Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:19 PM EDT

PDB ID	:	2B7S / pdb_00002b7s
Title	:	R381K mutant of flavocytochrome c3
Authors	:	Pankhurst, K.L.; Mowat, C.G.; Rothery, E.L.; Miles, C.S.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on	:	2005-10-05
Resolution	:	2.12 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 (i) 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 (i)) were used in the production of this report:

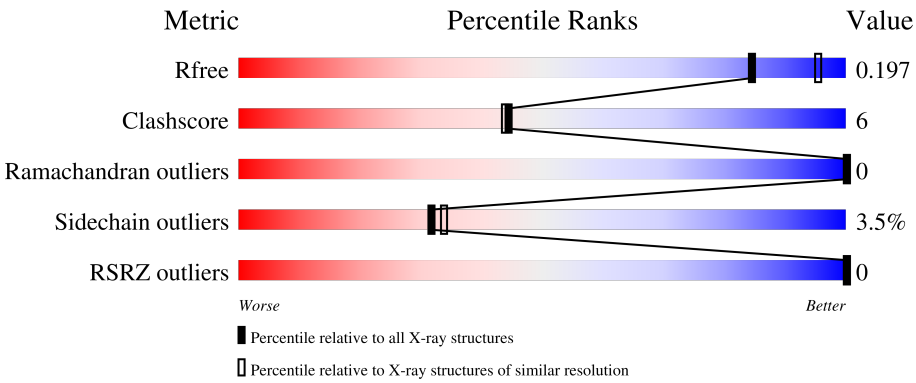
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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% 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	571	90% 9% ••

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	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	A	802	X	-	-	-
3	HEC	A	803	X	-	-	-
3	HEC	A	804	X	-	-	-
4	FAD	A	1805	X	-	-	-
5	FUM	A	1806	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5192 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
			Total	C	N	O	S			
1	A	568	4185	2601	736	823	25	0	0	0

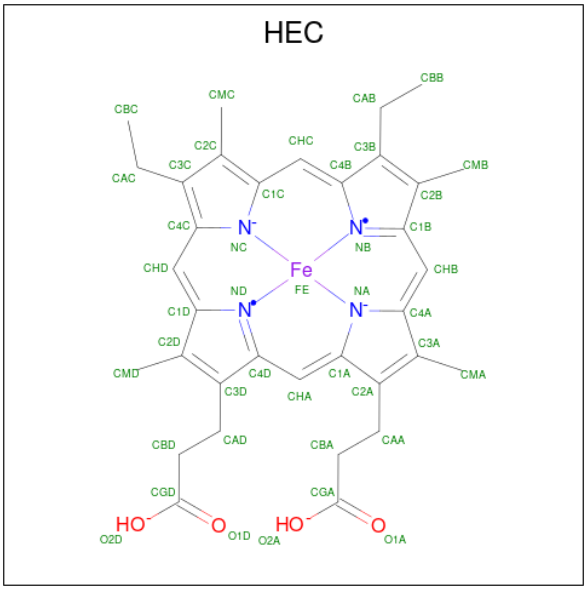
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LYS	ARG	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

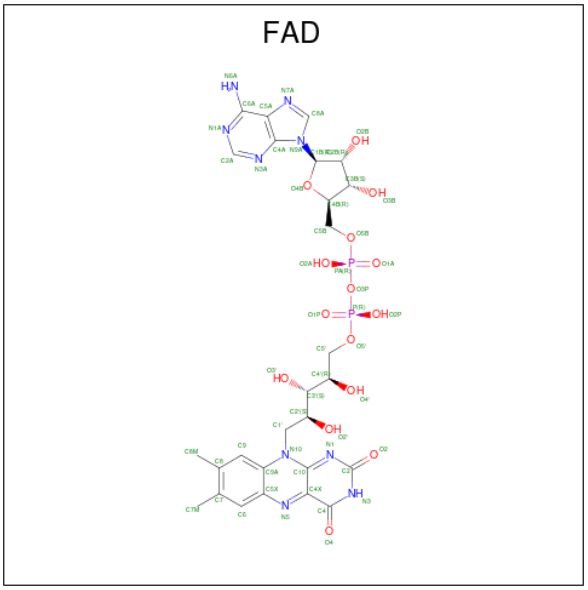
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



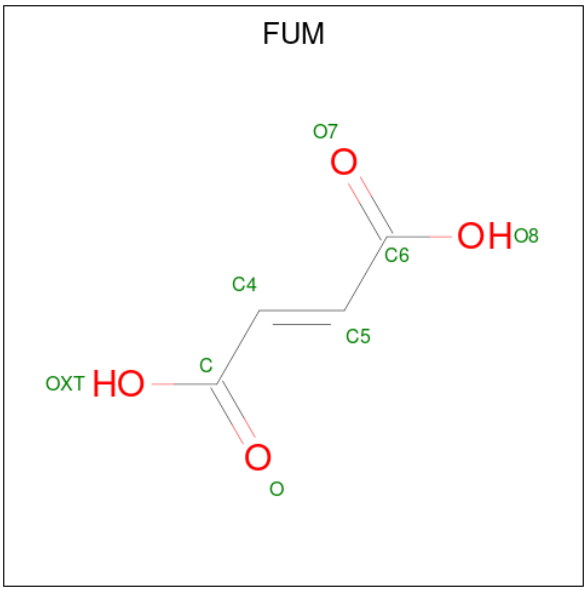
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



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

- Molecule 6 is water.

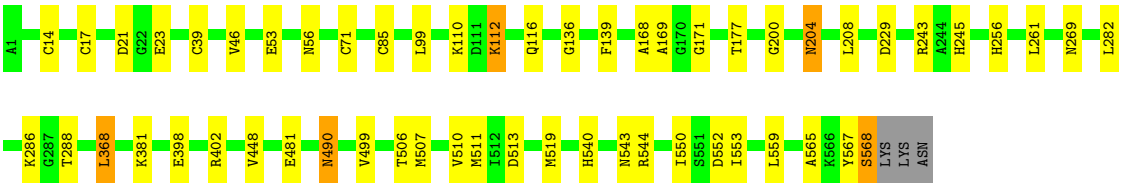
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	773	773	773	0	0

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 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: Fumarate reductase flavoprotein subunit

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.23Å 91.36Å 78.19Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	35.00 – 2.12 35.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.00-2.12) 98.5 (35.00-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.144 , 0.197 0.145 , 0.197	Depositor DCC
R_{free} test set	1763 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.95	2/4255 (0.0%)	1.00	1/5757 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	THR	CA-CB	5.45	1.60	1.53
1	A	169	ALA	C-O	5.12	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	GLY	N-CA-C	6.81	119.83	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	567	TYR	Peptide

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	4185	0	4098	51	0
2	A	1	0	0	0	0
3	A	172	0	124	21	0
4	A	53	0	28	2	0
5	A	8	0	1	1	0
6	A	773	0	0	4	0
All	All	5192	0	4251	52	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 6.

All (52) 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:14:CYS:SG	3:A:801:HEC:CAB	2.05	1.42
1:A:17:CYS:SG	3:A:801:HEC:CAC	2.15	1.35
1:A:71:CYS:SG	3:A:803:HEC:CAC	2.12	1.35
1:A:17:CYS:SG	3:A:801:HEC:HAC	1.70	1.30
1:A:85:CYS:SG	3:A:804:HEC:CAC	2.36	1.13
1:A:71:CYS:SG	3:A:803:HEC:HAC	1.88	1.13
1:A:39:CYS:SG	3:A:802:HEC:CAC	2.43	1.07
1:A:39:CYS:SG	3:A:802:HEC:HBC3	2.07	0.95
1:A:204:ASN:HD22	1:A:204:ASN:H	1.16	0.93
1:A:229:ASP:H	1:A:256:HIS:HE1	1.16	0.90
1:A:39:CYS:SG	3:A:802:HEC:CBC	2.60	0.89
1:A:17:CYS:HG	3:A:801:HEC:HAC	1.41	0.83
1:A:229:ASP:H	1:A:256:HIS:CE1	1.97	0.82
1:A:402:ARG:HH22	5:A:1806:FUM:C4	1.98	0.77
1:A:85:CYS:SG	3:A:804:HEC:HAC	2.26	0.76
1:A:71:CYS:SG	3:A:803:HEC:CBC	2.77	0.73
1:A:368:LEU:HB2	6:A:2391:HOH:O	1.87	0.73
1:A:204:ASN:H	1:A:204:ASN:ND2	1.87	0.68
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.78	0.66
1:A:381:LYS:HD2	1:A:398:GLU:HB3	1.79	0.63
1:A:17:CYS:SG	3:A:801:HEC:C3C	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:CYS:SG	3:A:802:HEC:C3C	2.86	0.63
1:A:229:ASP:N	1:A:256:HIS:HE1	1.92	0.63
1:A:71:CYS:SG	3:A:803:HEC:C3C	2.88	0.59
1:A:14:CYS:SG	3:A:801:HEC:C3B	2.89	0.58
1:A:14:CYS:SG	3:A:801:HEC:CBB	2.87	0.57
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.71	0.55
1:A:85:CYS:SG	3:A:804:HEC:C3C	2.95	0.55
1:A:490:ASN:HD22	1:A:490:ASN:C	2.17	0.52
1:A:168:ALA:HA	4:A:1805:FAD:N5	2.25	0.51
1:A:85:CYS:SG	3:A:804:HEC:CBC	2.96	0.50
1:A:21:ASP:OD1	1:A:23:GLU:CG	2.61	0.49
1:A:481:GLU:HB2	6:A:2464:HOH:O	2.14	0.47
1:A:204:ASN:ND2	1:A:204:ASN:N	2.58	0.47
1:A:565:ALA:O	1:A:568:SER:HA	2.15	0.47
1:A:53:GLU:OE2	6:A:1981:HOH:O	2.20	0.47
1:A:513:ASP:HB2	6:A:1985:HOH:O	2.15	0.46
1:A:540:HIS:HE1	1:A:552:ASP:OD2	2.00	0.45
1:A:46:VAL:HG21	3:A:803:HEC:HMB2	1.98	0.44
1:A:550:ILE:HG12	4:A:1805:FAD:C2	2.48	0.44
3:A:804:HEC:HHA	3:A:804:HEC:HBD2	1.99	0.44
1:A:243:ARG:O	1:A:245:HIS:HD2	2.01	0.43
1:A:490:ASN:C	1:A:490:ASN:ND2	2.77	0.43
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.54	0.43
1:A:112:LYS:HD2	1:A:112:LYS:HA	1.71	0.42
1:A:136:GLY:HA3	1:A:553:ILE:HD12	2.01	0.42
1:A:139:PHE:HB3	1:A:261:LEU:HB3	2.02	0.41
1:A:112:LYS:O	1:A:116:GLN:HG3	2.20	0.41
1:A:507:MET:HE3	1:A:543:ASN:HA	2.02	0.40
1:A:511:MET:HE3	1:A:519:MET:HE3	2.02	0.40
1:A:56:ASN:HD22	1:A:56:ASN:C	2.29	0.40
1:A:368:LEU:O	1:A:499:VAL:HA	2.21	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%)	547 (97%)	19 (3%)	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	431/445 (97%)	416 (96%)	15 (4%)	32	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	110	LYS
1	A	112	LYS
1	A	204	ASN
1	A	208	LEU
1	A	269	ASN
1	A	282	LEU
1	A	286	LYS
1	A	288	THR
1	A	368	LEU
1	A	448	VAL
1	A	490	ASN
1	A	510	VAL
1	A	559	LEU
1	A	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	56	ASN
1	A	91	ASN
1	A	202	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	FAD	A	1805	-	58,58,58	2.33	24 (41%)	85,89,89	2.45	31 (36%)
3	HEC	A	804	1	50,50,50	2.03	11 (22%)	68,82,82	1.67	14 (20%)
5	FUM	A	1806	-	7,7,7	2.80	4 (57%)	8,8,8	1.23	0
3	HEC	A	803	1	50,50,50	2.06	9 (18%)	68,82,82	1.97	22 (32%)
3	HEC	A	802	1	50,50,50	2.16	12 (24%)	68,82,82	2.00	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	A	801	1	50,50,50	2.24	12 (24%)	68,82,82	1.82	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1805	-	1/1/9/9	7/34/50/50	0/6/6/6
3	HEC	A	804	1	1/1/3/7	9/14/54/54	-
5	FUM	A	1806	-	-	4/5/5/5	-
3	HEC	A	803	1	1/1/3/7	6/14/54/54	-
3	HEC	A	802	1	1/1/3/7	7/14/54/54	-
3	HEC	A	801	1	1/1/3/7	8/14/54/54	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEC	C3D-C2D	8.11	1.54	1.36
3	A	804	HEC	C3D-C2D	7.91	1.53	1.36
3	A	801	HEC	C3D-C2D	7.66	1.53	1.36
4	A	1805	FAD	C6-C5X	7.18	1.50	1.40
3	A	803	HEC	C3D-C2D	6.88	1.51	1.36
3	A	801	HEC	FE-ND	6.82	2.15	1.94
3	A	802	HEC	FE-ND	6.46	2.14	1.94
3	A	803	HEC	FE-ND	6.40	2.14	1.94
3	A	804	HEC	FE-ND	6.26	2.14	1.94
3	A	803	HEC	FE-NC	5.52	2.13	1.95
3	A	801	HEC	FE-NB	5.33	2.11	1.94
4	A	1805	FAD	C4'-C3'	4.80	1.61	1.53
4	A	1805	FAD	O2'-C2'	4.59	1.53	1.43
4	A	1805	FAD	P-O3P	4.45	1.64	1.59
3	A	802	HEC	CBC-CAC	-4.23	1.33	1.51
5	A	1806	FUM	O-C	4.20	1.33	1.23
3	A	801	HEC	FE-NC	4.07	2.08	1.95
4	A	1805	FAD	C6-C7	-4.07	1.34	1.39
3	A	804	HEC	CBC-CAC	-4.03	1.34	1.51
5	A	1806	FUM	O8-C6	-3.90	1.20	1.30
4	A	1805	FAD	C9A-N10	3.83	1.47	1.41
3	A	803	HEC	CBC-CAC	-3.80	1.35	1.51
3	A	803	HEC	CBB-CAB	-3.79	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	HEC	FE-NA	3.79	2.07	1.95
3	A	802	HEC	FE-NB	3.72	2.06	1.94
3	A	801	HEC	CBC-CAC	-3.61	1.36	1.51
3	A	802	HEC	FE-NA	3.60	2.07	1.95
3	A	804	HEC	FE-NA	3.59	2.07	1.95
3	A	802	HEC	CBB-CAB	-3.59	1.36	1.51
3	A	804	HEC	FE-NC	3.51	2.06	1.95
3	A	801	HEC	CBB-CAB	-3.50	1.36	1.51
4	A	1805	FAD	C10-N1	-3.50	1.26	1.33
3	A	801	HEC	CMA-C3A	3.43	1.57	1.50
4	A	1805	FAD	C5X-N5	3.29	1.45	1.39
3	A	804	HEC	CBB-CAB	-3.29	1.37	1.51
5	A	1806	FUM	O7-C6	3.28	1.31	1.23
4	A	1805	FAD	O4-C4	-3.27	1.17	1.23
5	A	1806	FUM	OXT-C	-3.20	1.22	1.30
4	A	1805	FAD	C5'-C4'	-3.17	1.47	1.51
3	A	802	HEC	FE-NC	3.12	2.05	1.95
4	A	1805	FAD	C2-N1	3.09	1.43	1.36
4	A	1805	FAD	C9A-C5X	3.03	1.46	1.41
4	A	1805	FAD	O3B-C3B	3.03	1.50	1.43
3	A	802	HEC	CMA-C3A	3.00	1.56	1.50
4	A	1805	FAD	C9-C9A	2.93	1.44	1.39
4	A	1805	FAD	C2A-N3A	2.92	1.39	1.33
3	A	801	HEC	FE-NA	2.85	2.04	1.95
4	A	1805	FAD	O4B-C1B	-2.83	1.35	1.42
3	A	801	HEC	CMC-C2C	2.82	1.56	1.50
3	A	802	HEC	CMC-C2C	2.75	1.56	1.50
4	A	1805	FAD	C4A-N3A	2.61	1.39	1.34
3	A	803	HEC	CMD-C2D	2.59	1.56	1.50
4	A	1805	FAD	C1B-N9A	-2.58	1.39	1.46
3	A	803	HEC	CMB-C2B	2.54	1.56	1.50
4	A	1805	FAD	O2-C2	-2.54	1.19	1.24
3	A	804	HEC	CMA-C3A	2.51	1.55	1.50
3	A	804	HEC	CAC-C3C	2.49	1.57	1.51
3	A	802	HEC	CAC-C3C	2.48	1.57	1.51
3	A	804	HEC	FE-NB	2.48	2.02	1.94
4	A	1805	FAD	C2-N3	2.45	1.44	1.39
4	A	1805	FAD	C4X-C4	2.30	1.53	1.44
3	A	801	HEC	CMB-C2B	2.28	1.55	1.50
3	A	801	HEC	CMD-C2D	2.25	1.55	1.50
4	A	1805	FAD	C2A-N1A	-2.23	1.30	1.33
3	A	802	HEC	CMB-C2B	2.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEC	CMD-C2D	2.20	1.55	1.50
4	A	1805	FAD	C8-C7	2.18	1.46	1.40
3	A	804	HEC	CAB-C3B	2.17	1.56	1.51
3	A	804	HEC	CMB-C2B	2.09	1.55	1.50
3	A	803	HEC	FE-NB	2.09	2.01	1.94
3	A	801	HEC	CAC-C3C	2.08	1.56	1.51
4	A	1805	FAD	PA-O3P	2.03	1.61	1.59

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	HEC	C1D-ND-C4D	8.12	114.82	105.21
4	A	1805	FAD	C2B-C1B-N9A	7.29	131.43	113.30
3	A	801	HEC	C1D-ND-C4D	7.22	113.75	105.21
4	A	1805	FAD	O4'-C4'-C3'	-6.55	93.93	109.25
4	A	1805	FAD	O2B-C2B-C3B	6.42	132.39	111.82
3	A	804	HEC	C1D-ND-C4D	6.05	112.37	105.21
3	A	803	HEC	C1D-ND-C4D	5.58	111.82	105.21
4	A	1805	FAD	O4'-C4'-C5'	5.26	121.59	109.99
4	A	1805	FAD	O3'-C3'-C2'	-5.08	97.38	108.93
3	A	802	HEC	CBC-CAC-C3C	4.89	125.69	112.42
3	A	802	HEC	C4B-NB-C1B	4.66	110.72	105.21
4	A	1805	FAD	C9-C8-C7	4.56	126.39	119.69
4	A	1805	FAD	O3B-C3B-C2B	-4.54	97.27	111.82
4	A	1805	FAD	O5'-C5'-C4'	-4.41	97.58	109.36
3	A	802	HEC	C3D-C4D-ND	-4.38	106.12	110.35
3	A	803	HEC	C2A-C1A-NA	-4.15	106.31	110.32
3	A	802	HEC	C3B-C4B-NB	-3.93	105.86	110.17
3	A	801	HEC	C4B-NB-C1B	3.89	109.81	105.21
4	A	1805	FAD	N3A-C2A-N1A	-3.86	122.74	128.58
3	A	803	HEC	CBD-CAD-C3D	-3.83	101.94	112.53
3	A	803	HEC	CBC-CAC-C3C	3.76	122.62	112.42
3	A	801	HEC	CBC-CAC-C3C	3.74	122.56	112.42
4	A	1805	FAD	C2A-N1A-C6A	3.60	124.64	118.73
4	A	1805	FAD	O4B-C1B-N9A	3.55	114.91	108.09
4	A	1805	FAD	C8M-C8-C9	-3.47	113.46	119.57
3	A	804	HEC	C2A-C1A-NA	-3.47	106.97	110.32
3	A	804	HEC	CBC-CAC-C3C	3.44	121.75	112.42
4	A	1805	FAD	C9A-C5X-N5	-3.41	118.84	122.45
3	A	803	HEC	C3C-C4C-NC	-3.40	106.38	110.15
3	A	804	HEC	CMC-C2C-C1C	-3.31	120.37	125.42
3	A	801	HEC	C2B-C1B-NB	-3.27	106.12	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	HEC	C2B-C1B-NB	-3.25	106.15	109.90
3	A	802	HEC	C2A-C1A-NA	-3.24	107.19	110.32
3	A	804	HEC	CHA-C4D-ND	3.19	127.85	124.42
4	A	1805	FAD	C4X-C10-N10	3.19	121.04	116.48
4	A	1805	FAD	O2B-C2B-C1B	3.17	121.02	110.10
3	A	803	HEC	C3B-C4B-NB	-3.15	106.72	110.17
3	A	803	HEC	CMD-C2D-C1D	3.12	129.90	125.03
3	A	803	HEC	C3D-C4D-ND	-3.09	107.36	110.35
4	A	1805	FAD	O4-C4-N3	-3.07	114.34	120.11
3	A	801	HEC	C3C-C4C-NC	-3.07	106.75	110.15
3	A	803	HEC	C4C-NC-C1C	3.00	110.72	105.82
4	A	1805	FAD	C6-C5X-C9A	2.97	123.12	119.05
3	A	801	HEC	CBB-CAB-C3B	2.96	120.44	112.42
3	A	802	HEC	C3C-C4C-NC	-2.92	106.91	110.15
3	A	803	HEC	CHB-C1B-NB	2.89	127.53	124.42
3	A	803	HEC	CAB-C3B-C4B	2.89	128.55	124.79
4	A	1805	FAD	C5'-C4'-C3'	2.81	117.53	112.22
4	A	1805	FAD	C1B-N9A-C8A	-2.80	120.89	127.09
4	A	1805	FAD	C4A-N9A-C1B	2.79	133.16	126.63
3	A	803	HEC	C4B-NB-C1B	2.72	108.43	105.21
4	A	1805	FAD	C9-C9A-N10	2.70	125.49	121.85
3	A	802	HEC	C2D-C1D-ND	-2.68	106.76	109.84
4	A	1805	FAD	O2'-C2'-C1'	2.68	121.20	110.20
3	A	801	HEC	C3D-C4D-ND	-2.67	107.77	110.35
4	A	1805	FAD	C4-N3-C2	-2.67	120.91	125.64
3	A	802	HEC	CHB-C1B-NB	2.67	127.29	124.42
3	A	803	HEC	CMC-C2C-C1C	-2.65	121.38	125.42
3	A	804	HEC	C3D-C4D-ND	-2.62	107.82	110.35
3	A	804	HEC	C3C-C4C-NC	-2.59	107.28	110.15
3	A	803	HEC	C4A-NA-C1A	2.57	110.02	105.82
3	A	801	HEC	C3B-C4B-NB	-2.55	107.37	110.17
3	A	803	HEC	C2C-C1C-NC	-2.53	106.09	110.14
3	A	803	HEC	CAB-C3B-C2B	-2.52	122.92	127.56
3	A	803	HEC	CHA-C4D-ND	2.52	127.13	124.42
4	A	1805	FAD	O3P-P-O1P	-2.49	103.20	110.70
4	A	1805	FAD	O3'-C3'-C4'	-2.44	103.38	108.93
3	A	803	HEC	CBB-CAB-C3B	2.44	119.04	112.42
3	A	804	HEC	CAC-C3C-C2C	2.41	130.70	126.89
3	A	802	HEC	CHA-C4D-C3D	2.39	128.27	124.77
3	A	801	HEC	O2D-CGD-CBD	2.39	121.56	114.00
4	A	1805	FAD	O2A-PA-O1A	2.38	123.51	112.44
3	A	803	HEC	C1D-C2D-C3D	-2.33	104.53	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	804	HEC	CMB-C2B-C1B	-2.31	121.42	125.03
4	A	1805	FAD	C5X-N5-C4X	2.30	121.81	118.09
3	A	804	HEC	CAC-C3C-C4C	-2.28	121.77	124.91
4	A	1805	FAD	O2P-P-O1P	2.25	122.93	112.44
3	A	801	HEC	CBD-CAD-C3D	-2.23	106.36	112.53
3	A	802	HEC	CBD-CAD-C3D	-2.23	106.38	112.53
3	A	801	HEC	C2A-C1A-NA	-2.21	108.19	110.32
4	A	1805	FAD	C3B-C2B-C1B	2.17	105.57	101.46
3	A	803	HEC	CHA-C1A-C2A	2.16	128.27	124.86
4	A	1805	FAD	C6A-C5A-N7A	2.15	136.23	132.09
3	A	801	HEC	CBA-CAA-C2A	-2.15	106.60	112.53
3	A	801	HEC	CAB-C3B-C4B	-2.14	122.00	124.79
3	A	802	HEC	CBA-CAA-C2A	-2.14	106.63	112.53
3	A	804	HEC	C4B-NB-C1B	2.13	107.73	105.21
4	A	1805	FAD	O4-C4-C4X	2.09	132.05	126.53
3	A	801	HEC	O2D-CGD-O1D	-2.06	118.04	123.33
3	A	804	HEC	C4C-NC-C1C	2.04	109.15	105.82
3	A	803	HEC	CMC-C2C-C3C	2.04	129.94	125.62
3	A	804	HEC	C3B-C4B-NB	-2.03	107.94	110.17
3	A	801	HEC	C2D-C1D-ND	-2.02	107.52	109.84
3	A	804	HEC	CHB-C4A-NA	2.02	126.65	124.45
3	A	803	HEC	CAC-C3C-C4C	-2.01	122.14	124.91

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	801	HEC	NA
3	A	802	HEC	NA
3	A	803	HEC	NA
3	A	804	HEC	NA
4	A	1805	FAD	C2B

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1805	FAD	N10-C1'-C2'-O2'
4	A	1805	FAD	C2'-C3'-C4'-C5'
3	A	804	HEC	C4C-C3C-CAC-CBC
3	A	802	HEC	C4C-C3C-CAC-CBC
3	A	802	HEC	C2C-C3C-CAC-CBC
3	A	803	HEC	C4C-C3C-CAC-CBC
3	A	803	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	A	804	HEC	C2C-C3C-CAC-CBC
3	A	802	HEC	C2B-C3B-CAB-CBB
3	A	801	HEC	C2C-C3C-CAC-CBC
4	A	1805	FAD	C2'-C3'-C4'-O4'
5	A	1806	FUM	C4-C5-C6-O8
5	A	1806	FUM	C4-C5-C6-O7
3	A	801	HEC	C4C-C3C-CAC-CBC
3	A	804	HEC	C2B-C3B-CAB-CBB
3	A	802	HEC	C4B-C3B-CAB-CBB
4	A	1805	FAD	PA-O3P-P-O5'
5	A	1806	FUM	O-C-C4-C5
3	A	801	HEC	C2B-C3B-CAB-CBB
3	A	804	HEC	C4D-C3D-CAD-CBD
4	A	1805	FAD	N10-C1'-C2'-C3'
3	A	803	HEC	C2B-C3B-CAB-CBB
3	A	804	HEC	C2D-C3D-CAD-CBD
5	A	1806	FUM	OXT-C-C4-C5
3	A	803	HEC	CAA-CBA-CGA-O2A
3	A	801	HEC	C3D-CAD-CBD-CGD
3	A	803	HEC	CAA-CBA-CGA-O1A
3	A	804	HEC	CAA-CBA-CGA-O2A
3	A	804	HEC	CAA-CBA-CGA-O1A
3	A	801	HEC	CAD-CBD-CGD-O1D
3	A	801	HEC	CAD-CBD-CGD-O2D
4	A	1805	FAD	O3'-C3'-C4'-C5'
3	A	802	HEC	CAD-CBD-CGD-O2D
3	A	802	HEC	CAD-CBD-CGD-O1D
3	A	803	HEC	C4B-C3B-CAB-CBB
3	A	804	HEC	C4B-C3B-CAB-CBB
3	A	801	HEC	C4B-C3B-CAB-CBB
3	A	802	HEC	CAA-CBA-CGA-O2A
3	A	804	HEC	CAD-CBD-CGD-O2D
3	A	801	HEC	CAA-CBA-CGA-O2A
4	A	1805	FAD	P-O3P-PA-O2A

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1805	FAD	2	0
3	A	804	HEC	5	0
5	A	1806	FUM	1	0

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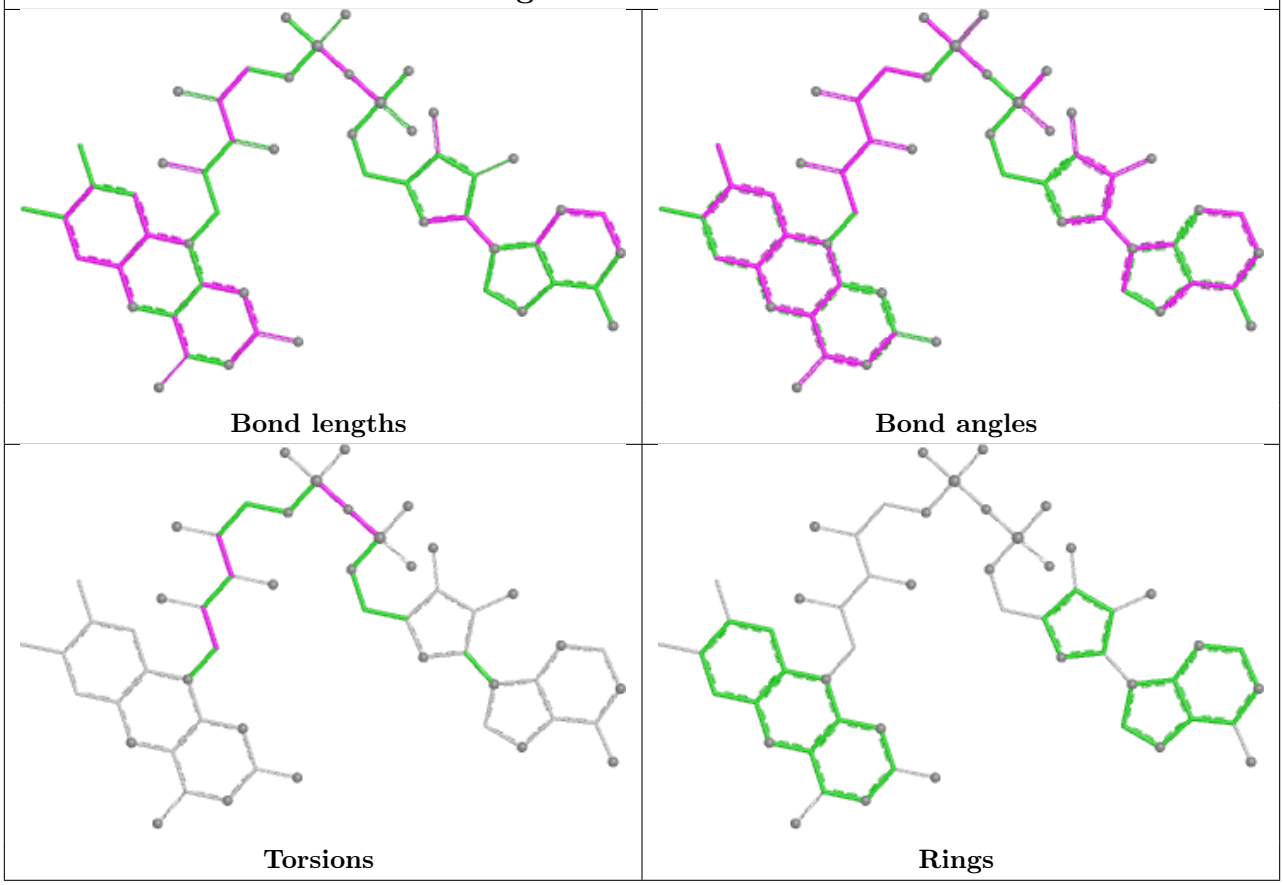
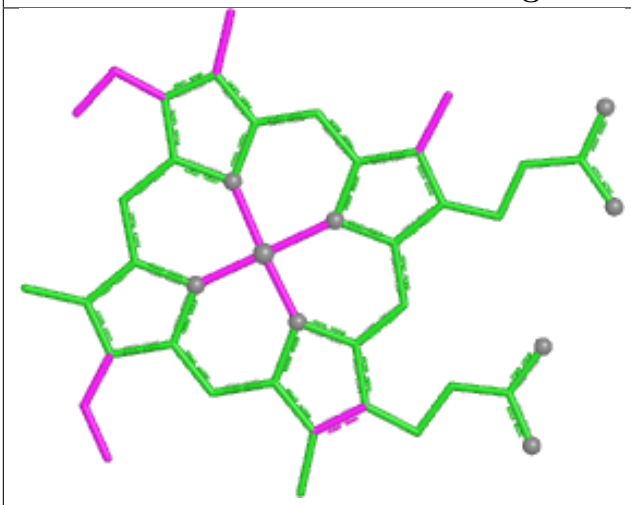
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	HEC	5	0
3	A	802	HEC	4	0
3	A	801	HEC	7	0

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.

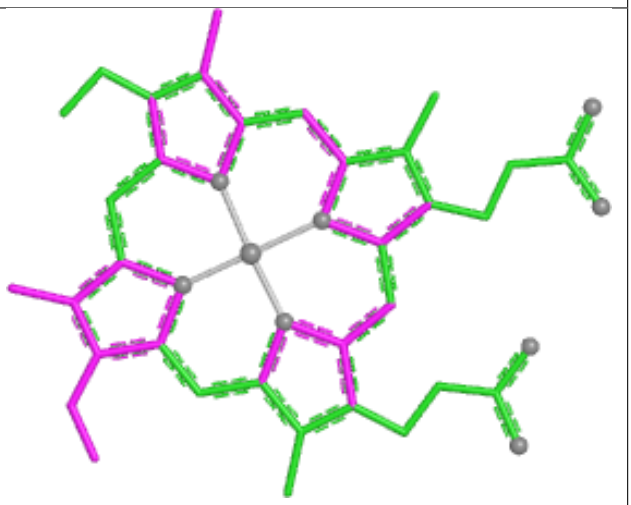
Ligand FAD A 1805



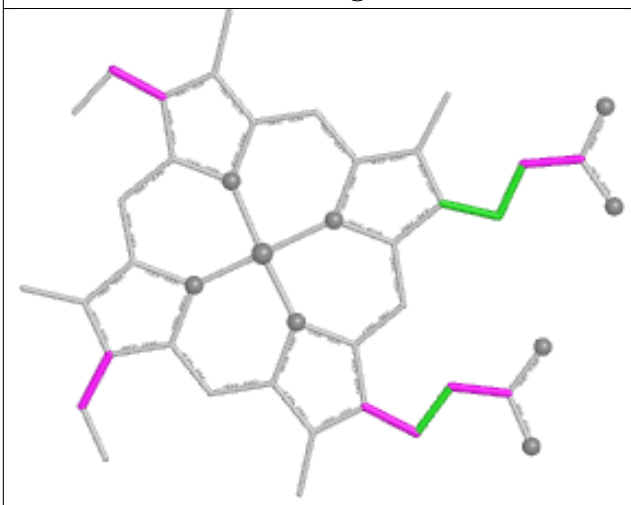
Ligand HEC A 804



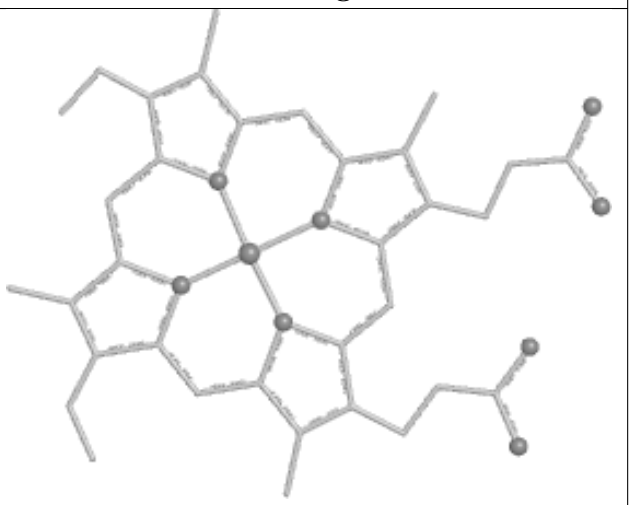
Bond lengths



Bond angles

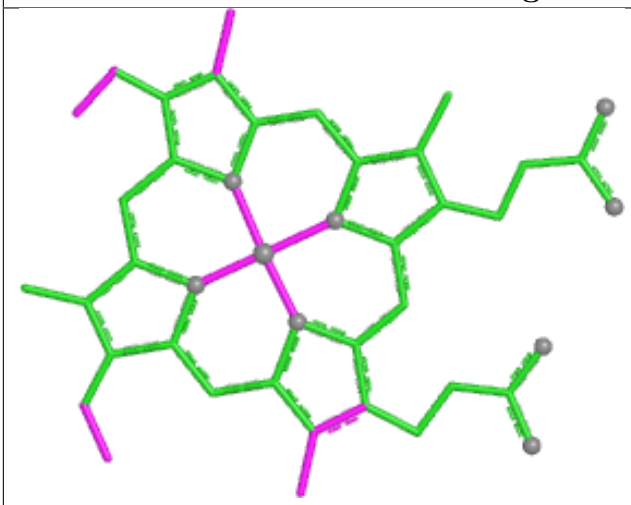


Torsions

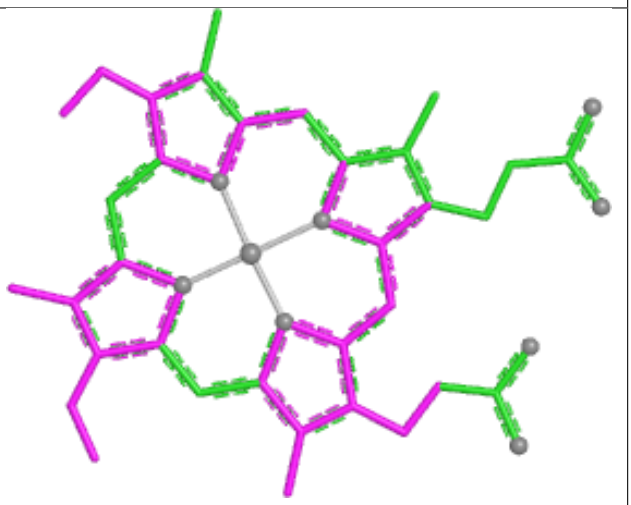


Rings

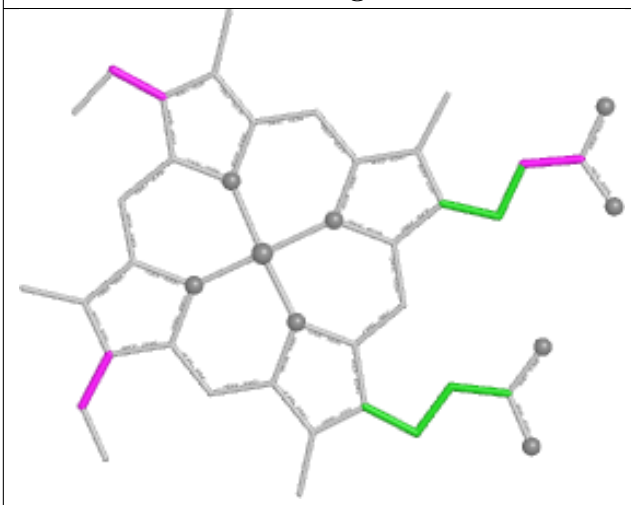
Ligand HEC A 803



Bond lengths



Bond angles



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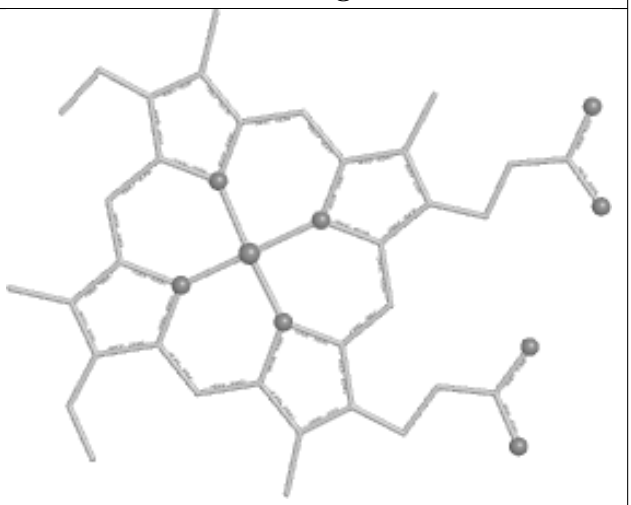
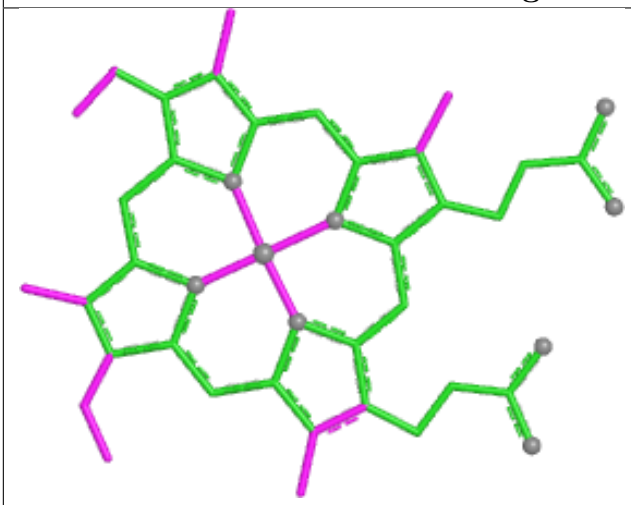
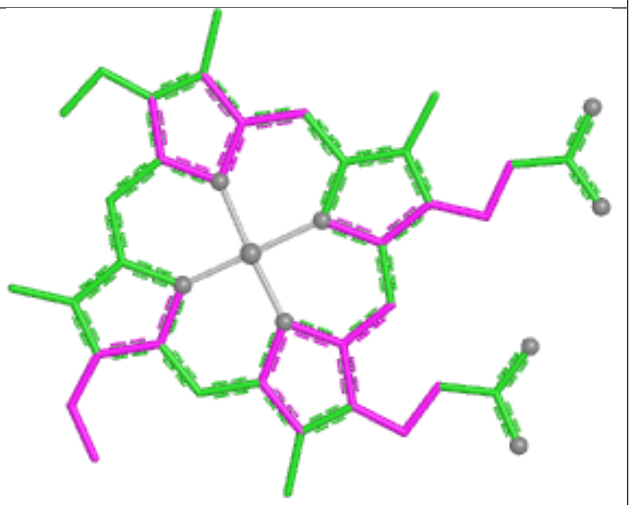


Rings

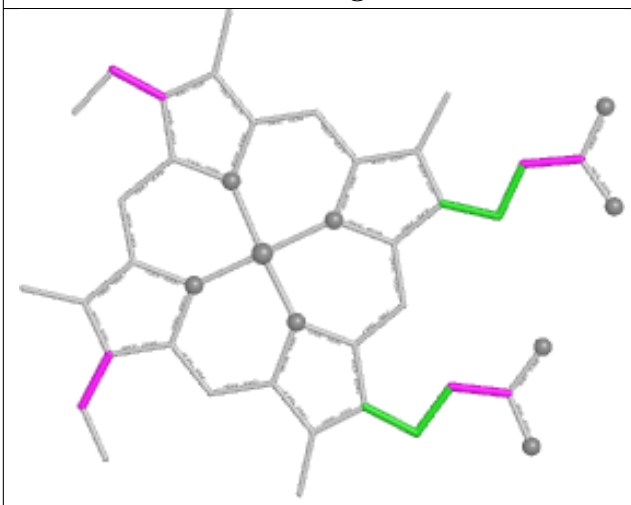
Ligand HEC A 802



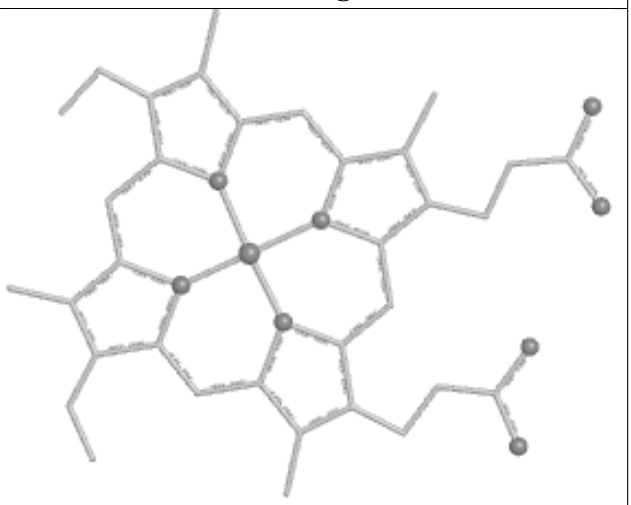
Bond lengths



Bond angles

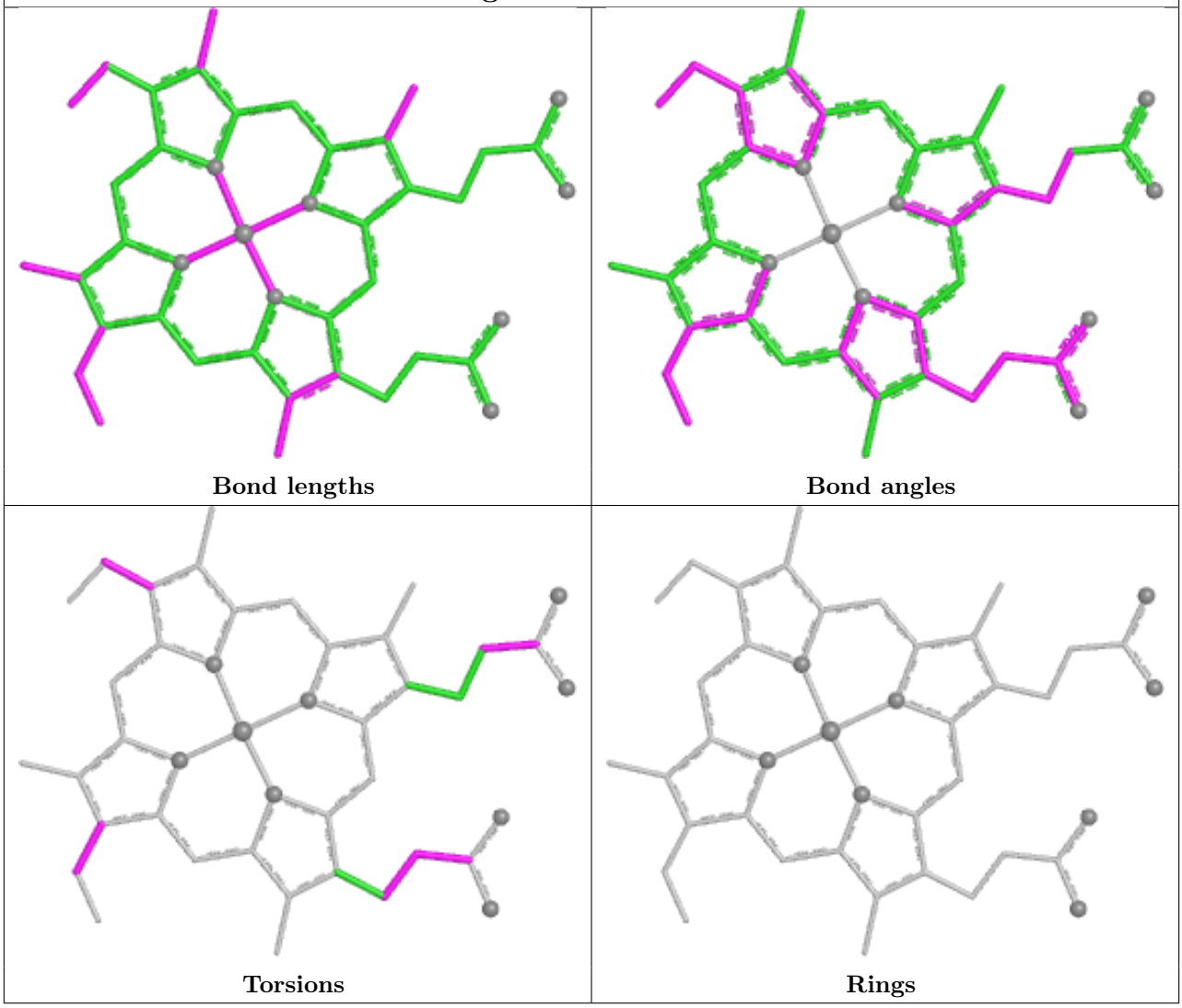


Torsions



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 (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	568/571 (99%)	-0.79	0 100 100	5, 12, 22, 35	0

There are no RSRZ outliers to report.

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.

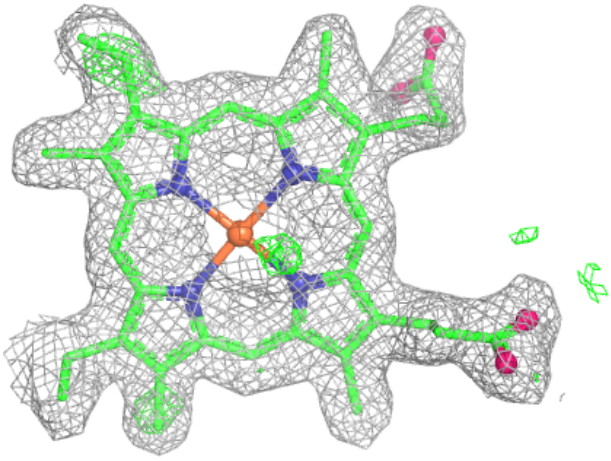
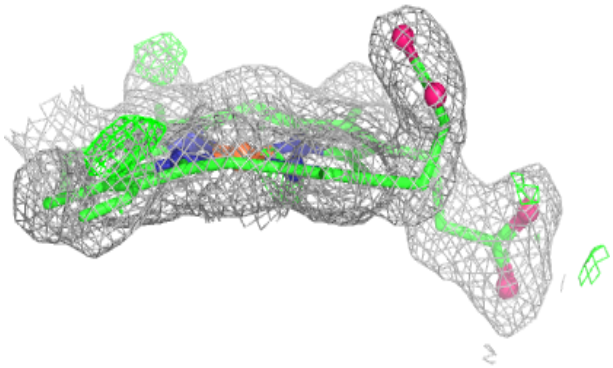
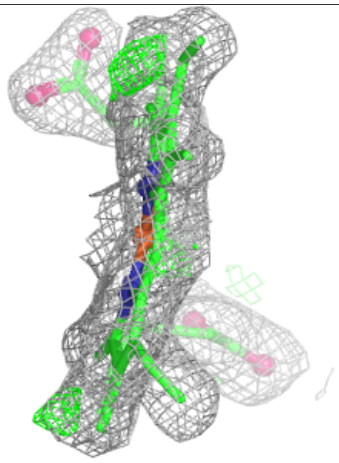
6.4 Ligands (i)

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(Å^2)	Q<0.9
5	FUM	A	1806	8/8	0.95	0.06	16,17,19,22	0
3	HEC	A	802	43/43	0.97	0.07	11,14,24,32	0
2	NA	A	1810	1/1	0.98	0.03	8,8,8,8	0
3	HEC	A	803	43/43	0.98	0.06	6,11,28,38	0
4	FAD	A	1805	53/53	0.98	0.05	5,9,15,17	0
3	HEC	A	801	43/43	0.98	0.06	9,13,19,25	0
3	HEC	A	804	43/43	0.99	0.05	4,8,13,16	0

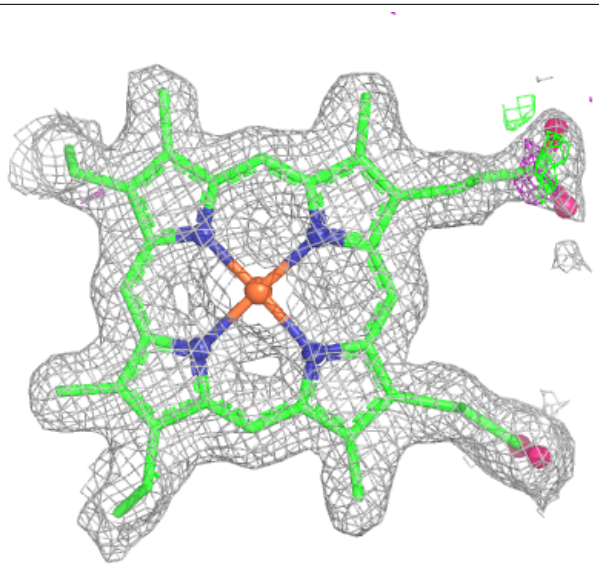
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

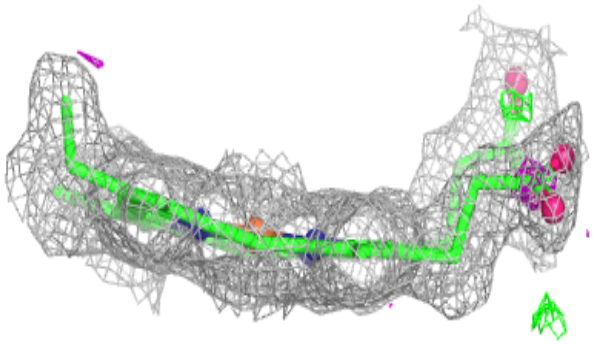
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

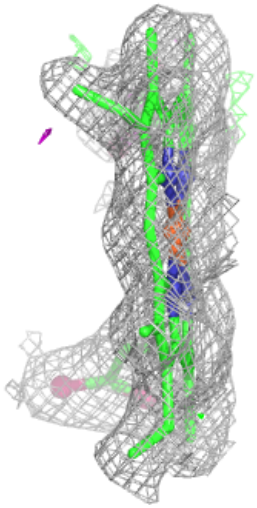
Electron density around HEC A 802: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HEC A 803:

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

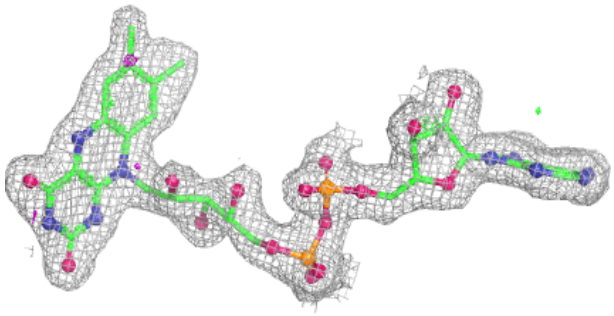


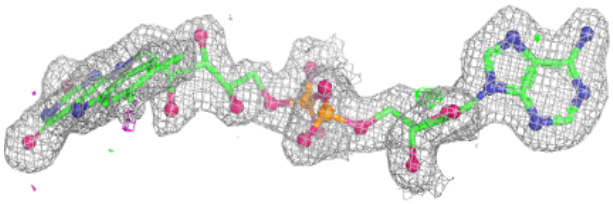


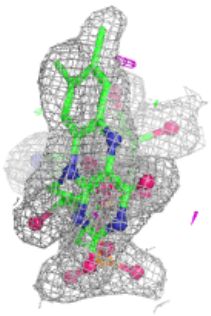


Electron density around FAD A 1805:

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

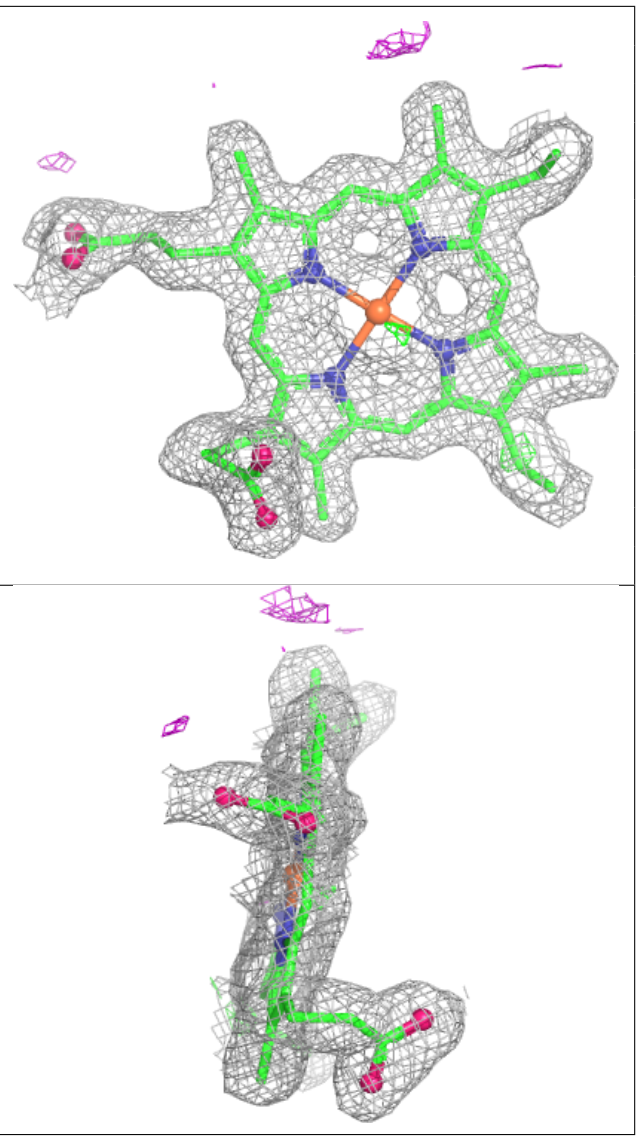






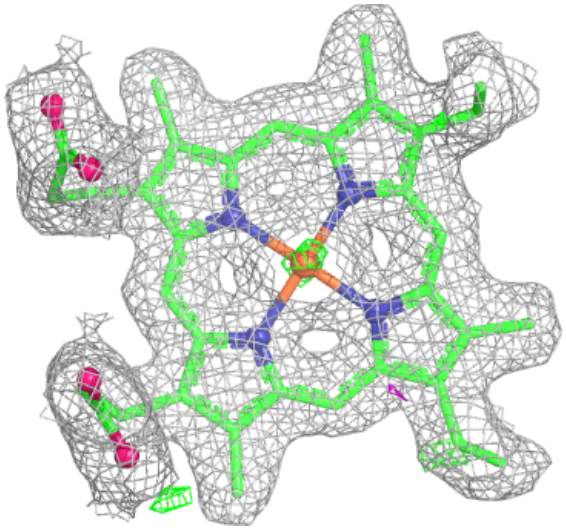
Electron density around HEC A 801:

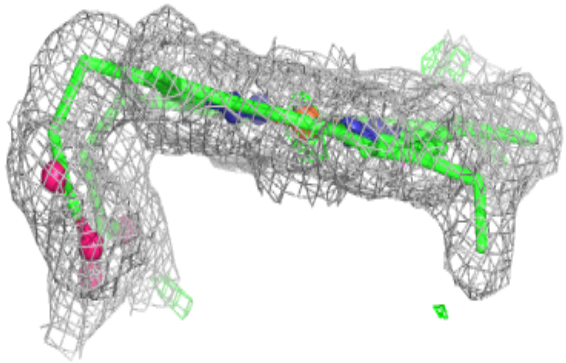
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

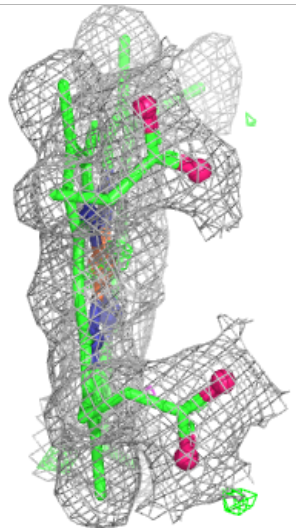


Electron density around HEC A 804:

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







6.5 Other polymers (i)

There are no such residues in this entry.