Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 04:05 AM EDT

PDB ID	:	1Q9I
Title	:	The A251C:S430C double mutant of flavocytochrome c3 from Shewanella frigidimarina
Authors	:	Rothery, E.L.; Mowat, C.G.; Miles, C.S.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on	:	2003-08-25
Resolution	:	1.60 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:

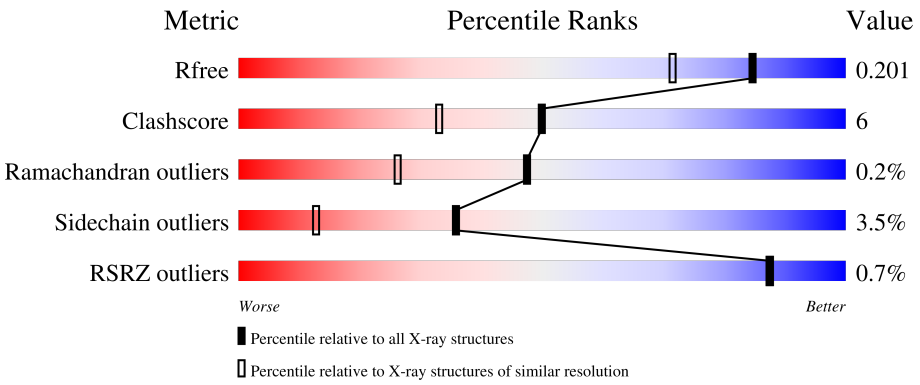
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

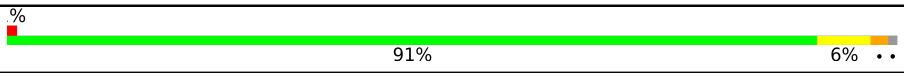
The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	

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
5	TEO	A	9806	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5653 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 flavocytochrome c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4190	2600	739	824	27	0	0	0

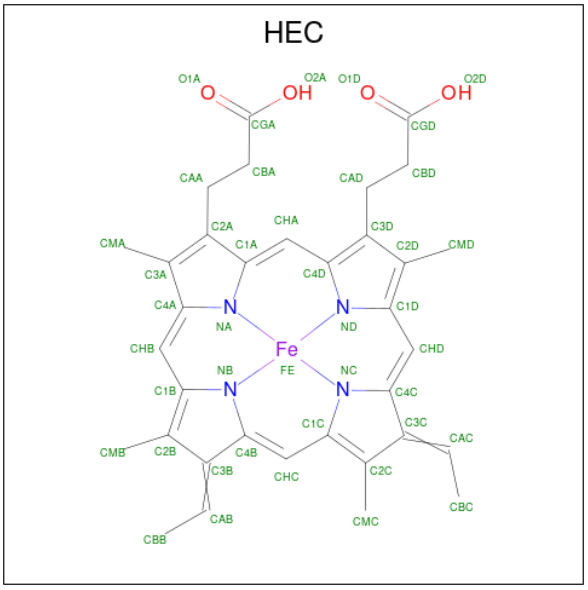
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	CYS	ALA	engineered mutation	UNP Q02469
A	430	CYS	SER	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

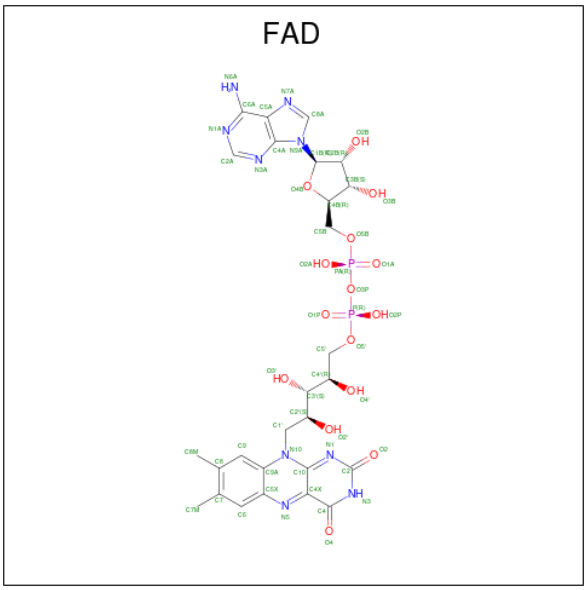
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



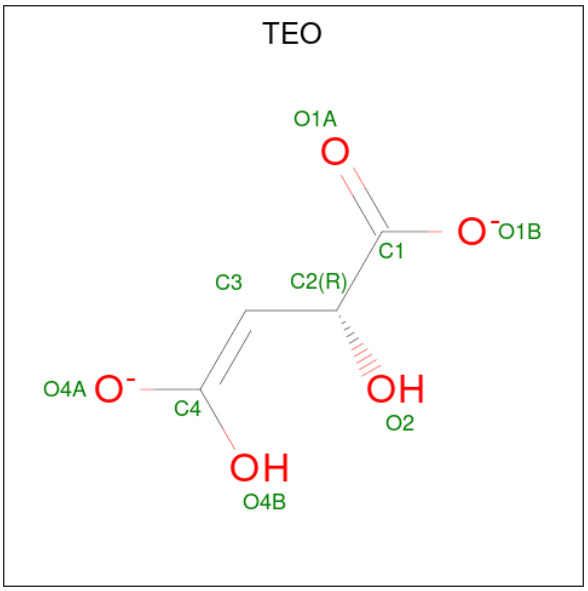
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: $C_4H_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0

- Molecule 6 is water.

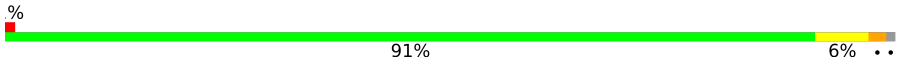
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1228	Total O 1228 1228	0	0

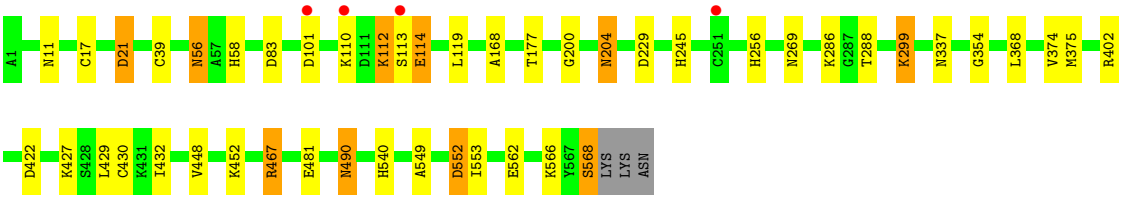
3 Residue-property plots (i)

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: flavocytochrome c3

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	45.29Å 91.89Å 78.31Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	24.00 – 1.60 22.64 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (24.00-1.60) 92.2 (22.64-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.155 , 0.197 0.158 , 0.201	Depositor DCC
R_{free} test set	3884 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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: HEC, FAD, TEO, 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	0.59	0/4260	0.81	5/5764 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	552	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	101	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	422	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	83	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	21	ASP	CB-CG-OD2	5.21	122.99	118.30

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	4190	0	4097	47	1
2	A	1	0	0	0	0
3	A	172	0	122	11	0
4	A	53	0	30	4	0
5	A	9	0	2	1	0
6	A	1228	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5653	0	4251	49	1

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 (49) 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:39:CYS:SG	3:A:802:HEC:CAC	2.16	1.34
1:A:17:CYS:SG	3:A:801:HEC:HAC	1.66	1.31
1:A:39:CYS:SG	3:A:802:HEC:HAC	1.81	1.18
1:A:368:LEU:HB2	6:A:1417:HOH:O	1.60	0.99
1:A:229:ASP:H	1:A:256:HIS:HE1	1.04	0.94
1:A:17:CYS:HG	3:A:801:HEC:HAC	1.38	0.88
1:A:204:ASN:HD22	1:A:204:ASN:H	1.18	0.88
1:A:229:ASP:H	1:A:256:HIS:CE1	1.92	0.86
1:A:481:GLU:CG	6:A:1385:HOH:O	2.28	0.81
1:A:299:LYS:HB2	6:A:1432:HOH:O	1.81	0.80
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.49	0.78
1:A:402:ARG:HH22	5:A:9806:TEO:C3	1.97	0.77
1:A:229:ASP:N	1:A:256:HIS:HE1	1.85	0.71
1:A:204:ASN:H	1:A:204:ASN:ND2	1.91	0.66
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.78	0.66
1:A:39:CYS:SG	3:A:802:HEC:C3C	2.84	0.65
1:A:17:CYS:SG	3:A:801:HEC:C3C	2.85	0.64
1:A:375:MET:HE2	4:A:9805:FAD:H6	1.83	0.60
1:A:17:CYS:SG	3:A:801:HEC:CBC	2.85	0.58
1:A:566:LYS:HG3	6:A:1357:HOH:O	2.05	0.55
1:A:568:SER:HB2	6:A:1136:HOH:O	2.06	0.55
1:A:540:HIS:HE1	1:A:552:ASP:OD2	1.91	0.53
1:A:56:ASN:HD22	1:A:58:HIS:H	1.57	0.51
1:A:354:GLY:N	6:A:1182:HOH:O	2.43	0.51
1:A:374:VAL:HB	3:A:804:HEC:HMD3	1.91	0.51
1:A:540:HIS:HD2	6:A:9822:HOH:O	1.94	0.50
1:A:448:VAL:HG12	6:A:1751:HOH:O	2.11	0.49
1:A:39:CYS:SG	3:A:802:HEC:CBC	2.94	0.49
1:A:113:SER:O	1:A:114:GLU:HB2	2.12	0.49
1:A:168:ALA:HA	4:A:9805:FAD:N5	2.29	0.48
3:A:802:HEC:HMB1	3:A:802:HEC:HBB3	1.96	0.48
1:A:204:ASN:ND2	1:A:204:ASN:N	2.62	0.47
1:A:467:ARG:NH2	6:A:1894:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:MET:HE2	4:A:9805:FAD:C6	2.45	0.46
1:A:427:LYS:NZ	6:A:1292:HOH:O	2.36	0.46
1:A:119:LEU:HD13	6:A:2039:HOH:O	2.16	0.45
3:A:803:HEC:HMB1	3:A:803:HEC:HBB3	1.99	0.45
1:A:56:ASN:ND2	1:A:58:HIS:H	2.14	0.45
1:A:490:ASN:HD22	1:A:490:ASN:C	2.21	0.44
1:A:549:ALA:O	1:A:553:ILE:HG23	2.18	0.43
1:A:562:GLU:O	1:A:566:LYS:HG3	2.19	0.42
1:A:427:LYS:CD	6:A:1292:HOH:O	2.67	0.42
1:A:113:SER:O	1:A:114:GLU:CB	2.68	0.41
1:A:429:LEU:HD23	1:A:432:ILE:HG13	2.02	0.41
1:A:427:LYS:HD3	6:A:1292:HOH:O	2.20	0.41
1:A:168:ALA:HA	4:A:9805:FAD:C5X	2.51	0.40
1:A:177:THR:OG1	1:A:245:HIS:CE1	2.67	0.40
1:A:568:SER:HB3	6:A:1248:HOH:O	2.20	0.40
1:A:112:LYS:HA	1:A:112:LYS:HZ3	1.87	0.40

All (1) 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:286:LYS:NZ	6:A:1145:HOH:O[2_646]	1.36	0.84

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%)	18 (3%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU

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	434/446 (97%)	419 (96%)	15 (4%)	36 13

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	21	ASP
1	A	56	ASN
1	A	110	LYS
1	A	112	LYS
1	A	204	ASN
1	A	269	ASN
1	A	288	THR
1	A	299	LYS
1	A	337	ASN
1	A	430	CYS
1	A	452	LYS
1	A	467	ARG
1	A	490	ASN
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	11	ASN
1	A	35	GLN
1	A	56	ASN
1	A	91	ASN
1	A	116	GLN
1	A	204	ASN

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Mol	Chain	Res	Type
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 monosaccharides 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	$\#\|Z\| > 2$
3	HEC	A	803	1	32,50,50	2.14	9 (28%)	24,82,82	1.99	8 (33%)
3	HEC	A	802	1	32,50,50	2.22	5 (15%)	24,82,82	1.73	6 (25%)
4	FAD	A	9805	-	53,58,58	2.13	19 (35%)	68,89,89	2.13	22 (32%)
3	HEC	A	801	1	32,50,50	2.15	6 (18%)	24,82,82	1.80	7 (29%)
5	TEO	A	9806	-	6,8,8	4.45	4 (66%)	4,10,10	3.18	3 (75%)
3	HEC	A	804	1	32,50,50	2.27	7 (21%)	24,82,82	1.66	7 (29%)

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	803	1	-	2/10/54/54	-
3	HEC	A	802	1	-	2/10/54/54	-
4	FAD	A	9805	-	-	7/30/50/50	0/6/6/6
3	HEC	A	801	1	-	3/10/54/54	-
5	TEO	A	9806	-	-	5/6/8/8	-
3	HEC	A	804	1	-	6/10/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	9806	TEO	O2-C2	-9.01	1.32	1.43
3	A	802	HEC	C2B-C3B	-6.78	1.33	1.40
3	A	804	HEC	C3C-C2C	-6.43	1.34	1.40
4	A	9805	FAD	C6-C5X	6.09	1.49	1.40
3	A	801	HEC	C2B-C3B	-5.99	1.34	1.40
3	A	803	HEC	C3C-C2C	-5.70	1.34	1.40
3	A	804	HEC	C2B-C3B	-5.57	1.34	1.40
3	A	803	HEC	C2B-C3B	-5.54	1.35	1.40
3	A	801	HEC	C3C-C2C	-5.35	1.35	1.40
4	A	9805	FAD	C2A-N3A	5.32	1.40	1.32
3	A	802	HEC	C3C-C2C	-5.06	1.35	1.40
4	A	9805	FAD	C6-C7	-4.85	1.32	1.39
3	A	802	HEC	C3D-C2D	4.81	1.51	1.37
3	A	804	HEC	C3D-C2D	4.77	1.51	1.37
3	A	803	HEC	C3D-C2D	4.68	1.51	1.37
3	A	801	HEC	C3D-C2D	4.12	1.49	1.37
3	A	802	HEC	CBC-CAC	-3.98	1.34	1.49
4	A	9805	FAD	O4-C4	-3.96	1.16	1.23
5	A	9806	TEO	O1B-C1	-3.81	1.18	1.30
5	A	9806	TEO	O4B-C4	3.62	1.48	1.30
3	A	801	HEC	CBB-CAB	-3.54	1.36	1.49
3	A	801	HEC	CBC-CAC	-3.47	1.36	1.49
3	A	804	HEC	CBC-CAC	-3.35	1.36	1.49
4	A	9805	FAD	C8-C7	3.28	1.49	1.40
4	A	9805	FAD	O2'-C2'	3.08	1.49	1.43
4	A	9805	FAD	C10-N1	-3.07	1.26	1.33
3	A	803	HEC	CBC-CAC	-3.02	1.38	1.49
3	A	803	HEC	CBB-CAB	-3.01	1.38	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	9805	FAD	C2-N1	3.00	1.43	1.36
5	A	9806	TEO	C2-C1	2.99	1.59	1.54
4	A	9805	FAD	O3B-C3B	2.90	1.49	1.43
4	A	9805	FAD	C4'-C3'	2.90	1.58	1.53
3	A	802	HEC	CBB-CAB	-2.82	1.38	1.49
3	A	804	HEC	CBB-CAB	-2.76	1.39	1.49
3	A	804	HEC	CAD-C3D	2.71	1.56	1.52
4	A	9805	FAD	C2-N3	2.64	1.45	1.39
3	A	803	HEC	CAA-C2A	2.57	1.56	1.52
4	A	9805	FAD	PA-O2A	-2.52	1.43	1.55
4	A	9805	FAD	P-O1P	-2.41	1.42	1.50
4	A	9805	FAD	C4X-C4	2.37	1.53	1.44
4	A	9805	FAD	C2'-C3'	2.36	1.57	1.53
4	A	9805	FAD	C5'-C4'	-2.35	1.48	1.51
4	A	9805	FAD	O4B-C1B	-2.26	1.37	1.41
3	A	803	HEC	C1D-ND	2.18	1.40	1.36
3	A	804	HEC	C1D-ND	2.17	1.40	1.36
4	A	9805	FAD	C9A-N10	2.09	1.44	1.41
3	A	803	HEC	C4D-ND	2.09	1.40	1.36
3	A	801	HEC	C1D-ND	2.06	1.40	1.36
3	A	803	HEC	C1B-NB	2.05	1.40	1.36
4	A	9805	FAD	C8A-N7A	-2.02	1.31	1.34

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	HEC	CBD-CAD-C3D	-6.03	102.33	112.62
4	A	9805	FAD	C9A-C5X-N5	-5.63	116.32	122.43
4	A	9805	FAD	O5'-C5'-C4'	-5.31	95.18	109.36
4	A	9805	FAD	O4'-C4'-C5'	5.23	121.67	109.92
5	A	9806	TEO	O1B-C1-O1A	4.67	134.69	124.09
4	A	9805	FAD	C8M-C8-C9	-4.34	111.47	119.49
4	A	9805	FAD	O2B-C2B-C3B	4.28	125.66	111.82
4	A	9805	FAD	O4'-C4'-C3'	-4.24	98.79	109.10
4	A	9805	FAD	C9-C8-C7	4.06	125.49	119.67
3	A	804	HEC	CMB-C2B-C1B	-3.99	122.33	128.46
3	A	801	HEC	CMB-C2B-C1B	-3.78	122.65	128.46
5	A	9806	TEO	O1B-C1-C2	-3.65	104.48	113.07
3	A	803	HEC	CMC-C2C-C1C	-3.60	122.93	128.46
3	A	802	HEC	CMC-C2C-C1C	-3.45	123.16	128.46
4	A	9805	FAD	O3'-C3'-C2'	-3.31	100.81	108.81
4	A	9805	FAD	C2A-N1A-C6A	3.21	124.24	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	HEC	CMC-C2C-C3C	3.10	129.46	125.82
3	A	802	HEC	CMB-C2B-C1B	-3.07	123.75	128.46
4	A	9805	FAD	C6-C5X-C9A	3.00	123.18	118.94
4	A	9805	FAD	C1B-N9A-C4A	2.99	131.89	126.64
3	A	801	HEC	CBA-CAA-C2A	-2.93	107.66	112.60
3	A	801	HEC	CBD-CAD-C3D	-2.92	107.64	112.62
3	A	803	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
3	A	804	HEC	CMB-C2B-C3B	2.91	129.24	125.82
4	A	9805	FAD	O3B-C3B-C2B	-2.89	102.46	111.82
3	A	801	HEC	CMB-C2B-C3B	2.89	129.21	125.82
3	A	804	HEC	CBA-CAA-C2A	-2.74	107.99	112.60
3	A	803	HEC	CMC-C2C-C3C	2.72	129.01	125.82
3	A	804	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
3	A	802	HEC	CBA-CAA-C2A	-2.67	108.11	112.60
3	A	802	HEC	C3B-C4B-NB	-2.55	106.13	110.94
4	A	9805	FAD	C4A-C5A-N7A	-2.54	106.76	109.40
4	A	9805	FAD	C5X-N5-C4X	2.52	122.27	118.07
3	A	802	HEC	C2B-C3B-C4B	2.50	109.05	106.35
4	A	9805	FAD	C6-C7-C8	-2.46	116.14	119.67
3	A	804	HEC	O1D-CGD-CBD	-2.43	115.27	123.08
3	A	801	HEC	CMC-C2C-C1C	-2.39	124.79	128.46
4	A	9805	FAD	C3B-C2B-C1B	2.37	104.55	100.98
4	A	9805	FAD	P-O3P-PA	-2.36	124.73	132.83
4	A	9805	FAD	C5A-C6A-N1A	-2.36	115.01	120.35
4	A	9805	FAD	C4-N3-C2	-2.31	121.38	125.64
3	A	803	HEC	C4C-C3C-C2C	2.28	108.81	106.35
4	A	9805	FAD	N6A-C6A-N1A	2.27	123.29	118.57
4	A	9805	FAD	O2'-C2'-C1'	2.26	115.27	109.80
3	A	803	HEC	C3C-C4C-NC	-2.25	106.69	110.94
4	A	9805	FAD	N3A-C2A-N1A	-2.25	125.16	128.68
3	A	803	HEC	CMB-C2B-C1B	-2.21	125.07	128.46
5	A	9806	TEO	O2-C2-C1	2.17	115.25	109.61
3	A	801	HEC	O1A-CGA-CBA	-2.17	116.11	123.08
3	A	804	HEC	C3B-C4B-NB	-2.16	106.87	110.94
3	A	801	HEC	C3B-C4B-NB	-2.12	106.95	110.94
3	A	804	HEC	O2D-CGD-CBD	2.08	120.70	114.03
3	A	803	HEC	CBA-CAA-C2A	-2.05	109.14	112.60

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	9805	FAD	N10-C1'-C2'-O2'
4	A	9805	FAD	C2'-C3'-C4'-C5'
5	A	9806	TEO	C1-C2-C3-C4
5	A	9806	TEO	O2-C2-C3-C4
5	A	9806	TEO	O1A-C1-C2-O2
5	A	9806	TEO	O1B-C1-C2-O2
4	A	9805	FAD	C2'-C3'-C4'-O4'
4	A	9805	FAD	P-O3P-PA-O1A
5	A	9806	TEO	O1B-C1-C2-C3
4	A	9805	FAD	O3'-C3'-C4'-C5'
3	A	804	HEC	C2D-C3D-CAD-CBD
3	A	804	HEC	C4D-C3D-CAD-CBD
3	A	801	HEC	CAD-CBD-CGD-O1D
3	A	804	HEC	CAA-CBA-CGA-O2A
3	A	803	HEC	CAA-CBA-CGA-O1A
3	A	802	HEC	CAD-CBD-CGD-O1D
3	A	804	HEC	CAA-CBA-CGA-O1A
3	A	802	HEC	CAD-CBD-CGD-O2D
3	A	801	HEC	CAD-CBD-CGD-O2D
3	A	803	HEC	CAA-CBA-CGA-O2A
3	A	801	HEC	C3D-CAD-CBD-CGD
4	A	9805	FAD	O4B-C4B-C5B-O5B
3	A	804	HEC	CAD-CBD-CGD-O1D
3	A	804	HEC	CAD-CBD-CGD-O2D
4	A	9805	FAD	P-O3P-PA-O2A

There are no ring outliers.

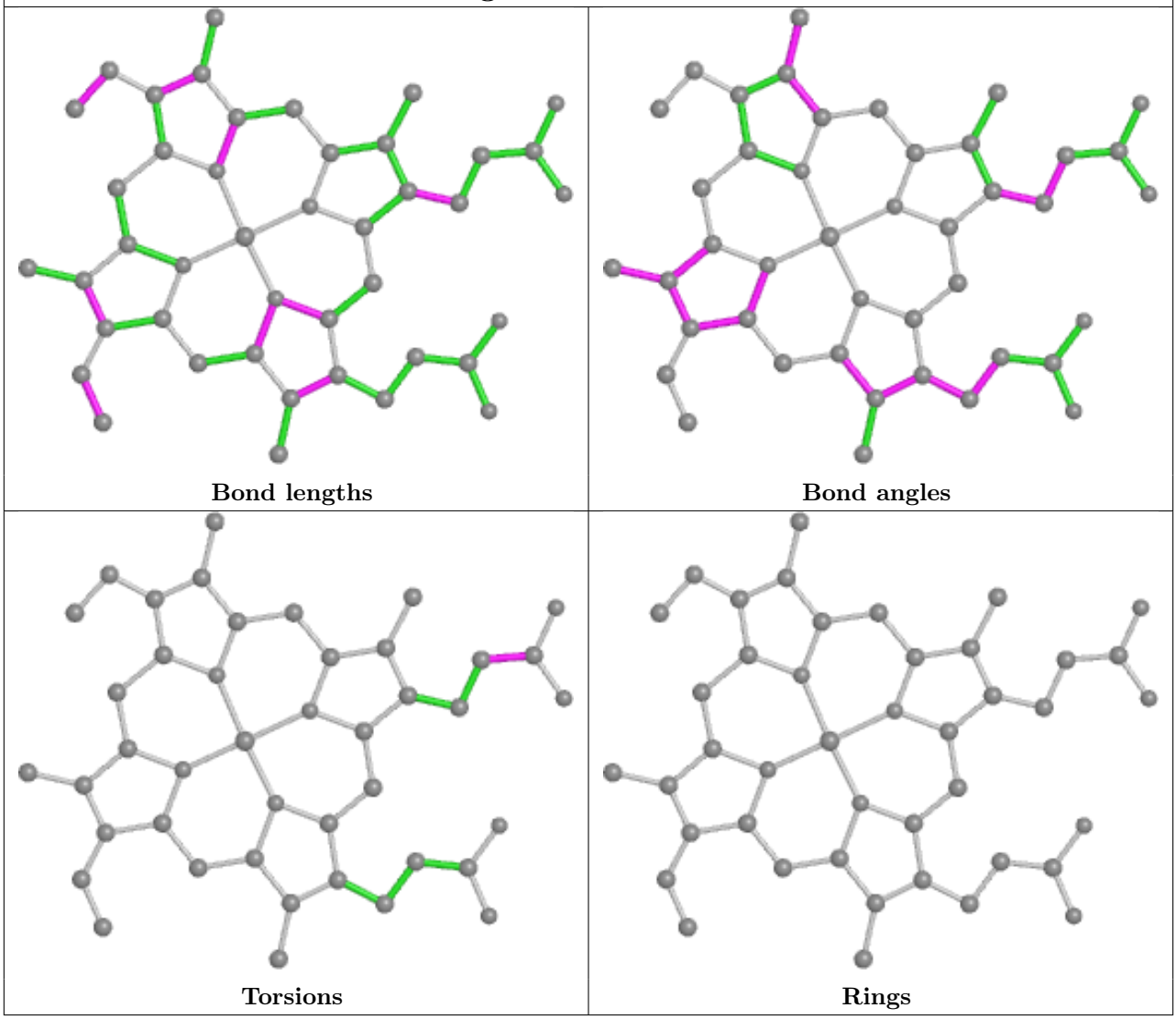
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	HEC	1	0
3	A	802	HEC	5	0
4	A	9805	FAD	4	0
3	A	801	HEC	4	0
5	A	9806	TEO	1	0
3	A	804	HEC	1	0

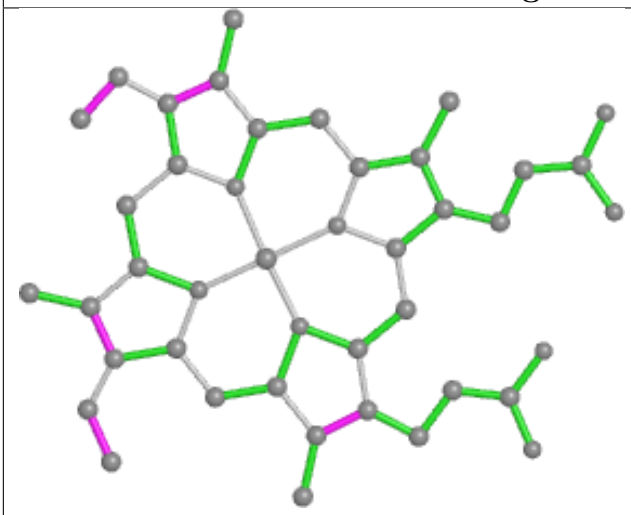
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

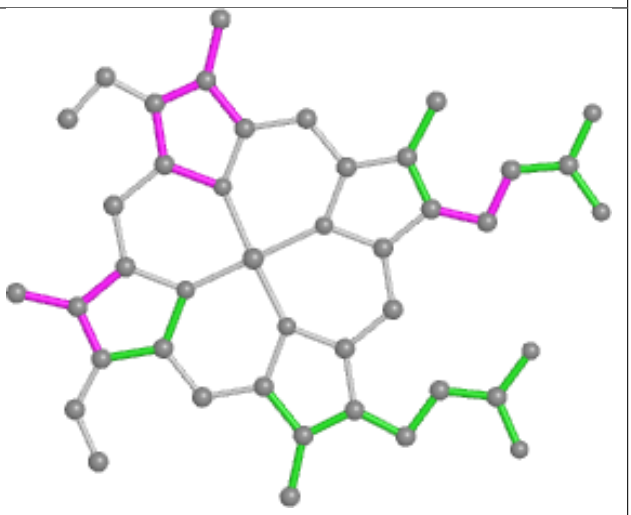
Ligand HEC A 803



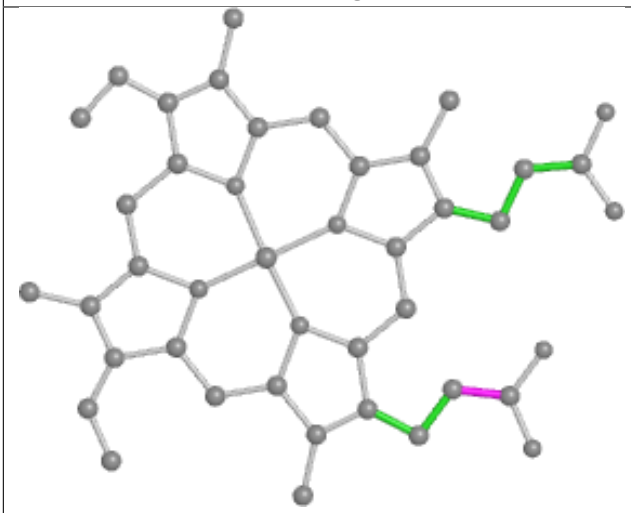
Ligand HEC A 802



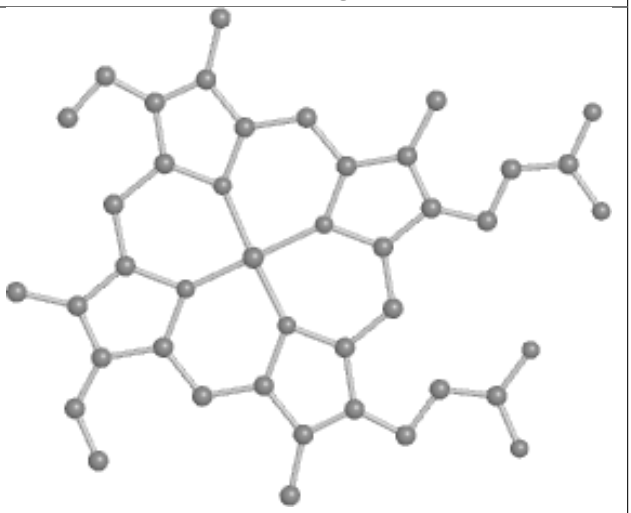
Bond lengths



Bond angles

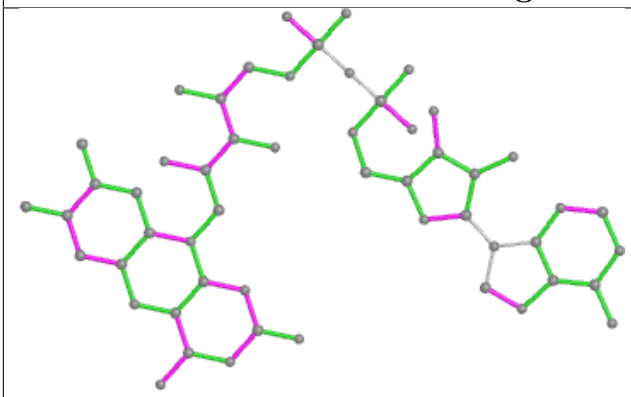


Torsions

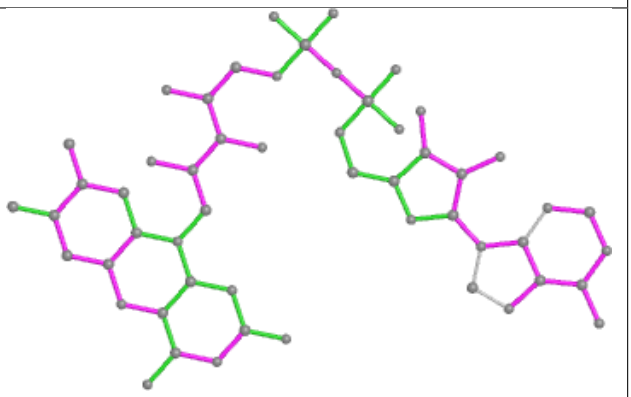


Rings

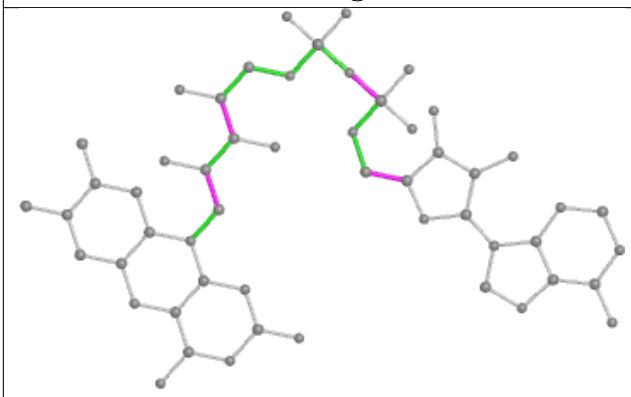
Ligand FAD A 9805



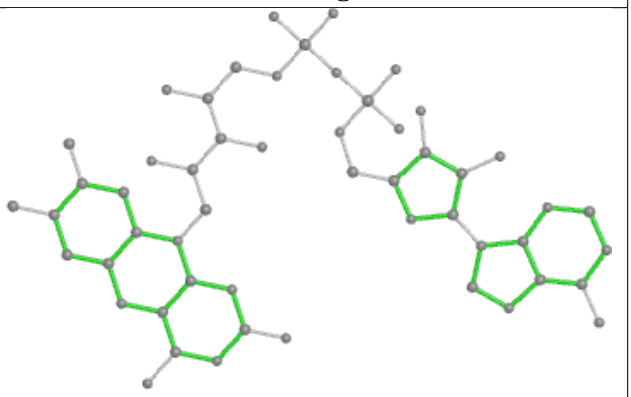
Bond lengths



Bond angles

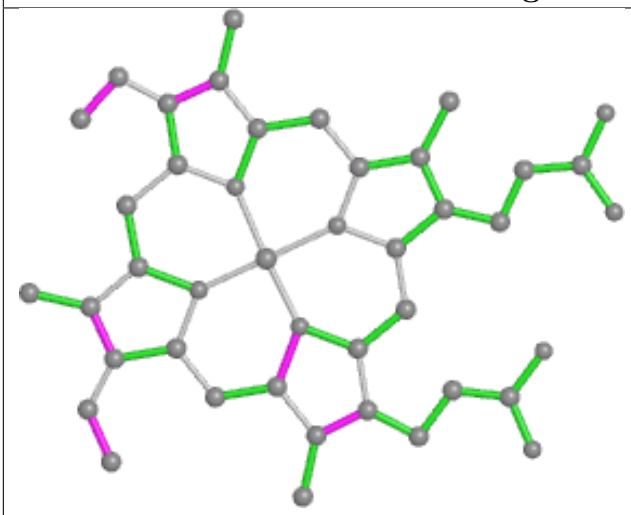


Torsions

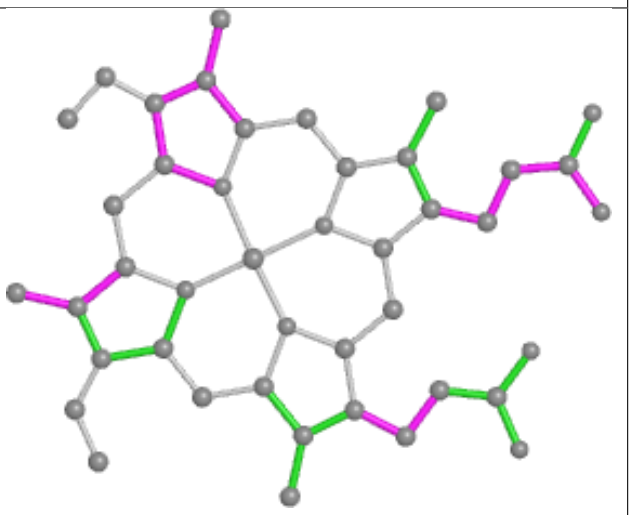


Rings

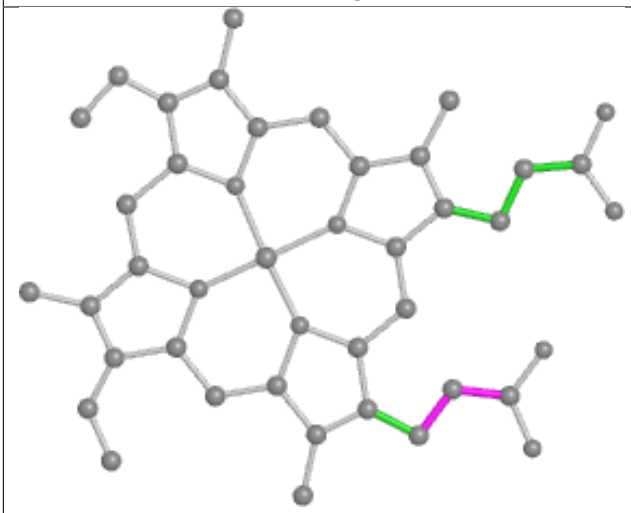
Ligand HEC A 801



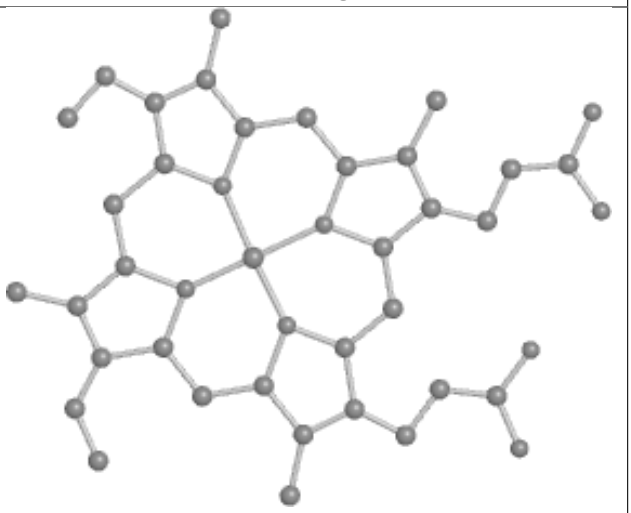
Bond lengths



Bond angles

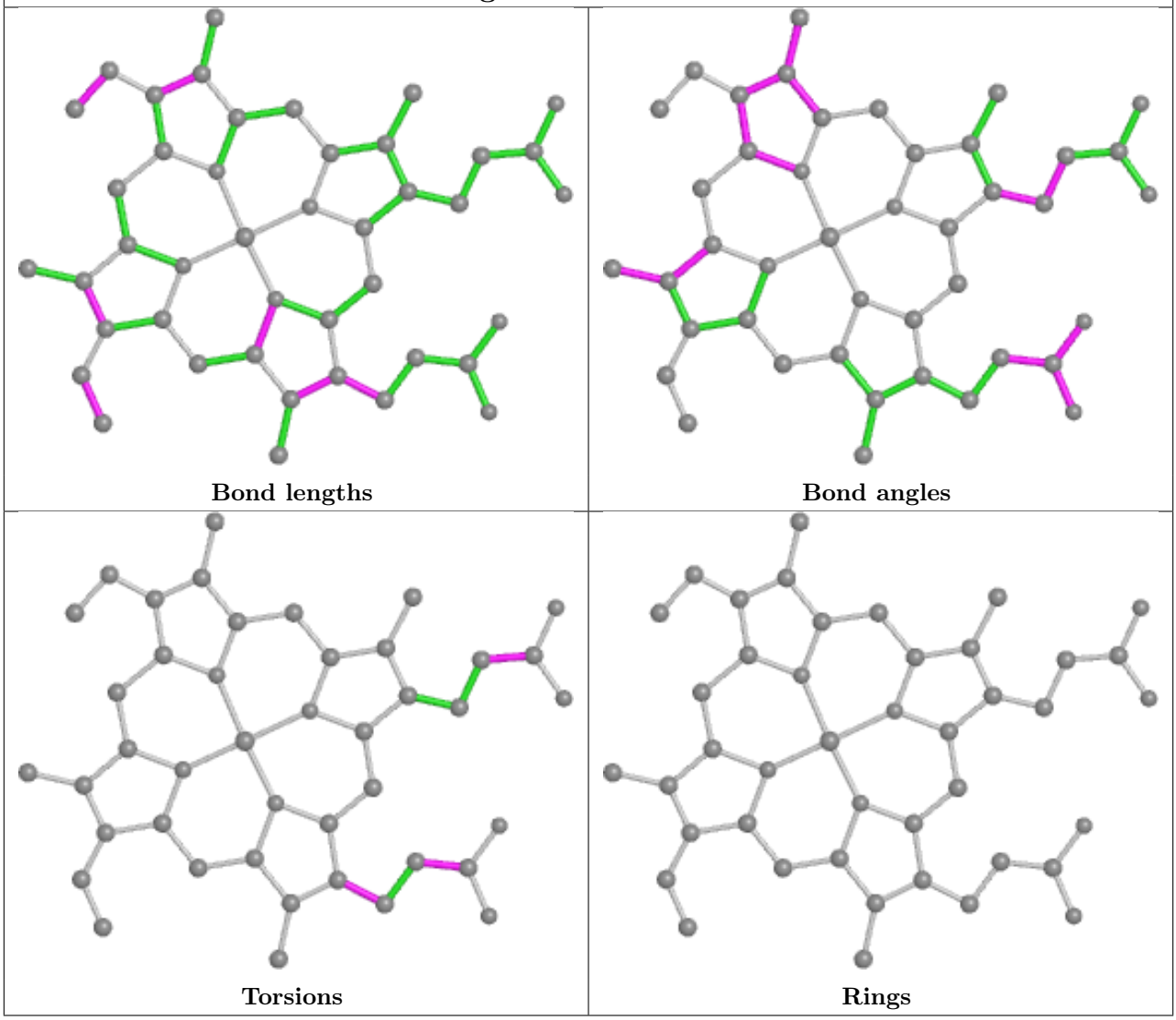


Torsions



Rings

Ligand HEC A 804



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%)	-0.34	4 (0%)	87	87	8, 15, 25, 37	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	SER	3.8
1	A	101	ASP	3.2
1	A	110	LYS	2.9
1	A	251	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	TEO	A	9806	9/9	0.94	0.10	13,17,22,25	0
3	HEC	A	802	43/43	0.95	0.10	13,18,27,32	0
3	HEC	A	803	43/43	0.97	0.10	11,16,29,36	0

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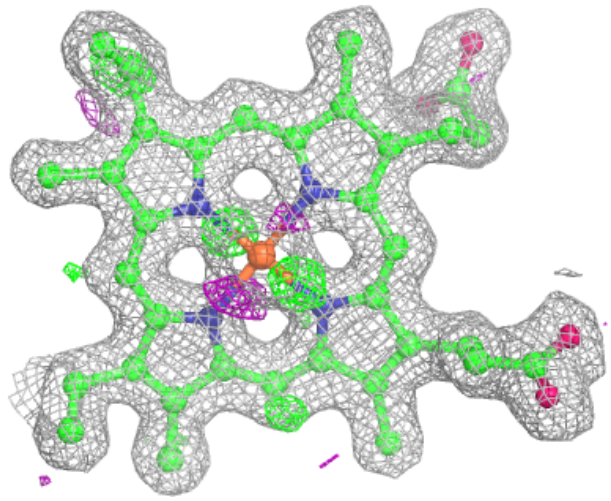
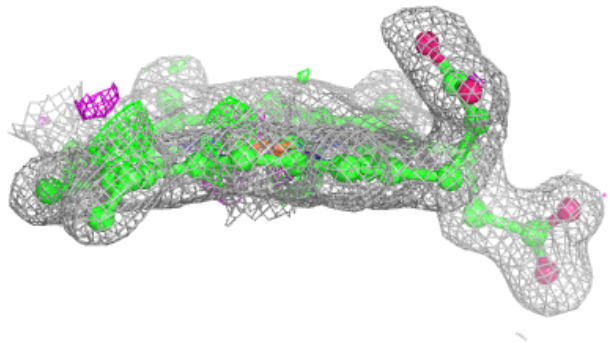
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	A	801	43/43	0.97	0.09	11,16,21,23	0
4	FAD	A	9805	53/53	0.98	0.06	7,10,15,16	0
3	HEC	A	804	43/43	0.98	0.08	9,11,17,19	0
2	NA	A	9810	1/1	1.00	0.04	9,9,9,9	0

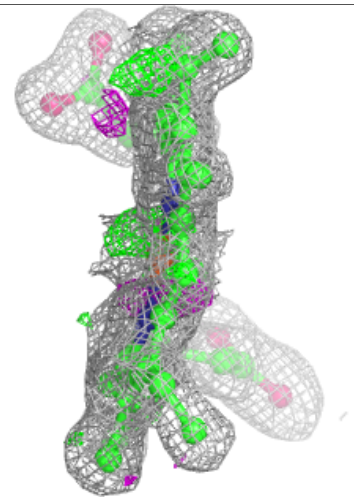
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

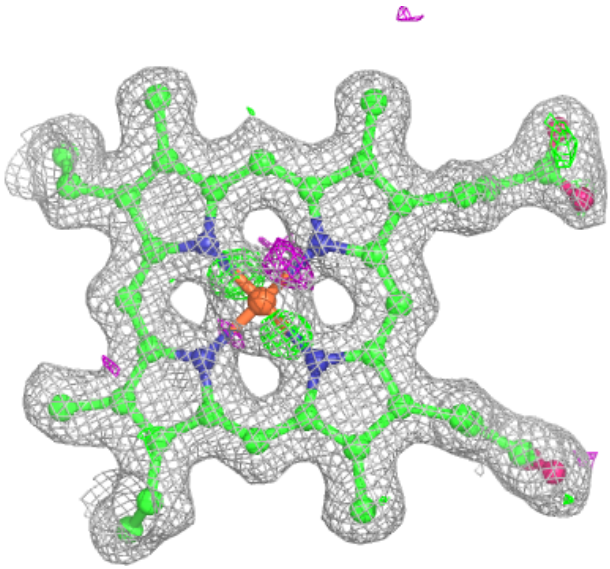


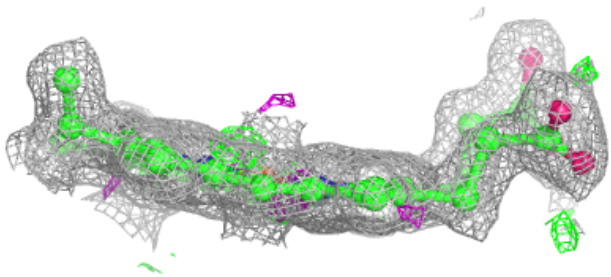


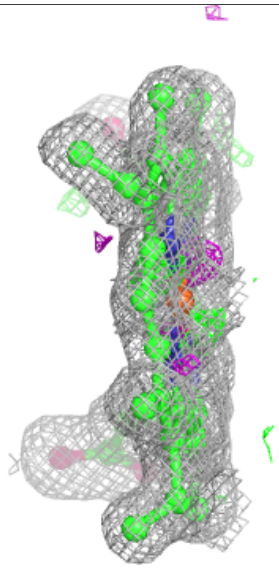


Electron density around HEC A 803:

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

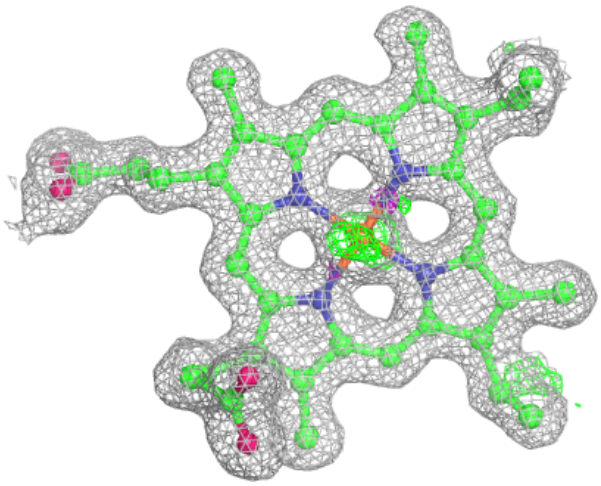


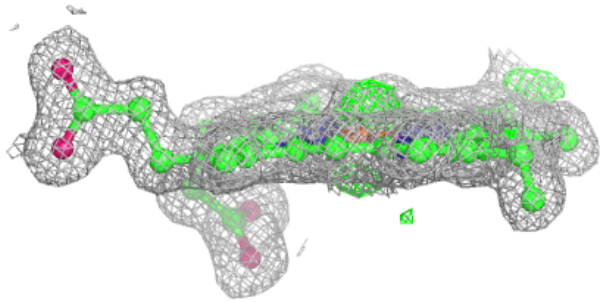


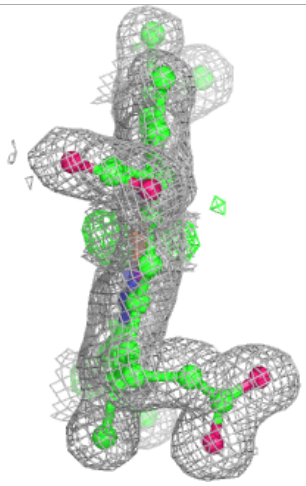


Electron density around HEC A 801:

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

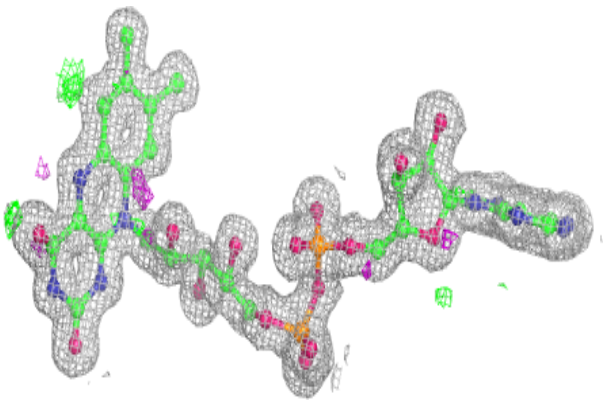


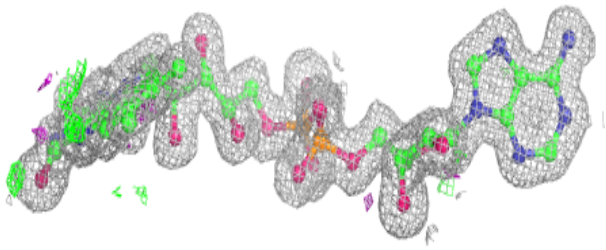


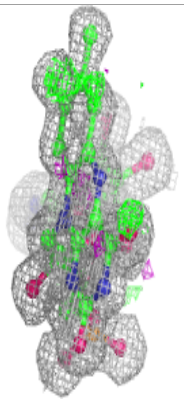


Electron density around FAD A 9805:

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

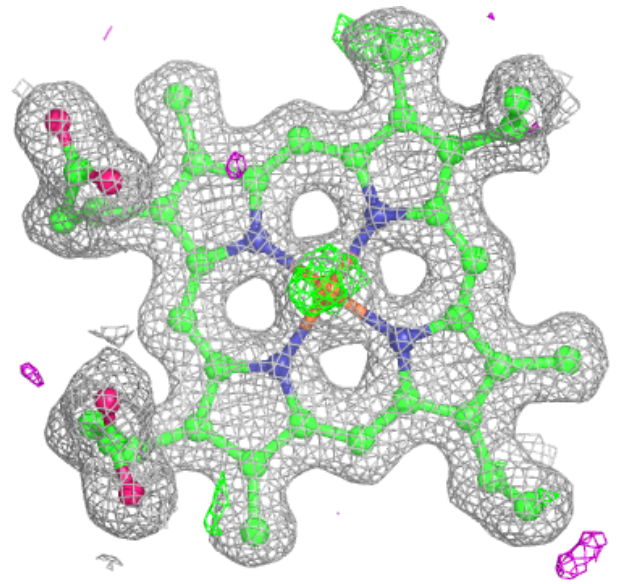


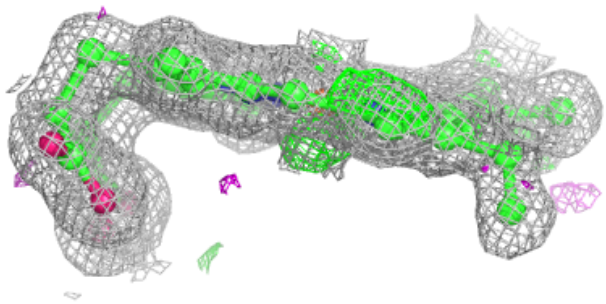


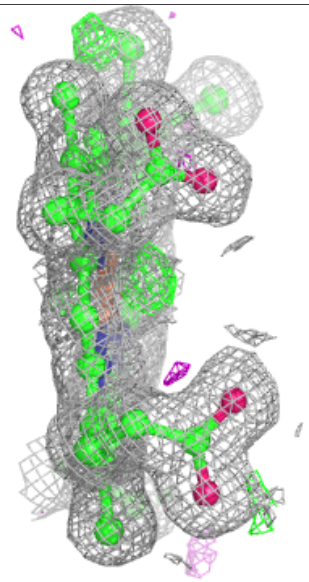


Electron density around HEC A 804:

$2mF_o$-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.