Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2024 – 12:40 pm GMT

PDB ID	:	8RVM
Title	:	Crystal structure of octaheme nitrite reductase from Trichlorobacter ammonificans in space group P63
Authors	:	Polyakov, K.M.; Safoonova, T.N.; Osipov, E.; Popov, A.N.; Tikhonova, T.V.; Popov, V.O.
Deposited on	:	2024-02-01
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 ⓘ 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:

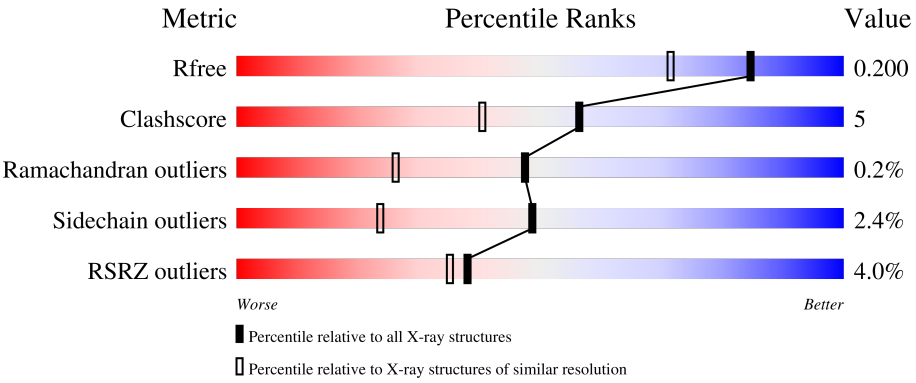
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	YYY	495	4% 91% 8%

2 Entry composition (i)

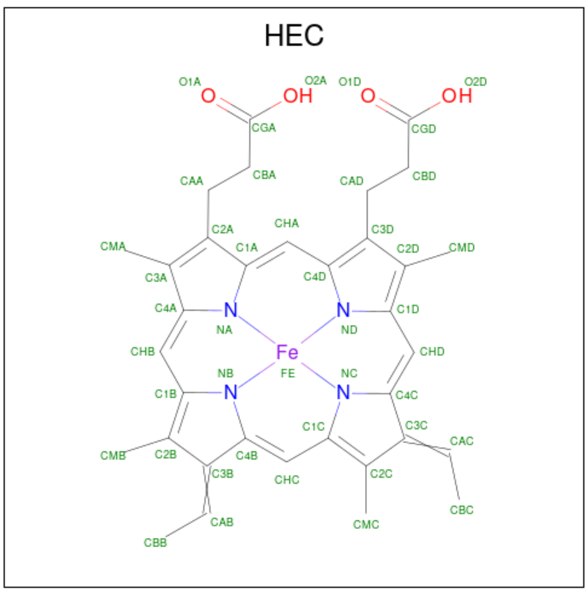
There are 5 unique types of molecules in this entry. The entry contains 4764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Octaheme nitrite c cytochrome c reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	YYY	495	Total 3909	C 2445	N 714	O 721	S 29	0	6	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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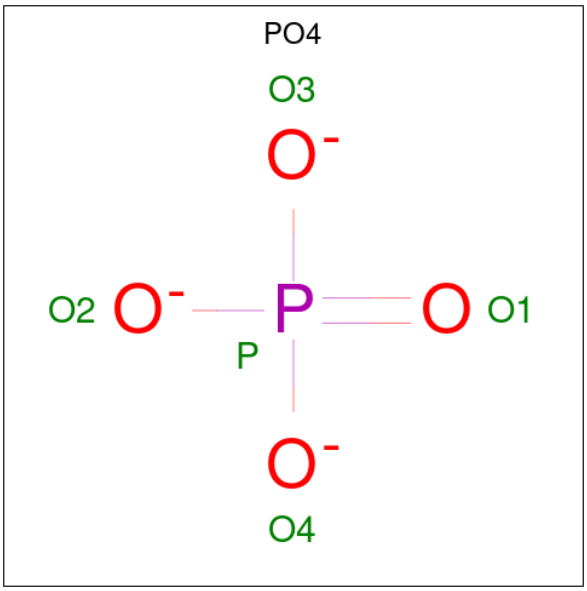
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	YYY	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	YYY	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

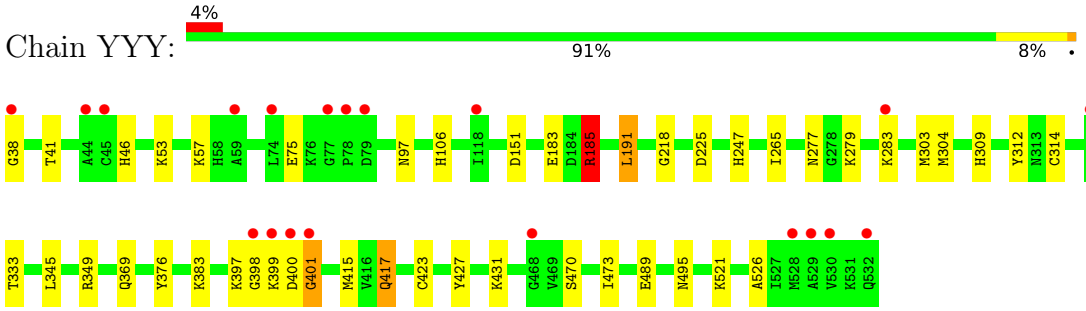
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	YYY	505	Total	O	0	0
			505	505		

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: Octaheme nitrite c cytochrome c reductase

Chain YYY:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	114.20Å 114.20Å 64.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	98.90 – 1.60 42.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.90-1.60) 99.9 (42.84-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.194 , 0.243 0.213 , 0.200	Depositor DCC
R_{free} test set	2685 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4764	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CA, PO4

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	YYY	0.76	1/4033 (0.0%)	0.88	3/5431 (0.1%)

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	YYY	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YYY	423	CYS	CB-SG	-5.03	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	YYY	417[A]	GLN	CA-CB-CG	-7.16	97.64	113.40
1	YYY	417[B]	GLN	CA-CB-CG	-7.16	97.64	113.40
1	YYY	185	ARG	NE-CZ-NH2	6.54	123.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	YYY	398	GLY	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	YYY	3909	0	3816	37	0
2	YYY	344	0	240	18	0
3	YYY	5	0	0	1	0
4	YYY	1	0	0	0	0
5	YYY	505	0	0	5	0
All	All	4764	0	4056	42	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 5.

All (42) 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:YYY:417[B]:GLN:HG3	5:YYY:1025:HOH:O	1.65	0.94
1:YYY:183:GLU:OE2	1:YYY:185:ARG:NH2	2.08	0.86
1:YYY:495:ASN:HB3	2:YYY:607:HEC:HAA1	1.66	0.75
1:YYY:277:ASN:ND2	5:YYY:701:HOH:O	2.21	0.71
1:YYY:400:ASP:OD2	1:YYY:401:GLY:N	2.24	0.71
1:YYY:312:TYR:CE2	2:YYY:604:HEC:HMC2	2.32	0.65
1:YYY:345:LEU:O	1:YYY:349:ARG:HG3	1.97	0.64
1:YYY:376:TYR:CE1	2:YYY:607:HEC:HMC2	2.35	0.62
1:YYY:495:ASN:HB3	2:YYY:607:HEC:CAA	2.30	0.61
2:YYY:608:HEC:HBC3	2:YYY:608:HEC:HMC1	1.82	0.61
1:YYY:185:ARG:HH21	1:YYY:185:ARG:HG2	1.69	0.58
1:YYY:265:ILE:HD13	1:YYY:303[A]:MET:CE	2.34	0.58
1:YYY:376:TYR:CZ	2:YYY:607:HEC:HMC2	2.42	0.54
2:YYY:606:HEC:HMA3	2:YYY:607:HEC:HBA1	1.90	0.53
1:YYY:265:ILE:CD1	1:YYY:303[A]:MET:HE2	2.38	0.53
1:YYY:97:ASN:HD21	1:YYY:399:LYS:HG2	1.73	0.52
1:YYY:46:HIS:CE1	2:YYY:601:HEC:ND	2.76	0.52
2:YYY:605:HEC:HBC3	2:YYY:605:HEC:HMC1	1.92	0.51
1:YYY:53:LYS:HD3	2:YYY:602:HEC:HBB2	1.94	0.50
1:YYY:247:HIS:CG	2:YYY:603:HEC:HMA1	2.47	0.50
1:YYY:185:ARG:HH21	1:YYY:185:ARG:CG	2.25	0.49
1:YYY:265:ILE:HD13	1:YYY:303[A]:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:314:CYS:HA	1:YYY:333:THR:O	2.13	0.48
1:YYY:218:GLY:O	1:YYY:225:ASP:HB2	2.13	0.48
1:YYY:312:TYR:CD2	2:YYY:604:HEC:HMC2	2.49	0.48
1:YYY:304:MET:SD	2:YYY:605:HEC:HMD3	2.53	0.47
1:YYY:473:ILE:HG21	1:YYY:526:ALA:CB	2.44	0.47
1:YYY:57:LYS:HG2	5:YYY:821:HOH:O	2.14	0.47
1:YYY:265:ILE:HD13	1:YYY:303[A]:MET:HE1	1.98	0.46
1:YYY:309:HIS:CE1	2:YYY:604:HEC:HMD1	2.51	0.45
1:YYY:473:ILE:HG21	1:YYY:526:ALA:HB2	1.99	0.45
1:YYY:38:GLY:N	5:YYY:718:HOH:O	2.49	0.45
1:YYY:369:GLN:HG2	3:YYY:609:PO4:O2	2.17	0.44
1:YYY:191:LEU:HD23	1:YYY:191:LEU:HA	1.90	0.43
1:YYY:427:TYR:CE1	1:YYY:431:LYS:HE2	2.55	0.42
1:YYY:151:ASP:OD2	2:YYY:606:HEC:O2D	2.38	0.41
1:YYY:97:ASN:ND2	1:YYY:399:LYS:HE3	2.36	0.41
2:YYY:607:HEC:HMC1	2:YYY:607:HEC:HBC3	2.02	0.41
1:YYY:41:THR:O	2:YYY:601:HEC:HMC3	2.21	0.41
1:YYY:106:HIS:HE1	5:YYY:880:HOH:O	2.04	0.41
2:YYY:607:HEC:HBB3	2:YYY:607:HEC:HMB1	2.03	0.41
1:YYY:383:LYS:HB2	1:YYY:383:LYS:HE3	1.91	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	YYY	499/495 (101%)	478 (96%)	20 (4%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	YYY	401	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	YYY	420/414 (101%)	409 (97%)	11 (3%)	46 21

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	YYY	75	GLU
1	YYY	185	ARG
1	YYY	191	LEU
1	YYY	279	LYS
1	YYY	283	LYS
1	YYY	397	LYS
1	YYY	415[A]	MET
1	YYY	415[B]	MET
1	YYY	470	SER
1	YYY	489	GLU
1	YYY	521	LYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	YYY	603	1	32,50,50	2.13	5 (15%)	24,82,82	2.54	6 (25%)
2	HEC	YYY	607	1	32,50,50	1.55	7 (21%)	24,82,82	2.27	8 (33%)
3	PO4	YYY	609	2	4,4,4	2.04	1 (25%)	6,6,6	0.75	0
2	HEC	YYY	602	1	32,50,50	2.08	9 (28%)	24,82,82	1.86	7 (29%)
2	HEC	YYY	608	1	32,50,50	1.80	4 (12%)	24,82,82	2.84	6 (25%)
2	HEC	YYY	605	1	32,50,50	1.75	7 (21%)	24,82,82	2.27	6 (25%)
2	HEC	YYY	606	1	32,50,50	1.59	8 (25%)	24,82,82	2.15	7 (29%)
2	HEC	YYY	604	3,1	32,50,50	1.87	7 (21%)	24,82,82	1.69	5 (20%)
2	HEC	YYY	601	1	32,50,50	1.97	7 (21%)	24,82,82	3.15	8 (33%)

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	YYY	603	1	-	2/10/54/54	-
2	HEC	YYY	607	1	-	4/10/54/54	-
2	HEC	YYY	602	1	-	3/10/54/54	-
2	HEC	YYY	608	1	-	2/10/54/54	-
2	HEC	YYY	605	1	-	2/10/54/54	-
2	HEC	YYY	606	1	-	1/10/54/54	-
2	HEC	YYY	604	3,1	-	2/10/54/54	-
2	HEC	YYY	601	1	-	6/10/54/54	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	602	HEC	C3C-C2C	6.93	1.48	1.40
2	YYY	603	HEC	C3C-C2C	6.50	1.47	1.40
2	YYY	608	HEC	C3C-C2C	6.39	1.47	1.40
2	YYY	603	HEC	C2B-C3B	6.25	1.47	1.40
2	YYY	601	HEC	C2B-C3B	6.17	1.47	1.40
2	YYY	604	HEC	C2B-C3B	5.22	1.46	1.40
2	YYY	604	HEC	C3C-C2C	5.13	1.46	1.40
2	YYY	601	HEC	C3C-C2C	4.97	1.45	1.40
2	YYY	605	HEC	C2B-C3B	4.84	1.45	1.40
2	YYY	602	HEC	C2B-C3B	4.10	1.45	1.40
2	YYY	607	HEC	C2B-C3B	3.89	1.44	1.40
3	YYY	609	PO4	P-O1	3.81	1.59	1.50
2	YYY	602	HEC	C4B-C3B	3.62	1.49	1.43
2	YYY	606	HEC	C3C-C2C	3.57	1.44	1.40
2	YYY	605	HEC	C3C-C2C	3.19	1.44	1.40
2	YYY	603	HEC	C3D-C2D	3.19	1.47	1.37
2	YYY	608	HEC	C3D-C2D	3.19	1.47	1.37
2	YYY	601	HEC	C3A-C4A	3.11	1.49	1.42
2	YYY	605	HEC	C2A-C1A	3.08	1.49	1.42
2	YYY	601	HEC	C2A-C3A	3.00	1.46	1.37
2	YYY	607	HEC	C3C-C2C	2.93	1.43	1.40
2	YYY	605	HEC	C1B-NB	-2.74	1.30	1.36
2	YYY	601	HEC	C1B-CHB	2.73	1.48	1.41
2	YYY	606	HEC	C2B-C3B	2.68	1.43	1.40
2	YYY	602	HEC	O1A-CGA	2.68	1.31	1.22
2	YYY	607	HEC	C3D-C2D	2.62	1.45	1.37
2	YYY	606	HEC	C4B-C3B	2.59	1.47	1.43
2	YYY	608	HEC	C4D-CHA	2.58	1.48	1.41
2	YYY	604	HEC	C2A-C3A	2.56	1.45	1.37
2	YYY	602	HEC	CAA-C2A	-2.48	1.47	1.52
2	YYY	605	HEC	C1C-CHC	2.46	1.47	1.41
2	YYY	605	HEC	C2A-C3A	2.44	1.44	1.37
2	YYY	608	HEC	CAA-C2A	-2.43	1.48	1.52
2	YYY	607	HEC	C1C-NC	-2.43	1.31	1.36
2	YYY	606	HEC	C3D-C2D	2.41	1.44	1.37
2	YYY	606	HEC	CAA-C2A	-2.39	1.48	1.52
2	YYY	606	HEC	C2A-C3A	2.39	1.44	1.37
2	YYY	601	HEC	C3D-C2D	2.38	1.44	1.37
2	YYY	602	HEC	C3D-C2D	2.35	1.44	1.37
2	YYY	605	HEC	C3D-C2D	2.32	1.44	1.37
2	YYY	602	HEC	C1D-ND	-2.30	1.31	1.36
2	YYY	603	HEC	CAA-C2A	-2.30	1.48	1.52
2	YYY	602	HEC	O1D-CGD	2.26	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YYY	607	HEC	O2D-CGD	-2.24	1.23	1.30
2	YYY	604	HEC	CAA-C2A	-2.24	1.48	1.52
2	YYY	604	HEC	CBD-CGD	2.23	1.55	1.50
2	YYY	602	HEC	C1C-CHC	2.22	1.47	1.41
2	YYY	601	HEC	C4D-ND	-2.20	1.31	1.36
2	YYY	604	HEC	C1C-CHC	2.18	1.47	1.41
2	YYY	603	HEC	C2A-C3A	2.17	1.44	1.37
2	YYY	607	HEC	C2A-C3A	2.13	1.44	1.37
2	YYY	604	HEC	C1D-CHD	2.12	1.46	1.41
2	YYY	607	HEC	C1D-CHD	2.07	1.46	1.41
2	YYY	606	HEC	C1D-ND	-2.01	1.32	1.36
2	YYY	606	HEC	C1D-CHD	2.01	1.46	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	YYY	608	HEC	CBA-CAA-C2A	-10.04	95.68	112.60
2	YYY	601	HEC	C1D-C2D-C3D	-9.22	100.58	107.00
2	YYY	605	HEC	C1D-C2D-C3D	-6.98	102.14	107.00
2	YYY	603	HEC	C1D-C2D-C3D	-6.92	102.18	107.00
2	YYY	601	HEC	CMB-C2B-C3B	6.05	132.93	125.82
2	YYY	603	HEC	CMB-C2B-C3B	5.76	132.59	125.82
2	YYY	606	HEC	CBA-CAA-C2A	-5.66	103.06	112.60
2	YYY	608	HEC	CMC-C2C-C3C	5.54	132.34	125.82
2	YYY	607	HEC	CBD-CAD-C3D	5.30	121.67	112.62
2	YYY	608	HEC	C1D-C2D-C3D	-5.29	103.32	107.00
2	YYY	601	HEC	CMC-C2C-C3C	5.03	131.73	125.82
2	YYY	602	HEC	CMC-C2C-C3C	5.03	131.73	125.82
2	YYY	601	HEC	CBA-CAA-C2A	4.86	120.79	112.60
2	YYY	607	HEC	C1D-C2D-C3D	-4.85	103.62	107.00
2	YYY	606	HEC	C1D-C2D-C3D	-4.73	103.70	107.00
2	YYY	603	HEC	CMC-C2C-C3C	4.65	131.29	125.82
2	YYY	601	HEC	CBD-CAD-C3D	4.62	120.51	112.62
2	YYY	603	HEC	CBD-CAD-C3D	-4.28	105.31	112.62
2	YYY	607	HEC	CBA-CAA-C2A	-4.27	105.41	112.60
2	YYY	604	HEC	CMB-C2B-C3B	4.01	130.53	125.82
2	YYY	602	HEC	CMB-C2B-C3B	4.01	130.53	125.82
2	YYY	605	HEC	CMB-C2B-C3B	3.62	130.07	125.82
2	YYY	604	HEC	C1D-C2D-C3D	-3.59	104.50	107.00
2	YYY	603	HEC	CAA-CBA-CGA	-3.58	103.72	113.76
2	YYY	601	HEC	CAD-CBD-CGD	-3.47	104.04	113.76
2	YYY	606	HEC	CMC-C2C-C3C	3.32	129.72	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	YYY	605	HEC	CBA-CAA-C2A	3.31	118.19	112.60
2	YYY	605	HEC	CBD-CAD-C3D	-3.28	107.02	112.62
2	YYY	604	HEC	CBD-CAD-C3D	-3.13	107.29	112.62
2	YYY	607	HEC	CMB-C2B-C3B	3.10	129.47	125.82
2	YYY	606	HEC	CMD-C2D-C3D	2.78	130.19	124.94
2	YYY	601	HEC	CAA-CBA-CGA	-2.73	106.11	113.76
2	YYY	606	HEC	C2B-C3B-C4B	-2.73	103.41	106.35
2	YYY	607	HEC	C4C-C3C-C2C	-2.70	103.44	106.35
2	YYY	602	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
2	YYY	606	HEC	CMB-C2B-C3B	2.62	128.90	125.82
2	YYY	608	HEC	CAD-CBD-CGD	-2.60	106.48	113.76
2	YYY	602	HEC	CMD-C2D-C3D	2.51	129.68	124.94
2	YYY	603	HEC	CMD-C2D-C3D	2.48	129.62	124.94
2	YYY	605	HEC	CAD-CBD-CGD	-2.47	106.84	113.76
2	YYY	608	HEC	CMB-C2B-C3B	2.46	128.71	125.82
2	YYY	607	HEC	CMC-C2C-C3C	2.36	128.59	125.82
2	YYY	604	HEC	CMC-C2C-C3C	2.32	128.54	125.82
2	YYY	602	HEC	CMD-C2D-C1D	-2.25	125.00	128.46
2	YYY	608	HEC	CAA-CBA-CGA	2.24	120.05	113.76
2	YYY	602	HEC	CAD-C3D-C2D	2.20	133.56	127.25
2	YYY	607	HEC	C3B-C4B-NB	2.19	115.09	110.94
2	YYY	607	HEC	CAD-CBD-CGD	-2.11	107.85	113.76
2	YYY	605	HEC	C2B-C3B-C4B	-2.10	104.08	106.35
2	YYY	601	HEC	CAD-C3D-C2D	2.10	133.29	127.25
2	YYY	606	HEC	CBD-CAD-C3D	-2.08	109.07	112.62
2	YYY	604	HEC	C2B-C3B-C4B	-2.04	104.15	106.35
2	YYY	602	HEC	C2B-C3B-C4B	-2.02	104.17	106.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	YYY	601	HEC	C2D-C3D-CAD-CBD
2	YYY	601	HEC	C4D-C3D-CAD-CBD
2	YYY	607	HEC	CAA-CBA-CGA-O2A
2	YYY	608	HEC	CAD-CBD-CGD-O1D
2	YYY	601	HEC	CAA-CBA-CGA-O1A
2	YYY	601	HEC	CAD-CBD-CGD-O2D
2	YYY	604	HEC	CAA-CBA-CGA-O1A
2	YYY	601	HEC	CAD-CBD-CGD-O1D
2	YYY	603	HEC	CAD-CBD-CGD-O1D
2	YYY	601	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	YYY	607	HEC	CAA-CBA-CGA-O1A
2	YYY	603	HEC	CAD-CBD-CGD-O2D
2	YYY	605	HEC	CAA-CBA-CGA-O2A
2	YYY	604	HEC	CAA-CBA-CGA-O2A
2	YYY	608	HEC	CAD-CBD-CGD-O2D
2	YYY	602	HEC	CAA-CBA-CGA-O2A
2	YYY	602	HEC	CAA-CBA-CGA-O1A
2	YYY	605	HEC	CAA-CBA-CGA-O1A
2	YYY	606	HEC	CAA-CBA-CGA-O1A
2	YYY	607	HEC	CAD-CBD-CGD-O2D
2	YYY	607	HEC	CAD-CBD-CGD-O1D
2	YYY	602	HEC	C3D-CAD-CBD-CGD

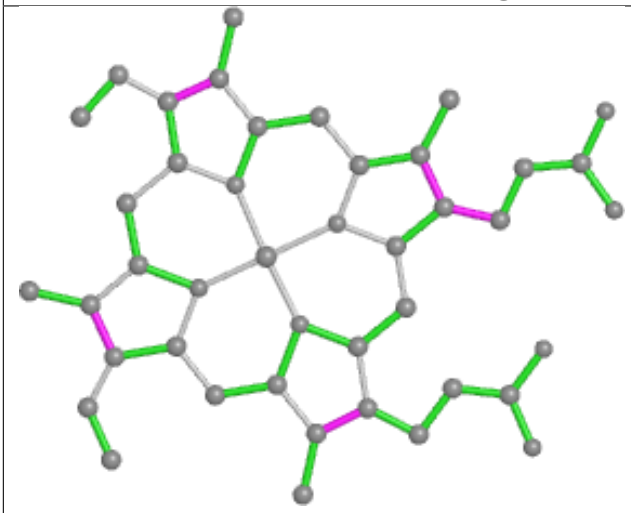
There are no ring outliers.

9 monomers are involved in 19 short contacts:

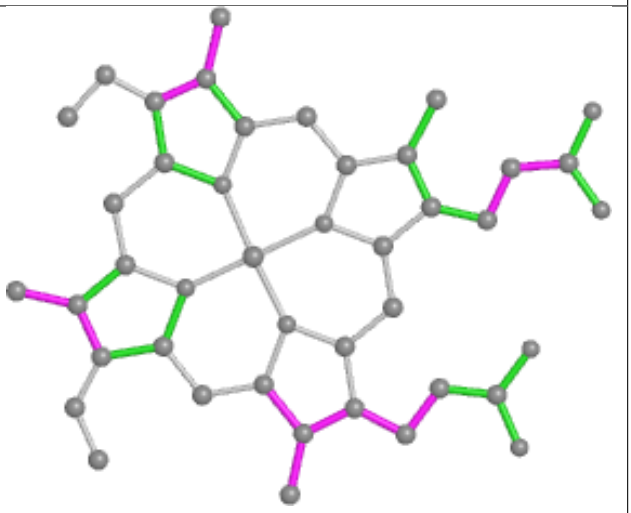
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	YYY	603	HEC	1	0
2	YYY	607	HEC	7	0
3	YYY	609	PO4	1	0
2	YYY	602	HEC	1	0
2	YYY	608	HEC	1	0
2	YYY	605	HEC	2	0
2	YYY	606	HEC	2	0
2	YYY	604	HEC	3	0
2	YYY	601	HEC	2	0

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

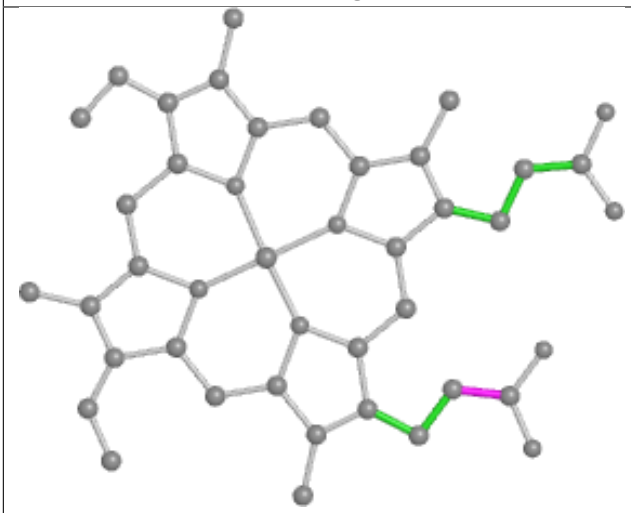
Ligand HEC YYY 603



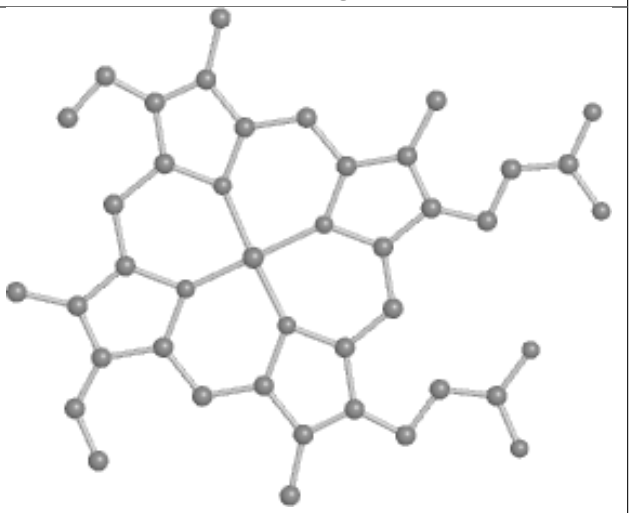
Bond lengths



Bond angles

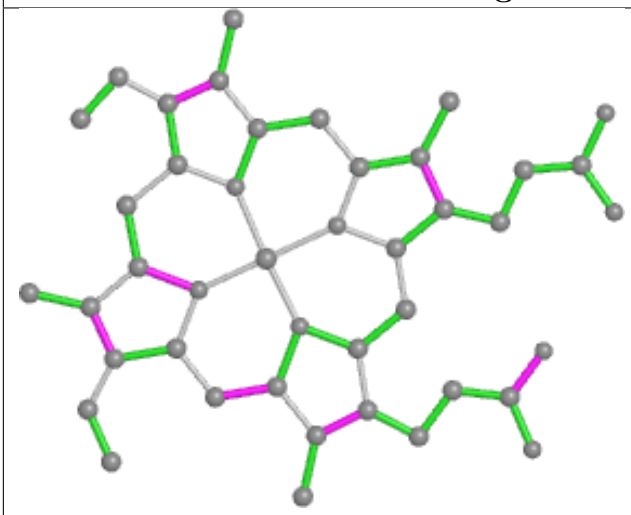


Torsions

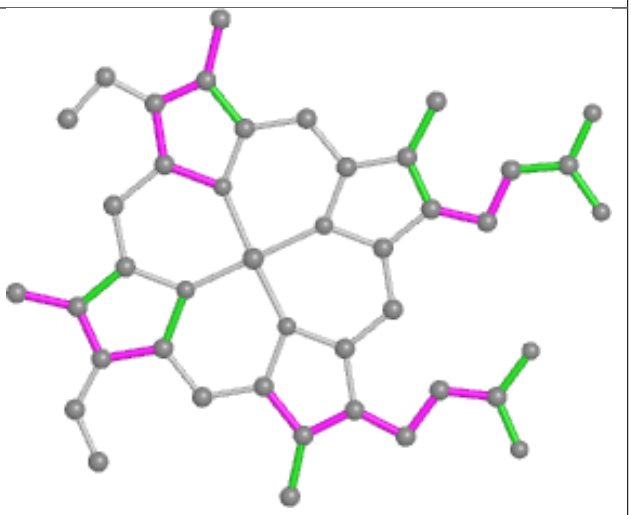


Rings

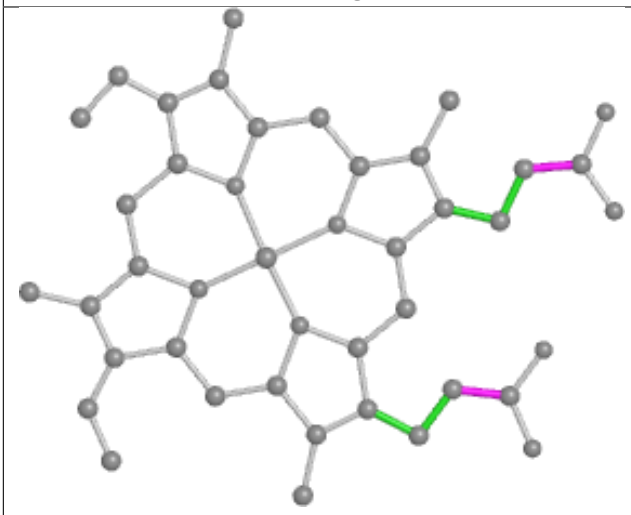
Ligand HEC YYY 607



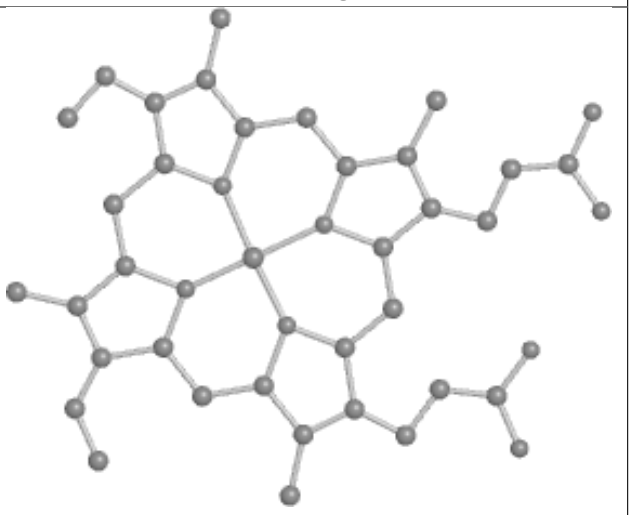
Bond lengths



Bond angles

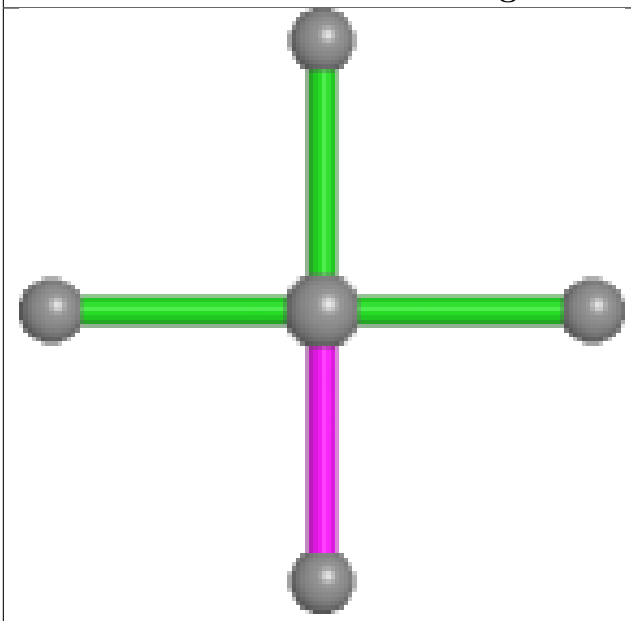


Torsions

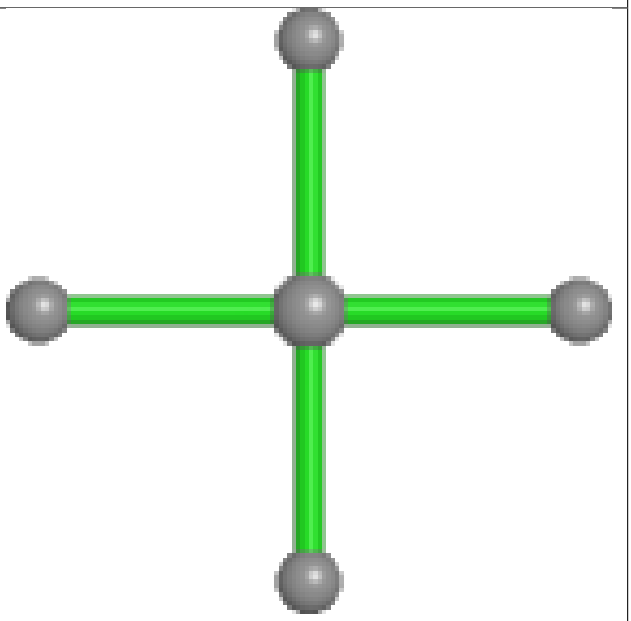


Rings

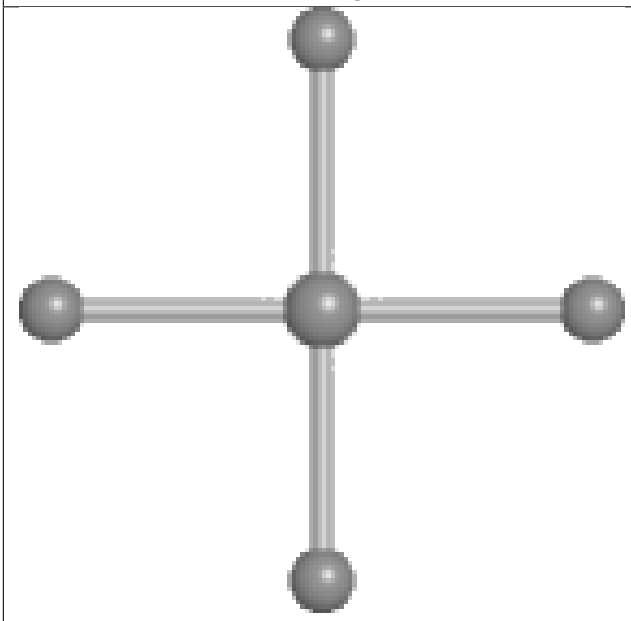
Ligand PO4 YYY 609



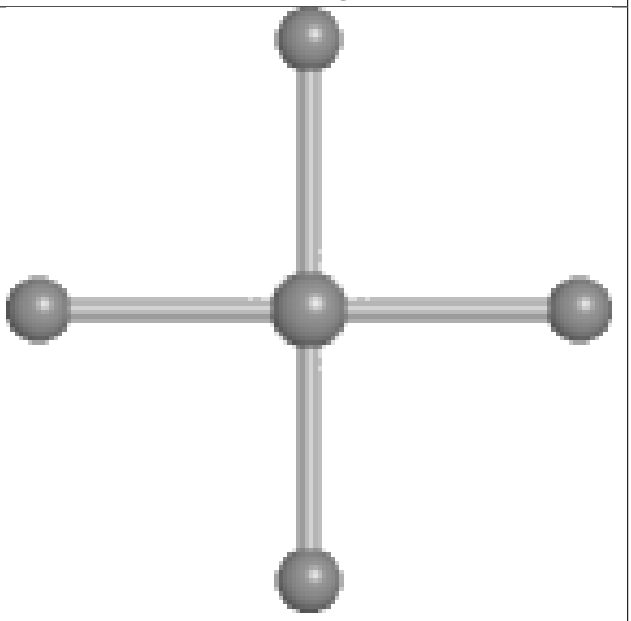
Bond lengths



Bond angles

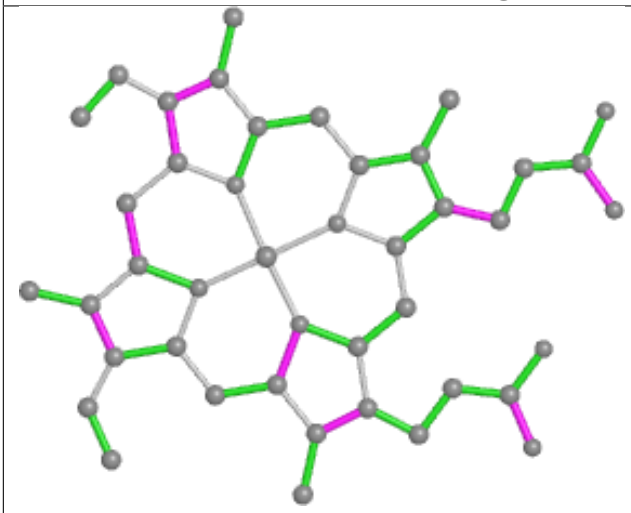


Torsions

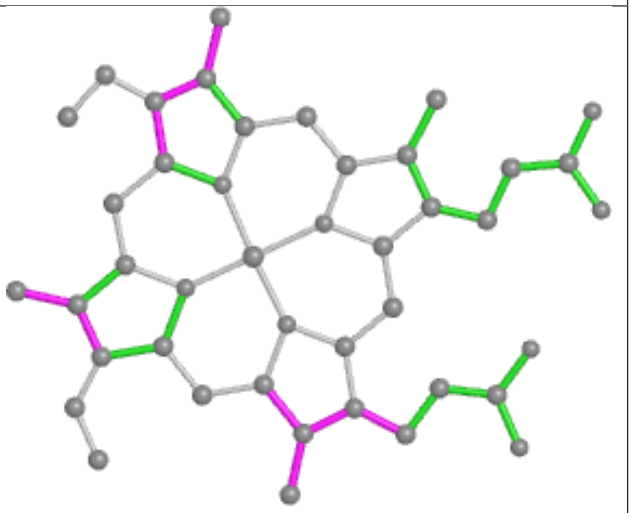


Rings

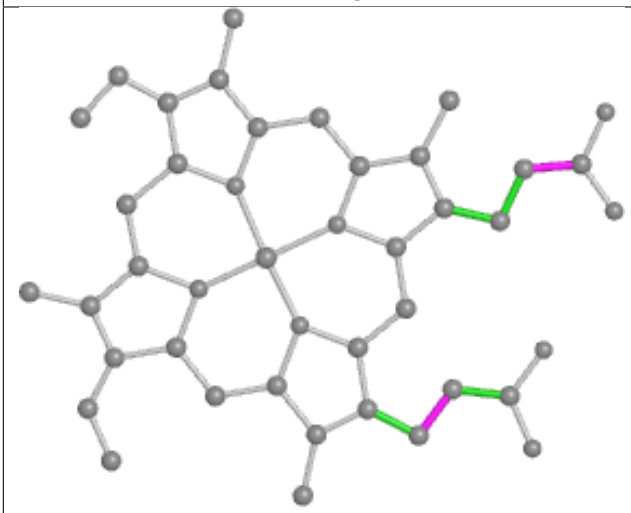
Ligand HEC YYY 602



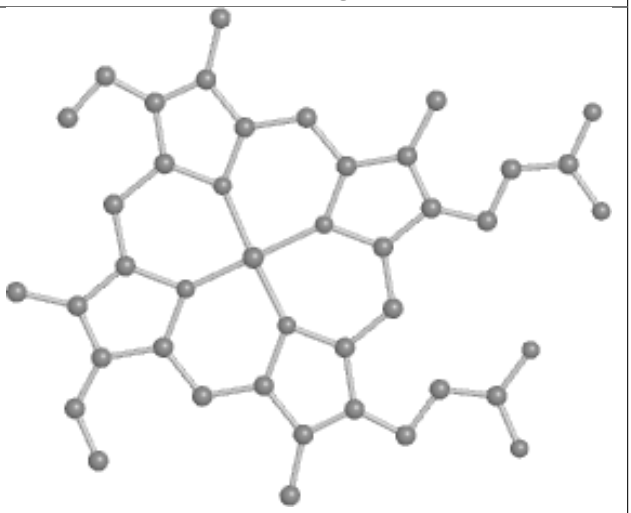
Bond lengths



Bond angles

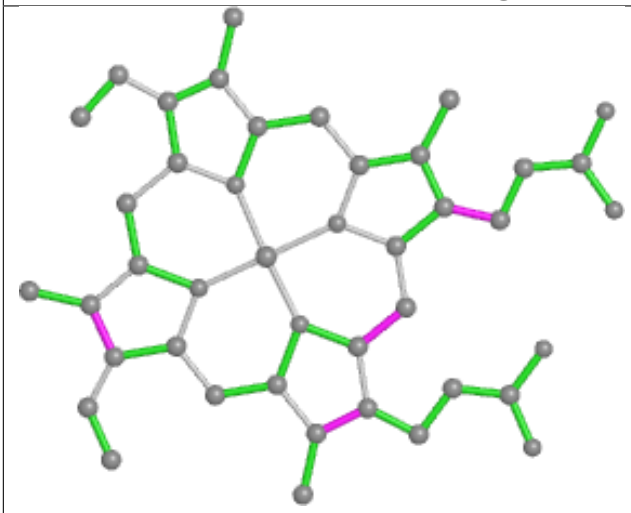


Torsions

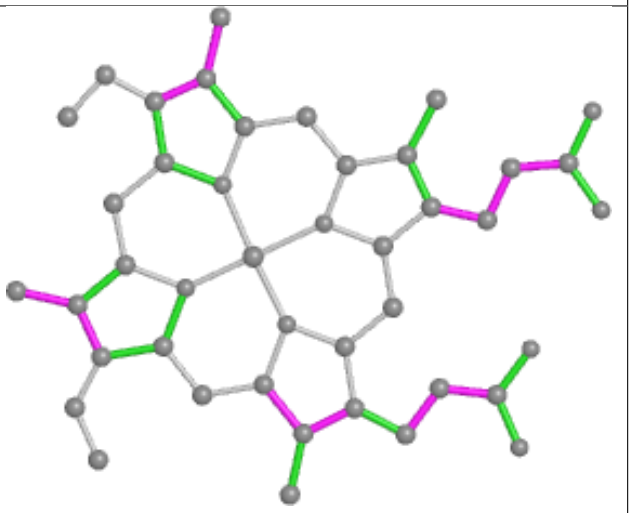


Rings

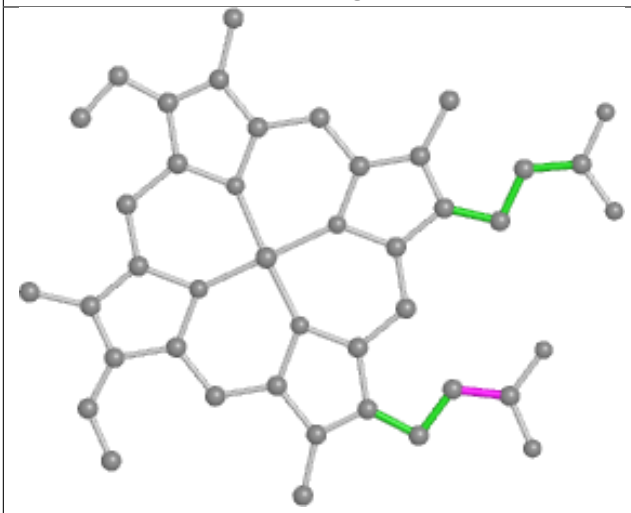
Ligand HEC YYY 608



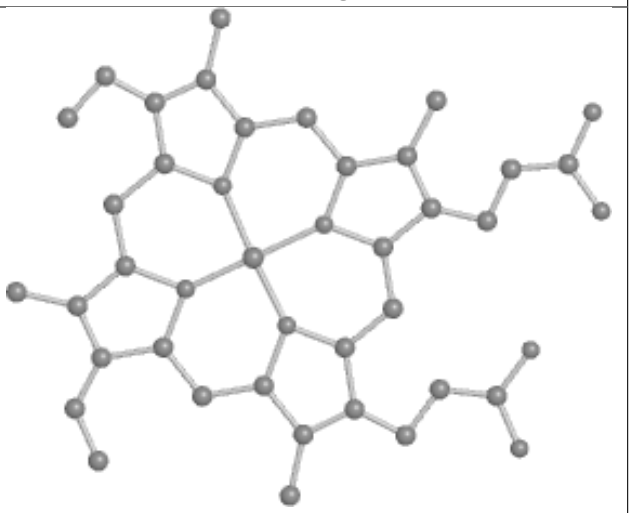
Bond lengths



Bond angles

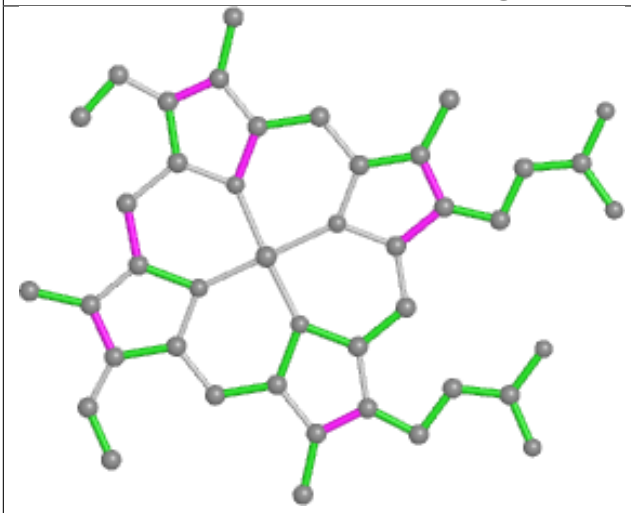


Torsions

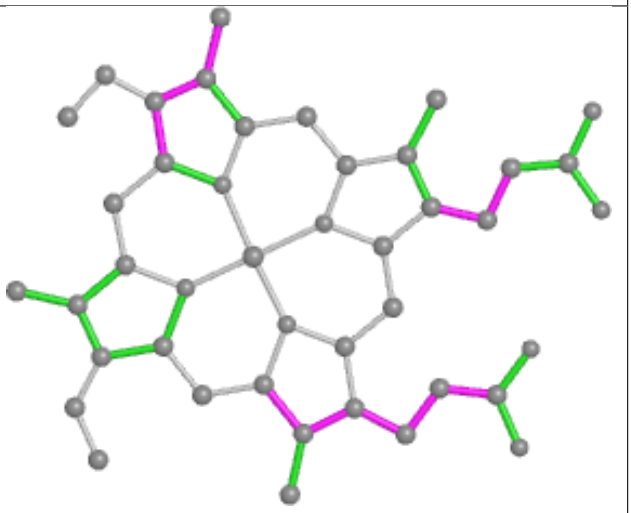


Rings

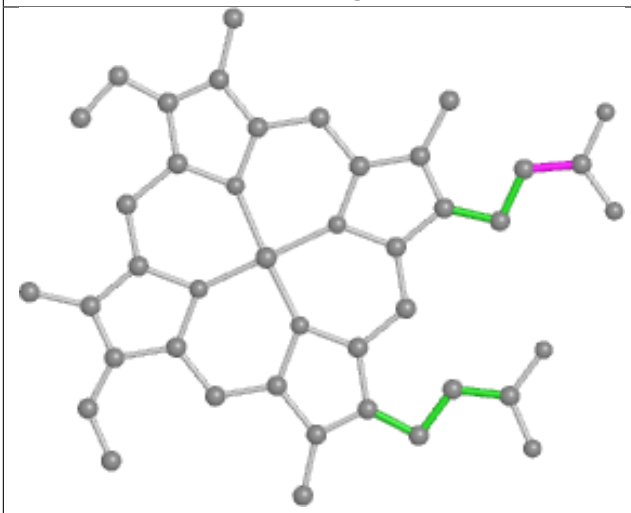
Ligand HEC YYY 605



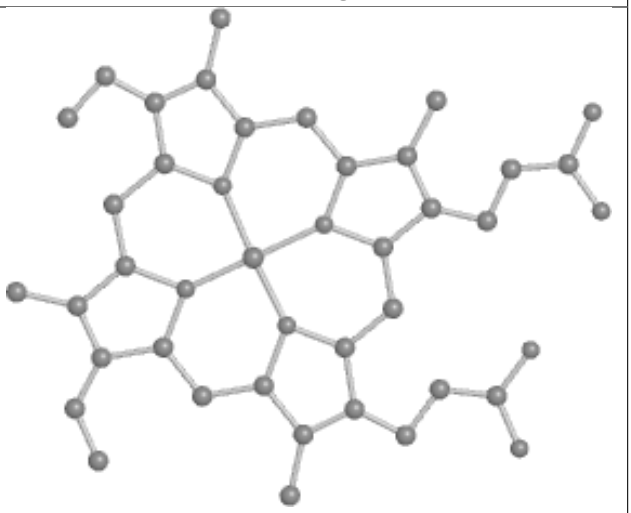
Bond lengths



Bond angles

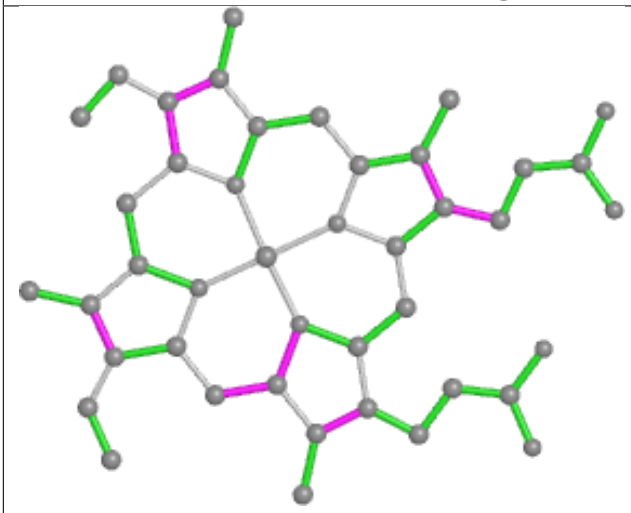


Torsions

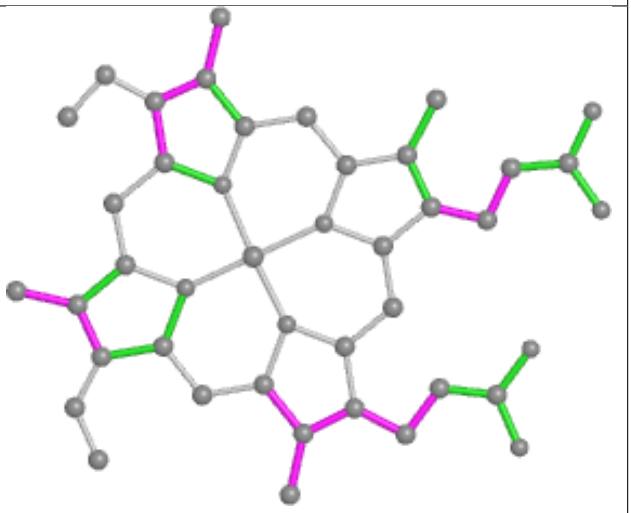


Rings

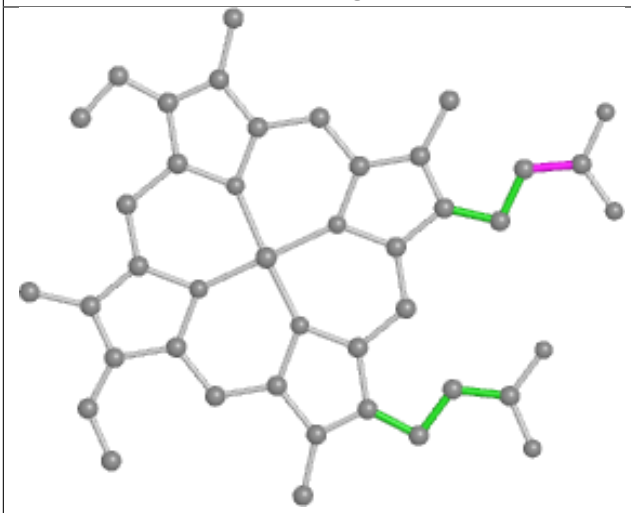
Ligand HEC YYY 606



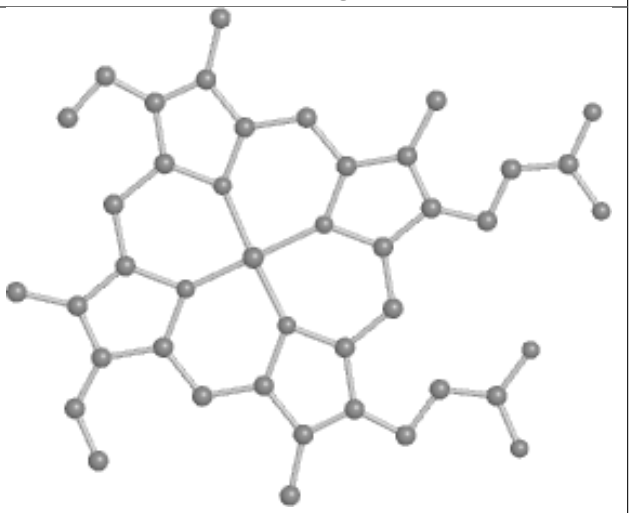
Bond lengths



Bond angles

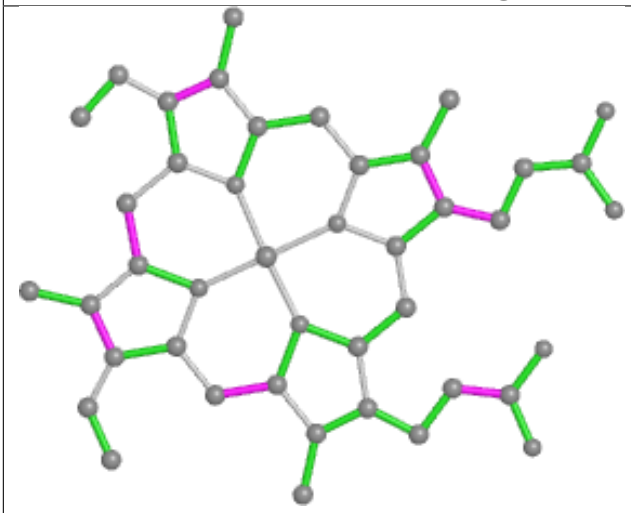


Torsions

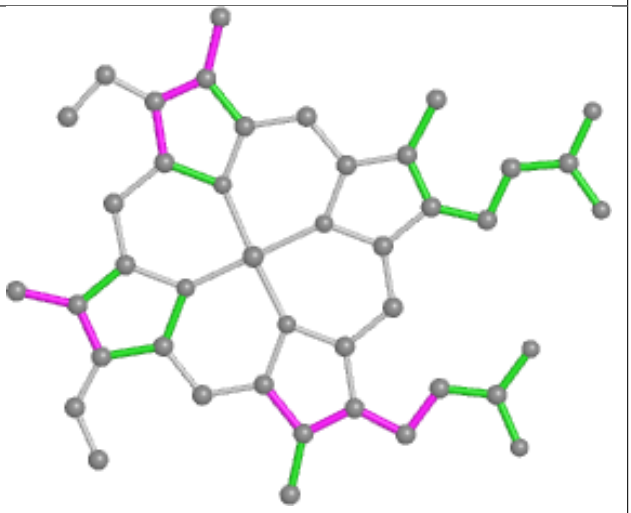


Rings

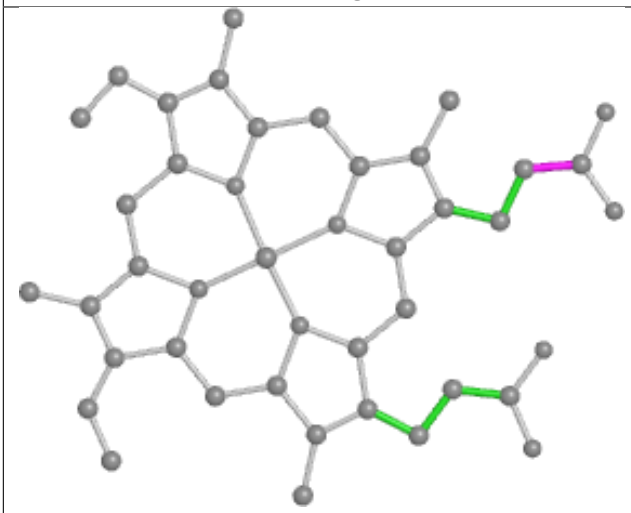
Ligand HEC YYY 604



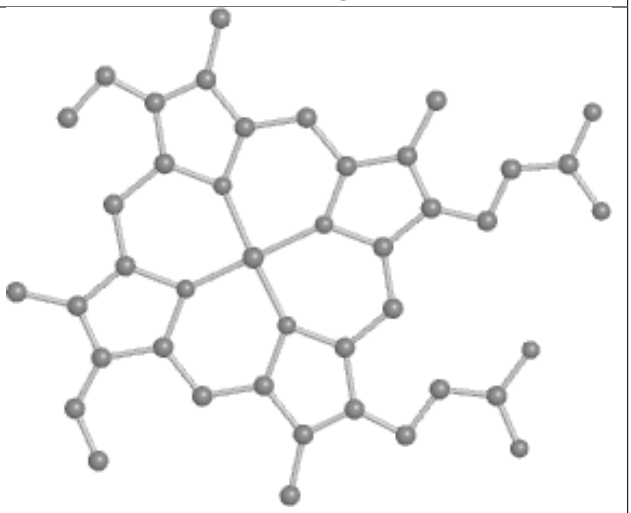
Bond lengths



Bond angles

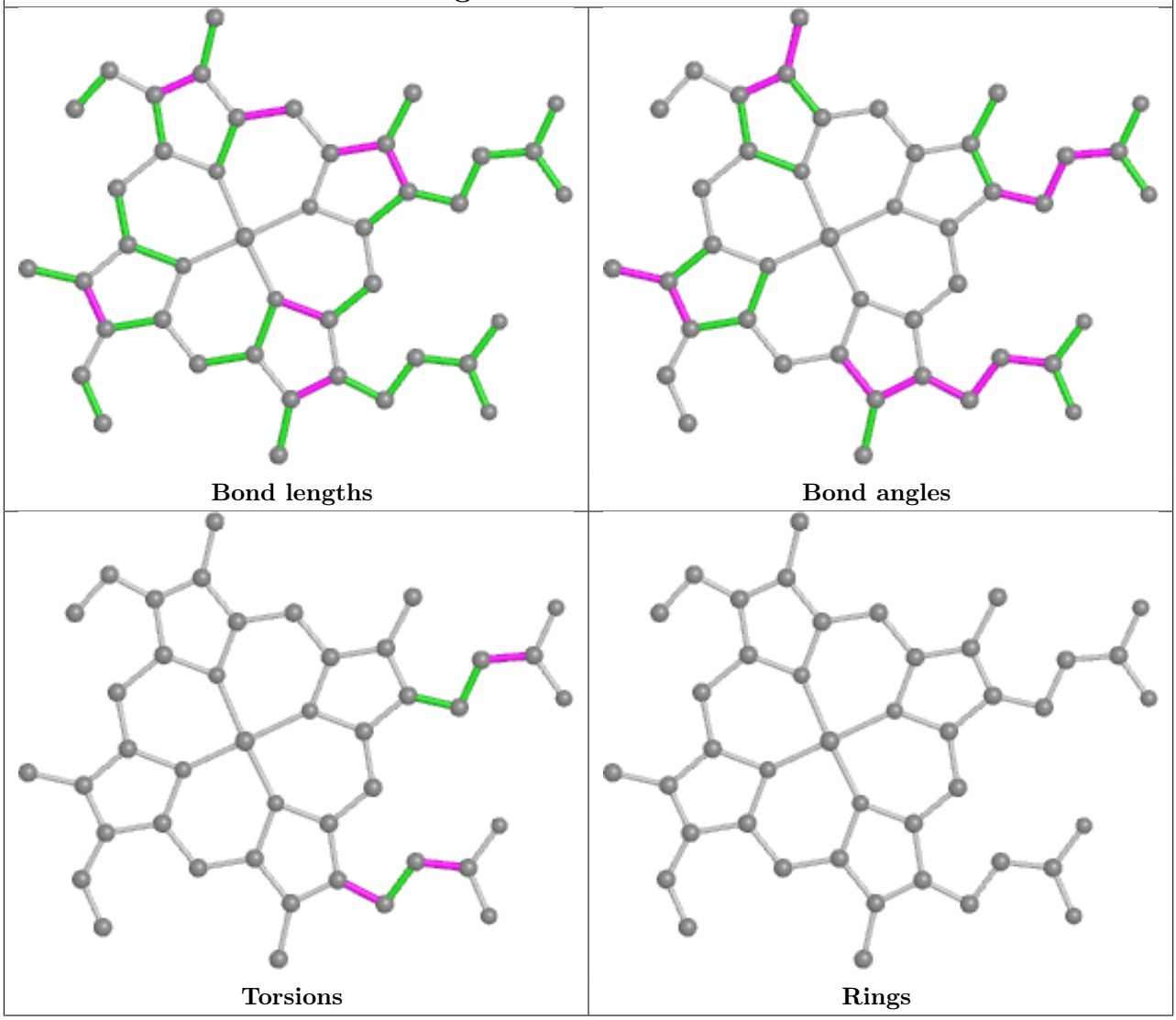


Torsions



Rings

Ligand HEC YYY 601



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

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, 95^{th} 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	YYY	495/495 (100%)	0.28	20 (4%) 38 35	10, 20, 42, 90	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	YYY	400	ASP	6.8
1	YYY	401	GLY	5.7
1	YYY	528	MET	5.4
1	YYY	399	LYS	4.1
1	YYY	530	VAL	3.6
1	YYY	38	GLY	3.4
1	YYY	468	GLY	3.3
1	YYY	79	ASP	3.3
1	YYY	45	CYS	3.2
1	YYY	74	LEU	2.8
1	YYY	59	ALA	2.7
1	YYY	78	PRO	2.7
1	YYY	532	GLN	2.6
1	YYY	529	ALA	2.5
1	YYY	283	LYS	2.3
1	YYY	77	GLY	2.2
1	YYY	398	GLY	2.2
1	YYY	322	ASP	2.2
1	YYY	44	ALA	2.1
1	YYY	118	ILE	2.0

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

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)

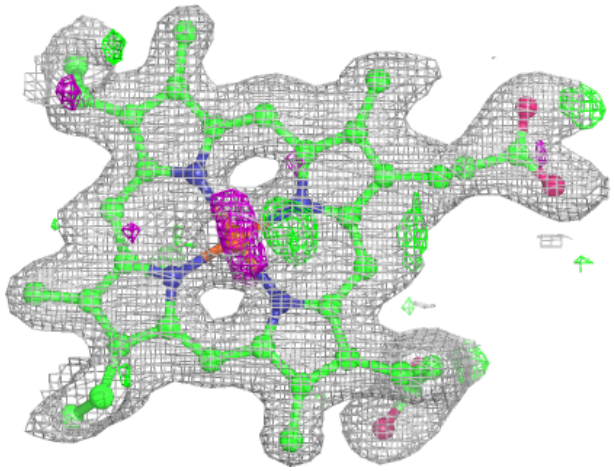
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

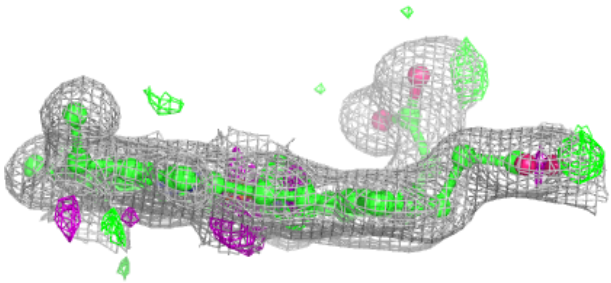
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	YYY	602	43/43	0.90	0.12	16,20,24,25	0
2	HEC	YYY	603	43/43	0.92	0.13	18,24,31,34	0
2	HEC	YYY	601	43/43	0.93	0.14	17,23,39,55	0
2	HEC	YYY	605	43/43	0.93	0.11	16,18,23,26	0
2	HEC	YYY	608	43/43	0.95	0.11	13,17,29,44	0
2	HEC	YYY	606	43/43	0.96	0.09	10,12,13,15	0
2	HEC	YYY	607	43/43	0.96	0.09	11,13,16,19	0
2	HEC	YYY	604	43/43	0.96	0.10	10,12,14,15	0
3	PO4	YYY	609	5/5	0.97	0.07	16,17,21,23	0
4	CA	YYY	610	1/1	0.99	0.06	15,15,15,15	0

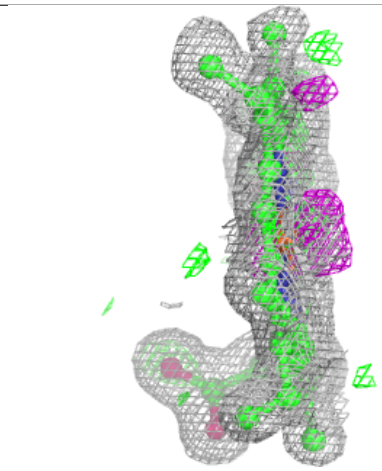
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC YYY 602:

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

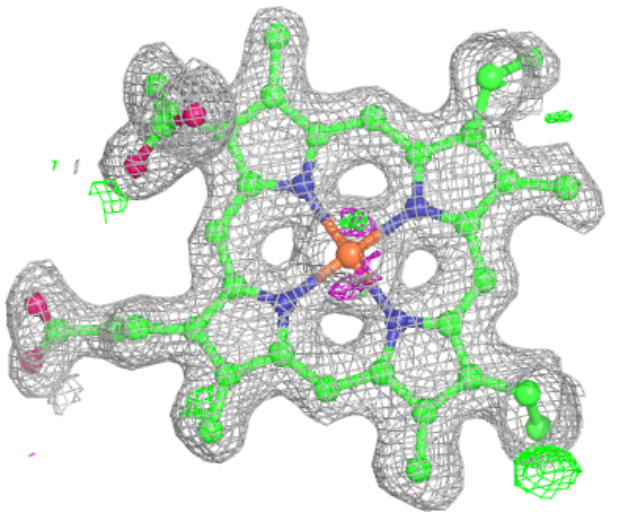


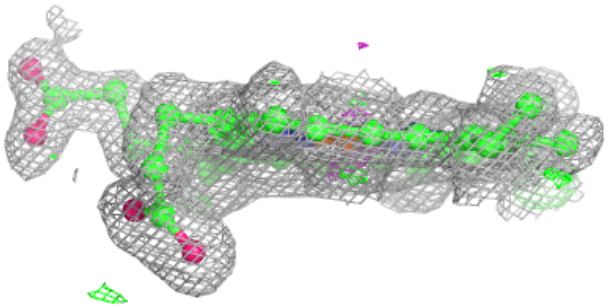


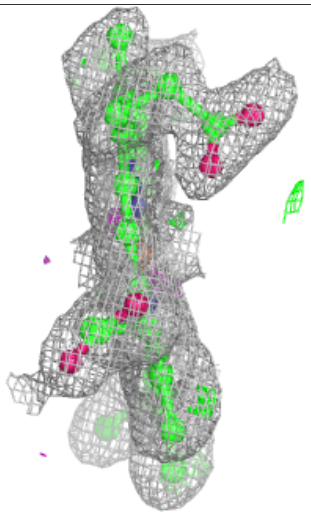


Electron density around HEC YYY 603:

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

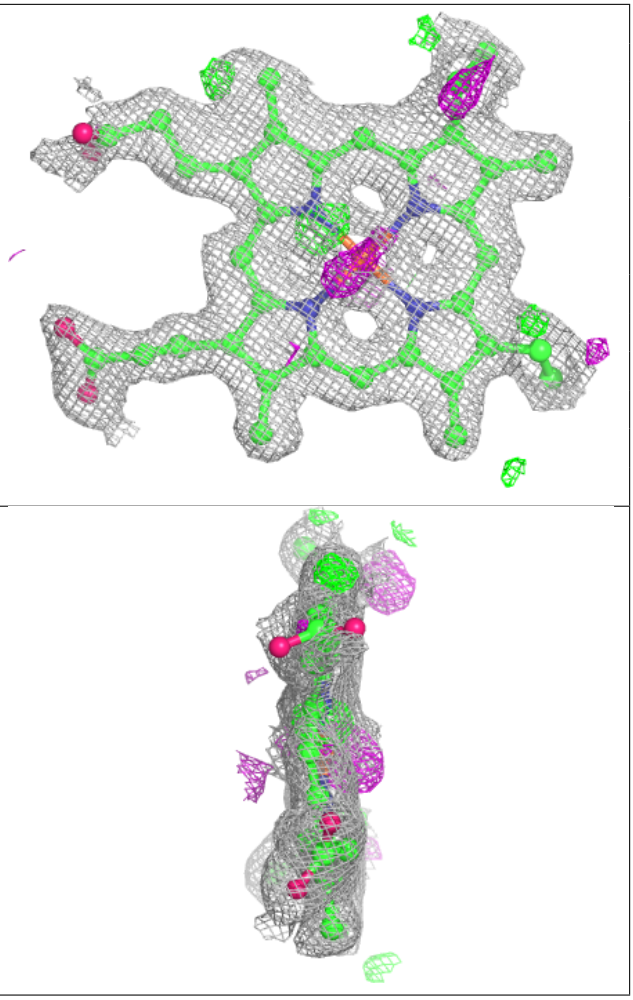






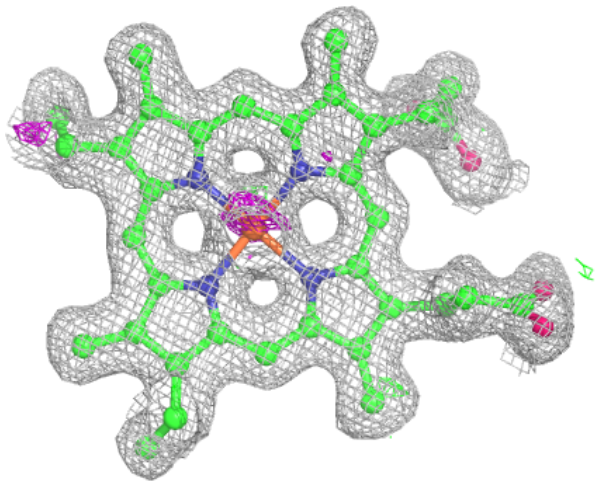
Electron density around HEC YYY 601:

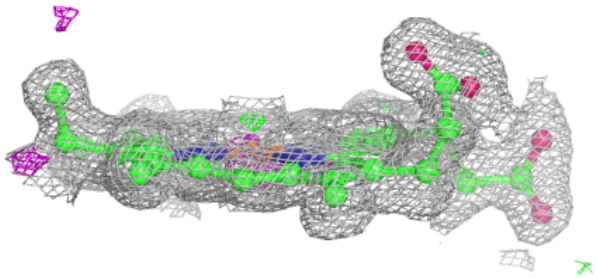
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

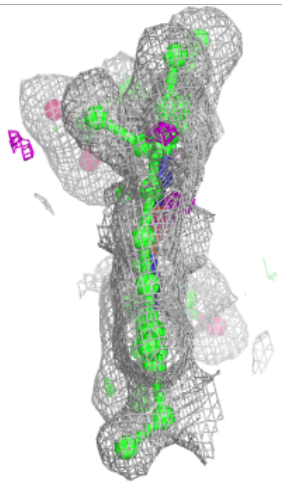


Electron density around HEC YYY 605:

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

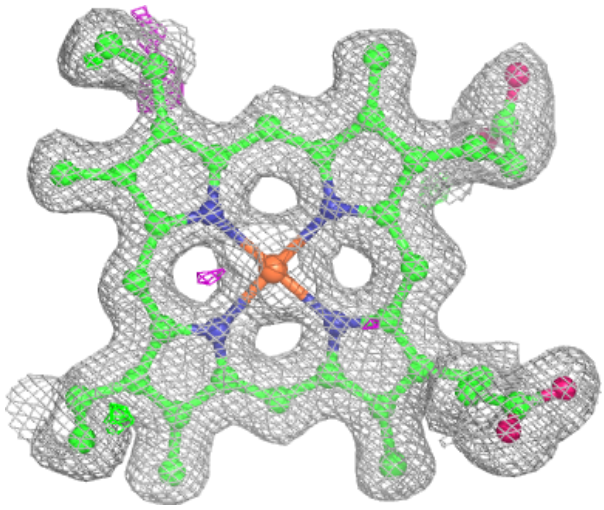


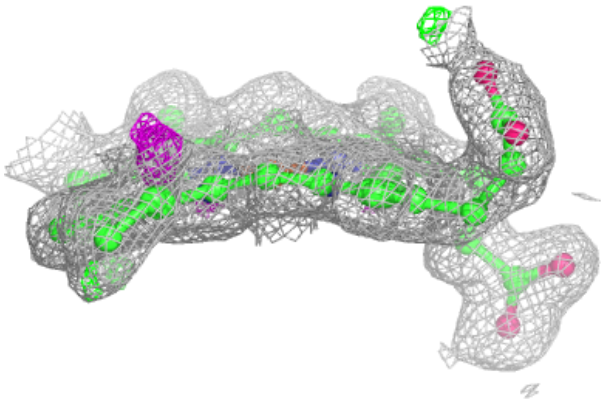


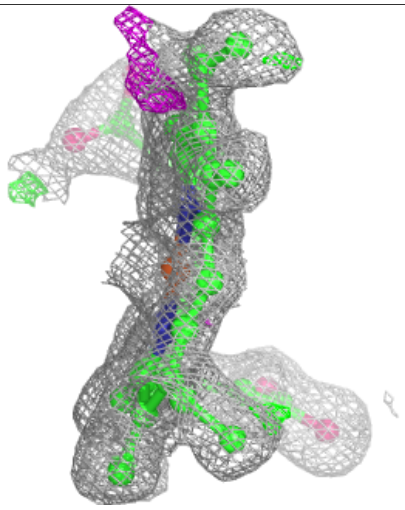


Electron density around HEC YYY 608:

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

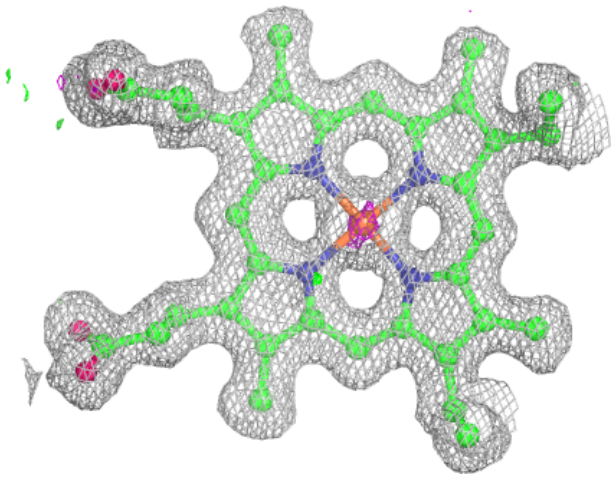


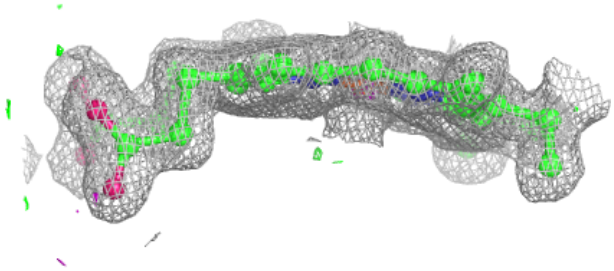


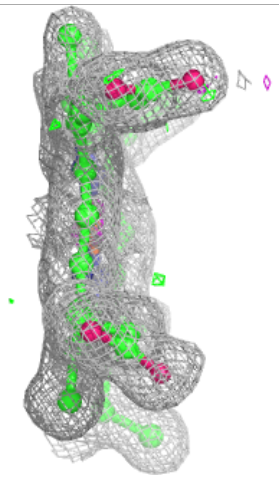


Electron density around HEC YYY 606:

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

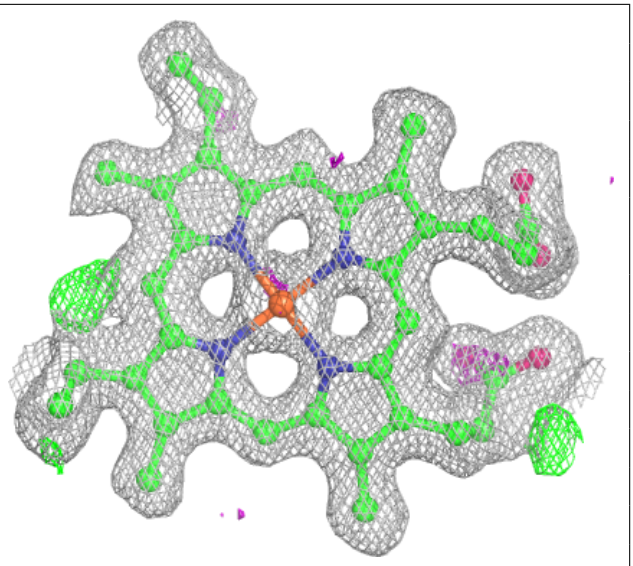


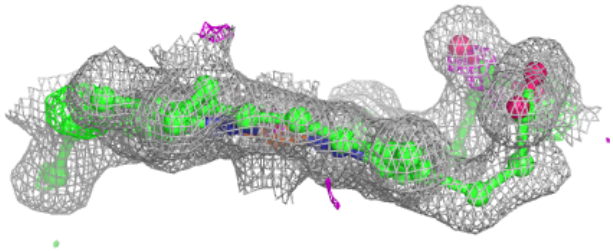


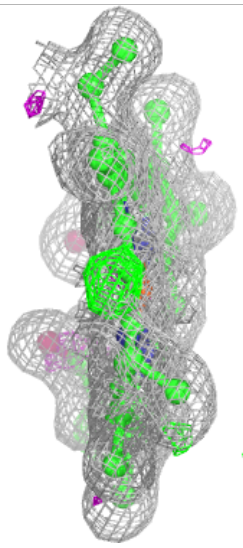


Electron density around HEC YYY 607:

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

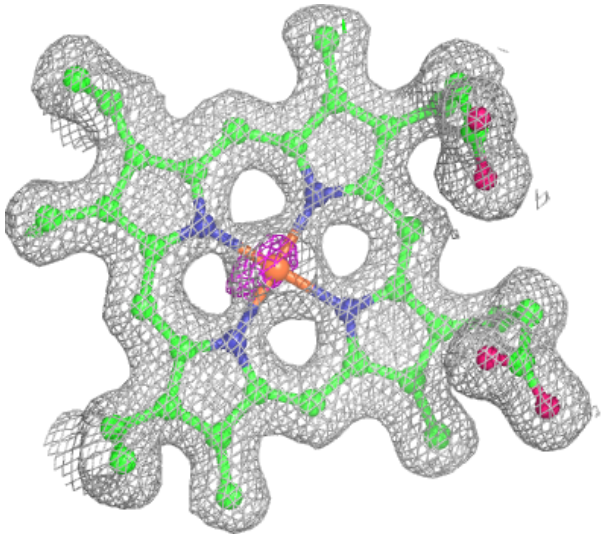


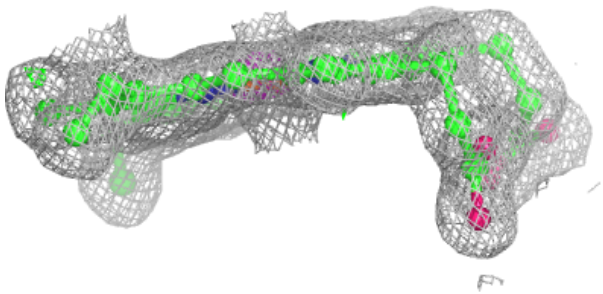


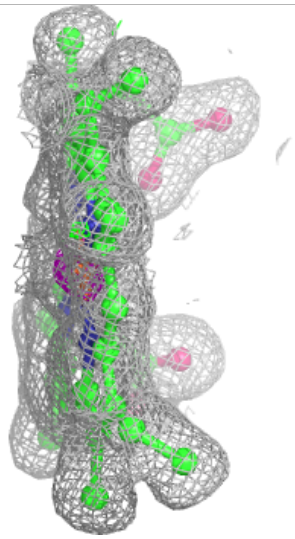


Electron density around HEC YYY 604:

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

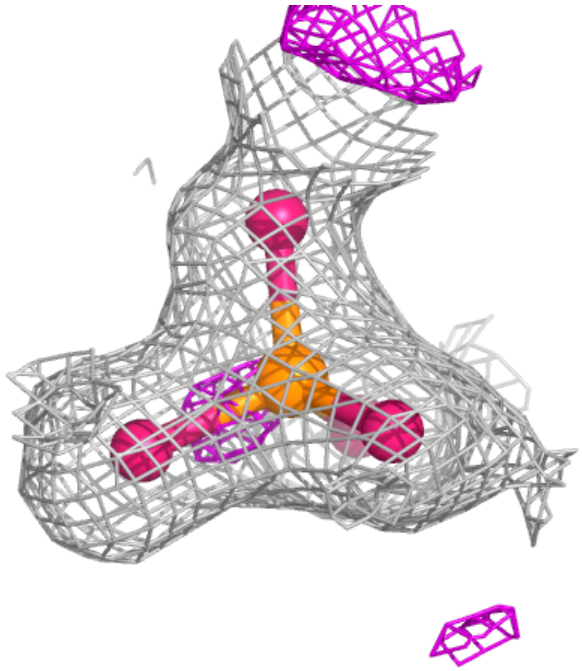


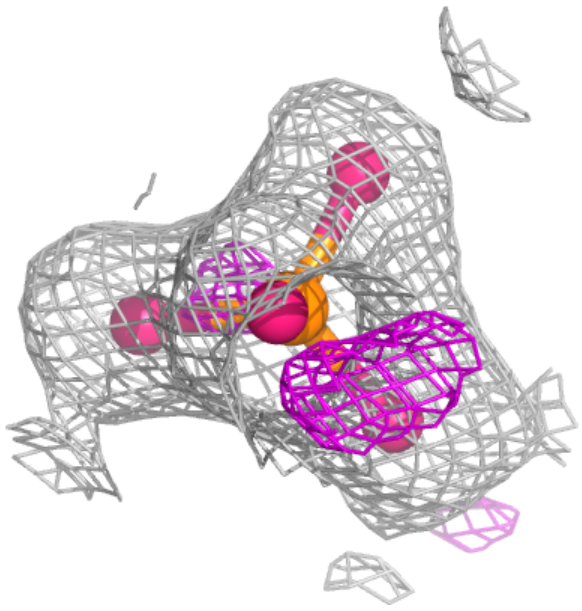


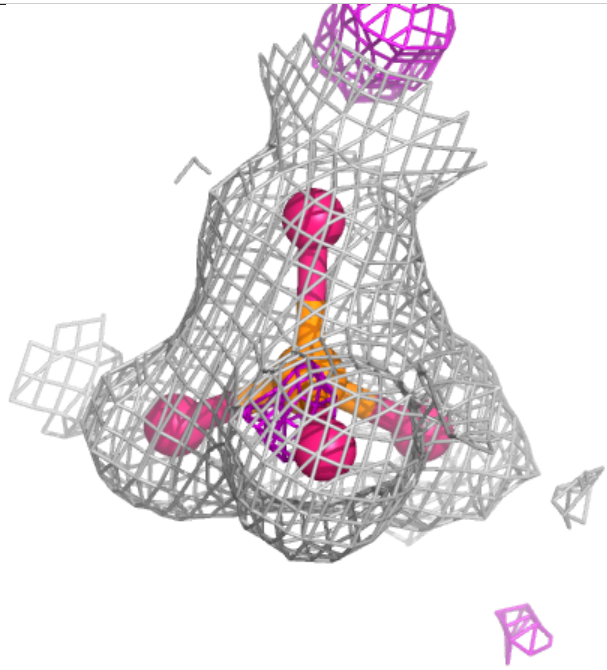


Electron density around PO4 YYY 609:

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

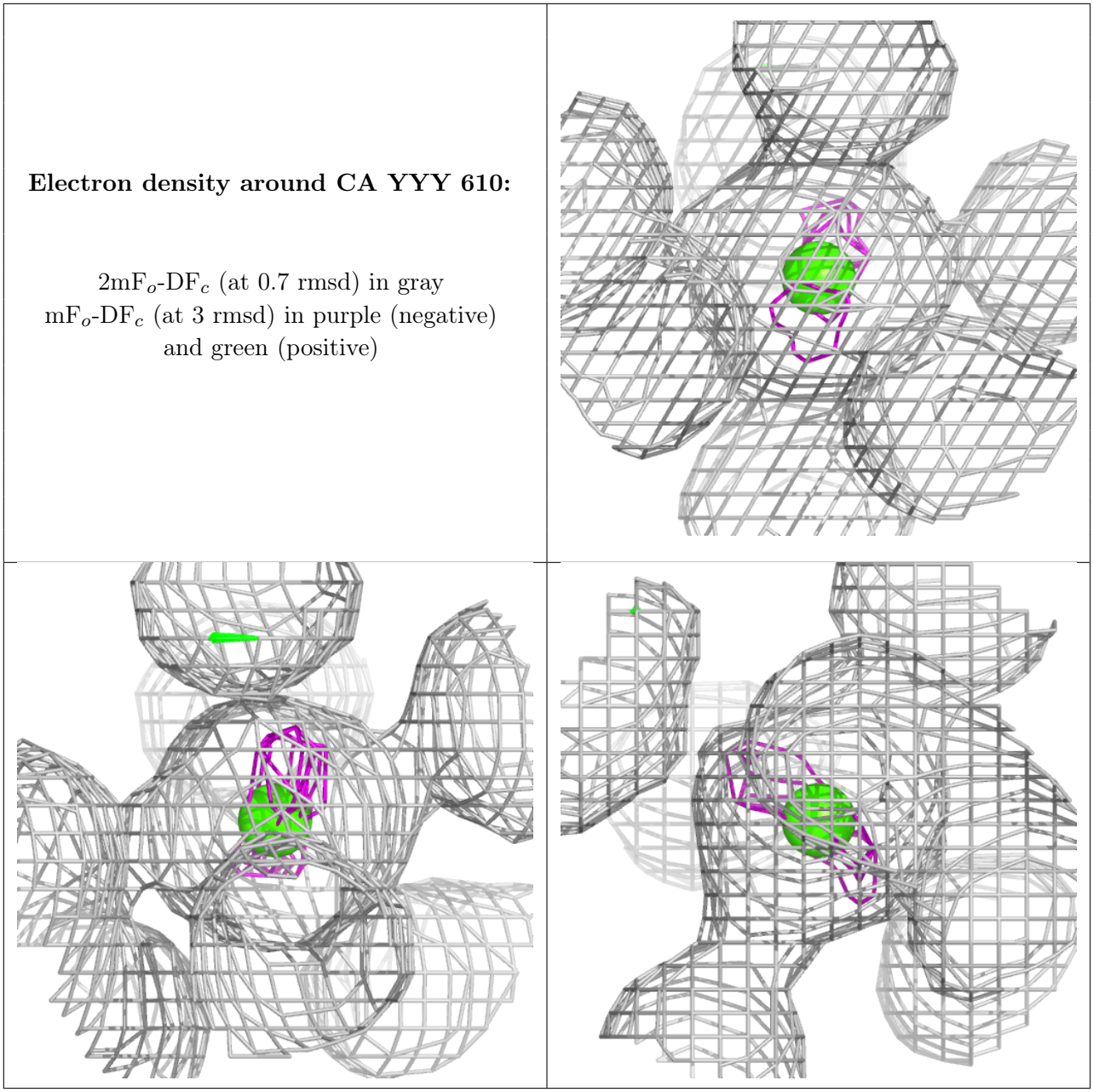






Electron density around CA YYY 610:

$2mF_o$-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.