A	801	HEC	FE-ND	2.00	2.01	1.94

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	805	FAD	O5'-C5'-C4'	-5.94	93.49	109.36

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	803	HEC	CHB-C4A-NA	-3.57	120.58	124.44
2	A	803	HEC	CHA-C1A-NA	-3.54	120.61	124.44
2	A	802	HEC	CBB-CAB-C3B	3.53	122.16	112.43
2	A	803	HEC	CAB-C3B-C4B	3.13	128.88	124.81
2	A	802	HEC	CBC-CAC-C3C	3.02	120.75	112.43
2	A	801	HEC	CBB-CAB-C3B	3.01	120.74	112.43
2	A	802	HEC	CHB-C1B-C2B	2.94	129.58	124.98
2	A	803	HEC	CHA-C4D-C3D	-2.80	120.72	124.84
2	A	802	HEC	CHB-C1B-NB	-2.77	121.40	124.42
3	A	805	FAD	O4B-C1B-C2B	-2.74	100.66	106.64
4	A	806	FUM	C5-C4-C	-2.67	113.55	127.26
2	A	802	HEC	CHA-C1A-C2A	-2.66	120.62	124.94
2	A	803	HEC	CBB-CAB-C3B	2.64	119.71	112.43
3	A	805	FAD	O4'-C4'-C3'	-2.61	102.75	109.10
2	A	801	HEC	CHA-C4D-ND	-2.53	121.67	124.42
2	A	802	HEC	C4B-NB-C1B	2.47	107.62	105.07
2	A	801	HEC	CHA-C1A-NA	2.44	127.08	124.44
2	A	803	HEC	CBC-CAC-C3C	2.43	119.14	112.43
2	A	801	HEC	CHA-C1A-C2A	-2.35	121.12	124.94
2	A	801	HEC	CBC-CAC-C3C	2.32	118.83	112.43
3	A	805	FAD	O2'-C2'-C3'	-2.32	103.47	109.10
2	A	802	HEC	CBA-CAA-C2A	2.27	118.92	112.63
3	A	805	FAD	C6-C5X-C9A	2.25	122.13	118.94
2	A	801	HEC	C4C-NC-C1C	-2.19	103.20	105.35
3	A	805	FAD	O2P-P-O1P	2.18	123.02	112.24
2	A	803	HEC	C4B-NB-C1B	-2.14	102.86	105.07
2	A	802	HEC	C4C-NC-C1C	-2.12	103.27	105.35
2	A	803	HEC	C3D-C4D-ND	2.12	112.41	110.36
2	A	803	HEC	CMC-C2C-C3C	2.10	130.16	125.61
3	A	805	FAD	O2A-PA-O1A	2.03	122.26	112.24

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	HEC	NA
2	A	802	HEC	NA
2	A	803	HEC	NA
2	A	804	HEC	NA

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	HEC	C3A-C2A-CAA-CBA
3	A	805	FAD	C2'-C3'-C4'-O4'
3	A	805	FAD	C2'-C3'-C4'-C5'
3	A	805	FAD	O3'-C3'-C4'-C5'
2	A	802	HEC	C2B-C3B-CAB-CBB
2	A	801	HEC	C4D-C3D-CAD-CBD
4	A	806	FUM	C-C4-C5-C6
3	A	805	FAD	O3'-C3'-C4'-O4'
2	A	802	HEC	C4C-C3C-CAC-CBC
2	A	803	HEC	C2C-C3C-CAC-CBC
2	A	801	HEC	C4C-C3C-CAC-CBC
4	A	806	FUM	C4-C5-C6-O8
4	A	806	FUM	C4-C5-C6-O7
2	A	803	HEC	C2B-C3B-CAB-CBB
2	A	802	HEC	C2C-C3C-CAC-CBC
2	A	803	HEC	C4C-C3C-CAC-CBC
2	A	802	HEC	C4B-C3B-CAB-CBB
2	A	801	HEC	C2B-C3B-CAB-CBB
6	A	850	GOL	O1-C1-C2-O2
2	A	804	HEC	C4C-C3C-CAC-CBC
6	A	850	GOL	O1-C1-C2-C3
6	A	850	GOL	O2-C2-C3-O3
2	A	802	HEC	CAD-CBD-CGD-O2D
2	A	804	HEC	C2B-C3B-CAB-CBB
2	A	803	HEC	CAA-CBA-CGA-O2A
2	A	804	HEC	CAA-CBA-CGA-O2A
2	A	804	HEC	CAA-CBA-CGA-O1A
2	A	803	HEC	CAA-CBA-CGA-O1A
2	A	802	HEC	CAD-CBD-CGD-O1D
2	A	801	HEC	C4B-C3B-CAB-CBB
3	A	805	FAD	P-O3P-PA-O1A
2	A	803	HEC	C3D-CAD-CBD-CGD
2	A	801	HEC	CAD-CBD-CGD-O1D
2	A	803	HEC	C4B-C3B-CAB-CBB
2	A	804	HEC	CAD-CBD-CGD-O1D
2	A	801	HEC	CAD-CBD-CGD-O2D
3	A	805	FAD	P-O3P-PA-O2A
2	A	804	HEC	C2A-CAA-CBA-CGA
3	A	805	FAD	O4B-C4B-C5B-O5B
2	A	804	HEC	CAD-CBD-CGD-O2D

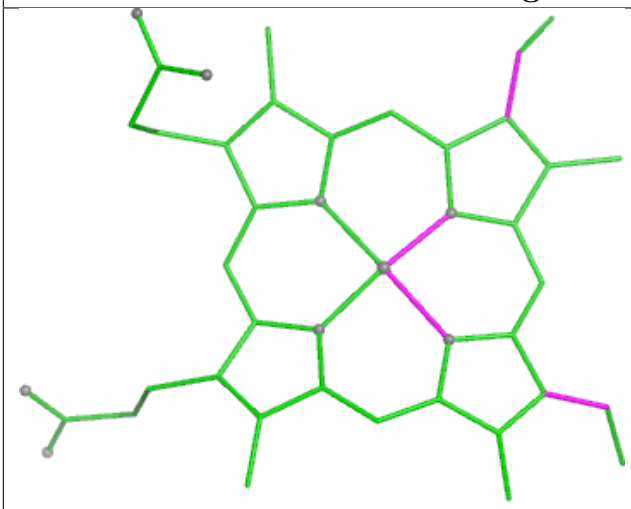
There are no ring outliers.

4 monomers are involved in 6 short contacts:

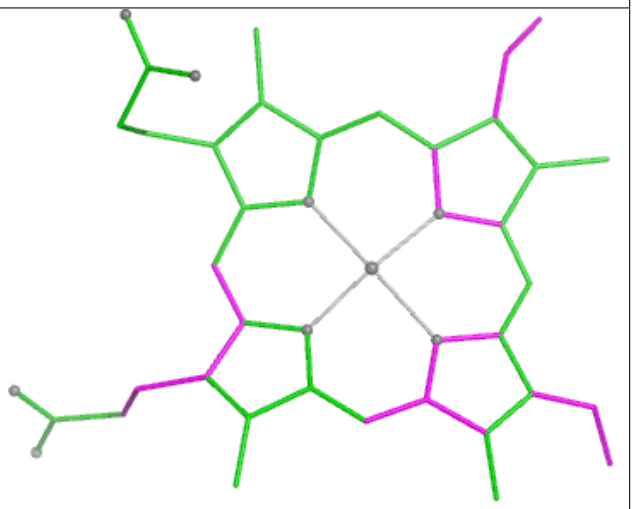
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	FAD	1	0
2	A	804	HEC	2	0
4	A	806	FUM	2	0
6	A	850	GOL	1	0

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

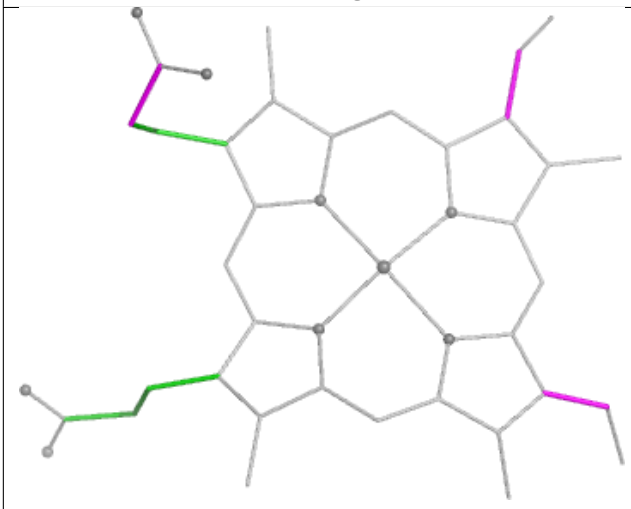
Ligand HEC A 802



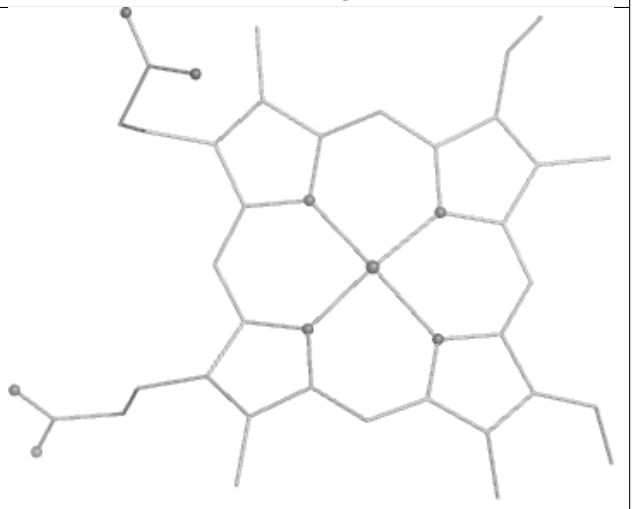
Bond lengths



Bond angles

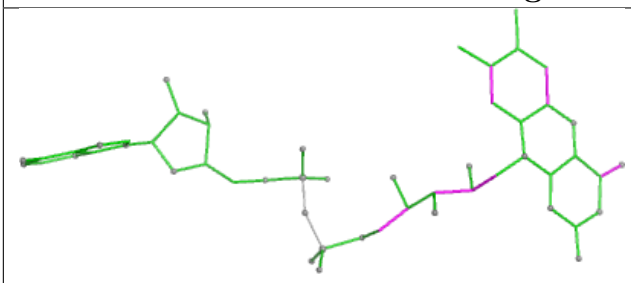


Torsions

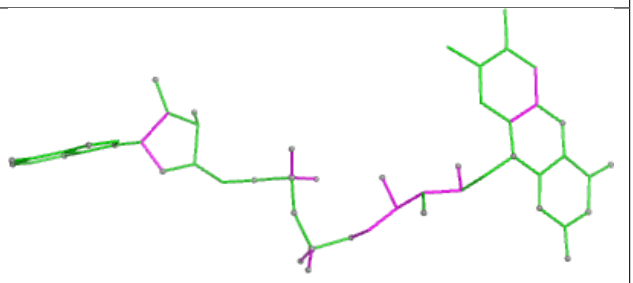


Rings

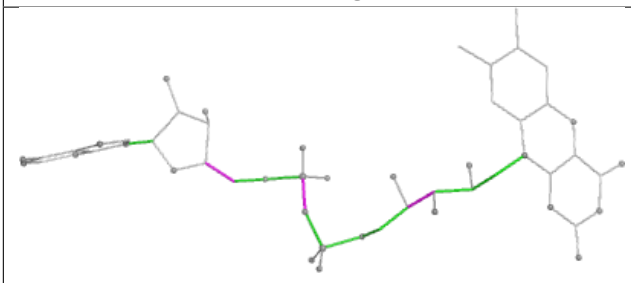
Ligand FAD A 805



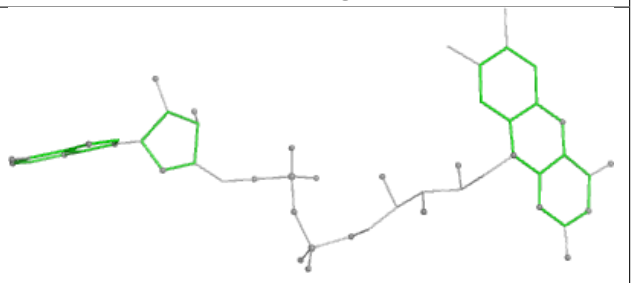
Bond lengths



Bond angles

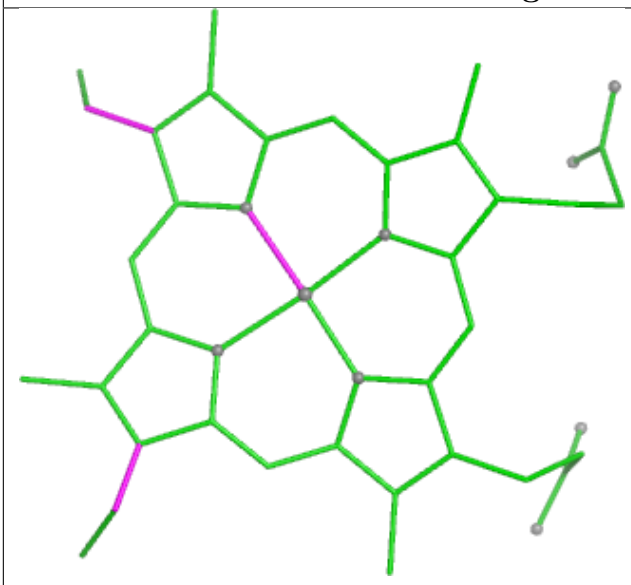


Torsions

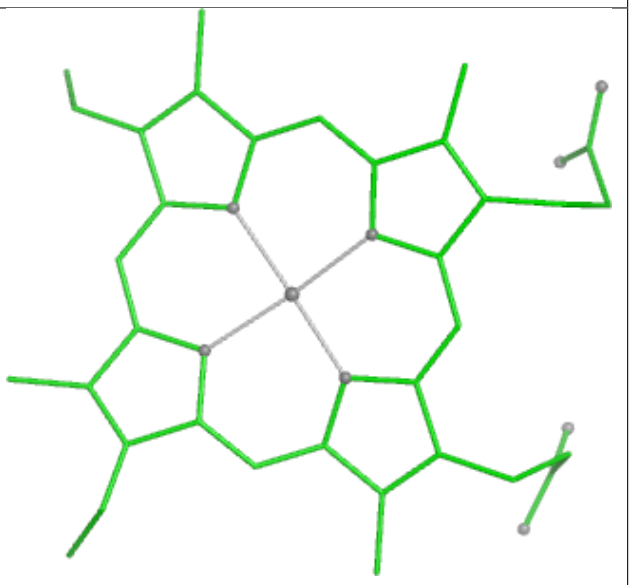


Rings

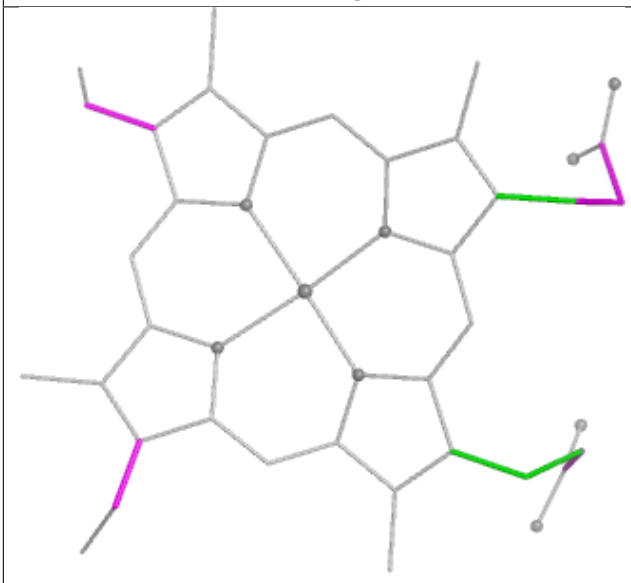
Ligand HEC A 804



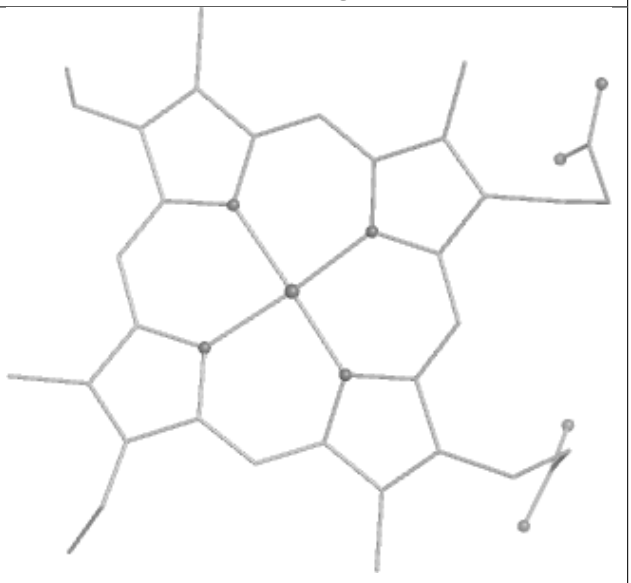
Bond lengths



Bond angles

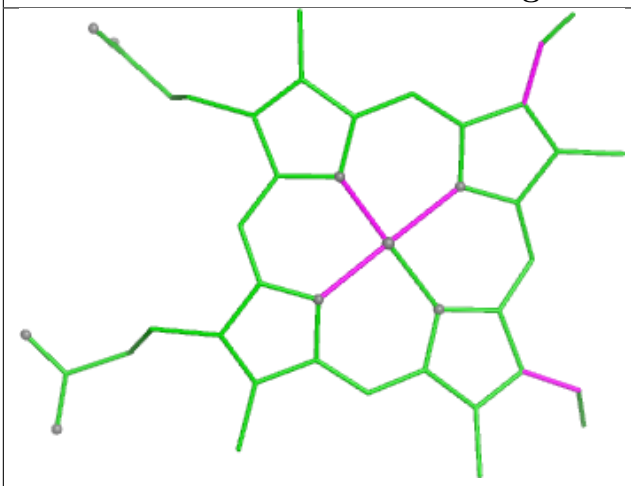


Torsions

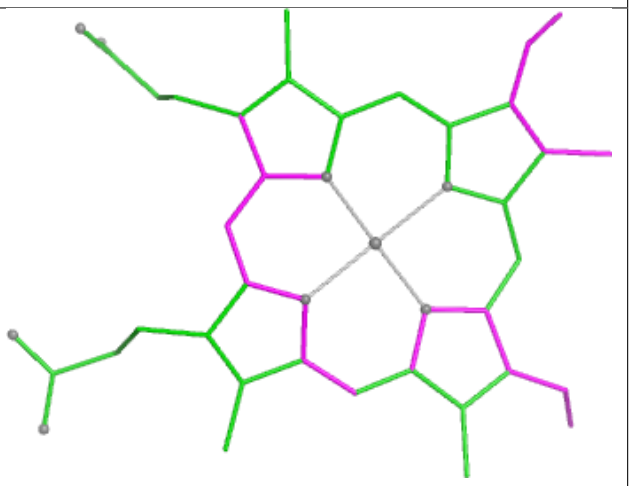


Rings

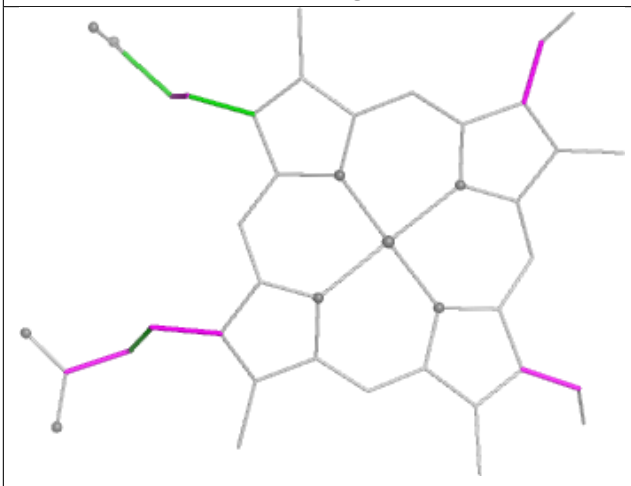
Ligand HEC A 803



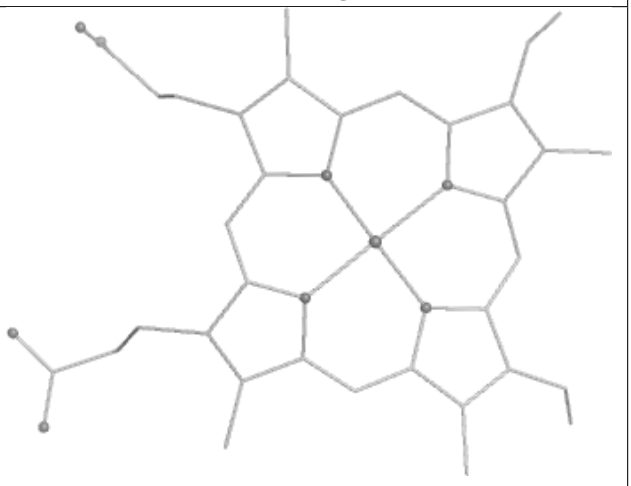
Bond lengths



Bond angles

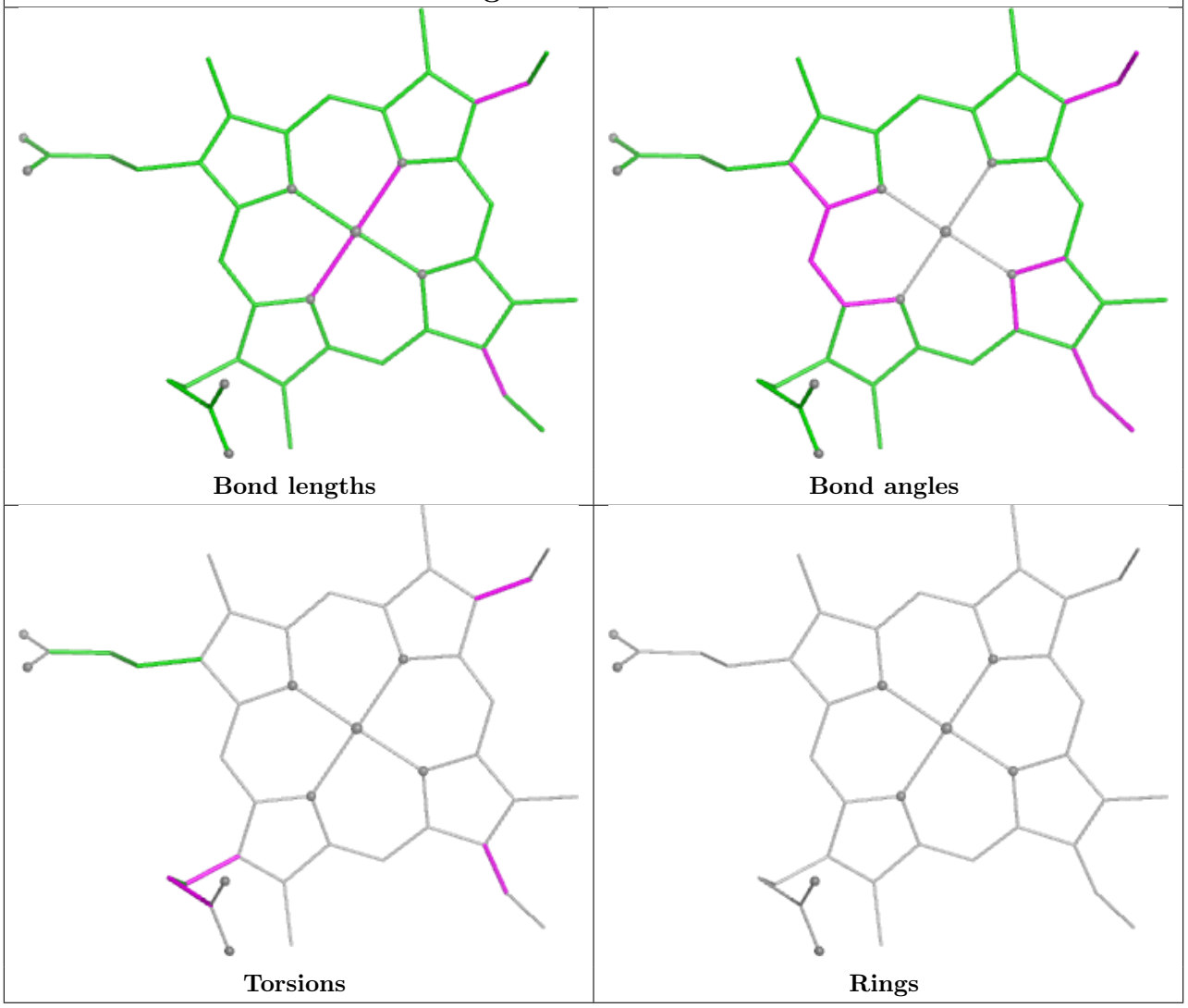


Torsions



Rings

Ligand HEC A 801



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.