Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2026 – 04:41 PM EDT

PDB ID	:	1AOF / pdb_00001aof
Title	:	CYTOCHROME CD1 NITRITE REDUCTASE, REDUCED FORM
Authors	:	Williams, P.A.; Fulop, V.
Deposited on	:	1997-07-02
Resolution	:	2.00 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:

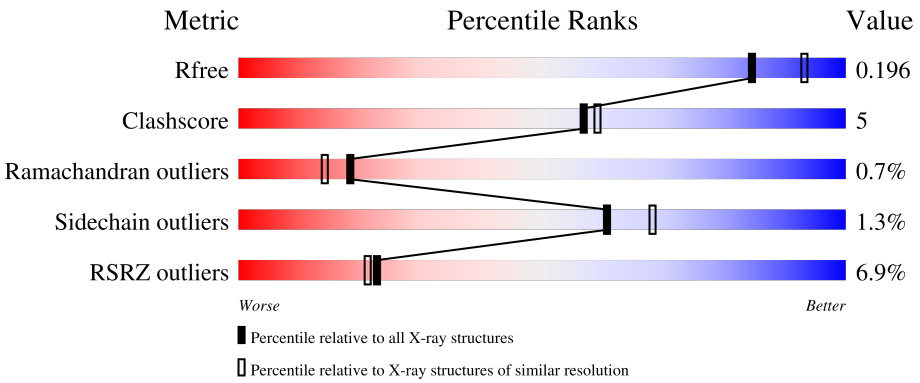
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	567	10% 82% 11% • 6%
1	B	567	3% 82% 13% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	601	X	-	-	-
2	HEC	B	601	X	-	-	-
3	DHE	A	602	X	-	-	-
3	DHE	B	602	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9085 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.

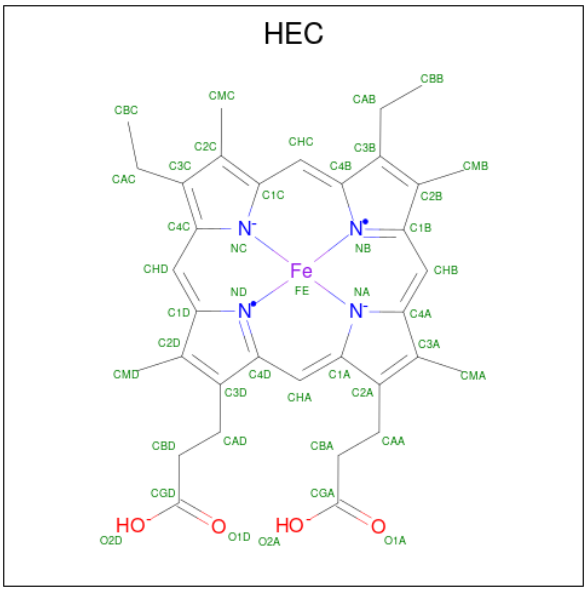
- Molecule 1 is a protein called NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4133	2618	689	811	15	0	0	0
1	B	542	4210	2664	702	829	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

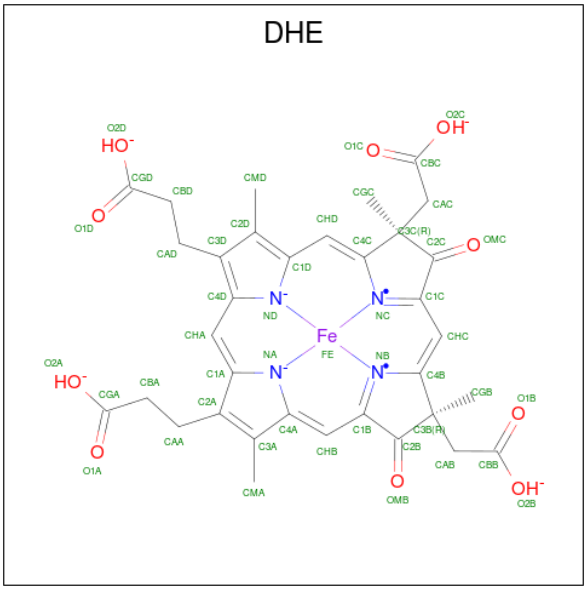
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	MET	GLU	conflict	UNP P72181
A	185	SER	THR	conflict	UNP P72181
A	191	THR	SER	conflict	UNP P72181
A	331	ASN	ASP	conflict	UNP P72181
B	160	MET	GLU	conflict	UNP P72181
B	185	SER	THR	conflict	UNP P72181
B	191	THR	SER	conflict	UNP P72181
B	331	ASN	ASP	conflict	UNP P72181

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



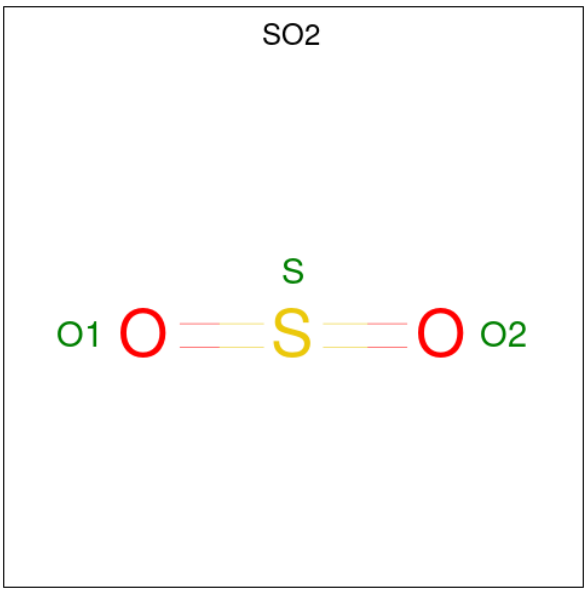
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is HEME D (CCD ID: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	49	34	1	4	10	0	0
			Total	C	Fe	N	O		
3	B	1	49	34	1	4	10	0	0

- Molecule 4 is SULFUR DIOXIDE (CCD ID: SO2) (formula: O_2S).



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

- Molecule 5 is water.

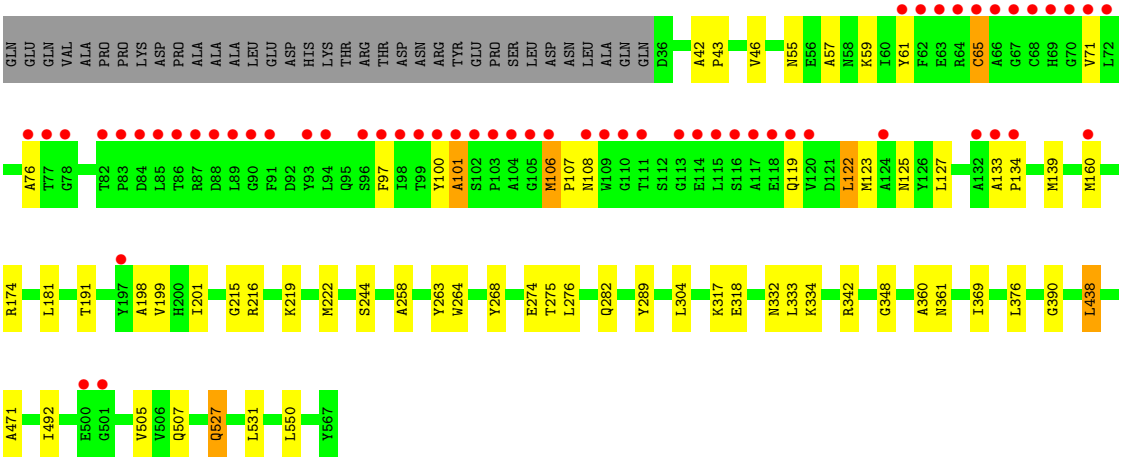
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	267	267	267	0	0
			Total	O		
5	B	285	285	285	0	0

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.

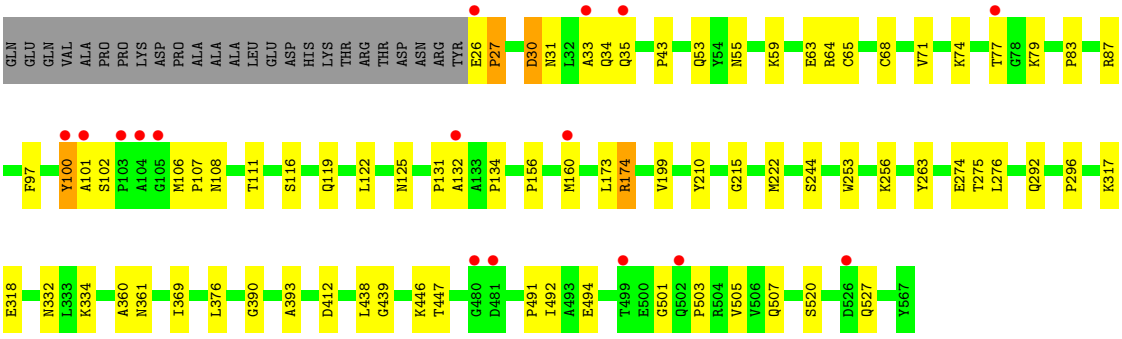
• Molecule 1: NITRITE REDUCTASE

Chain A:



• Molecule 1: NITRITE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.40Å 61.70Å 101.20Å 90.00° 112.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.00) 96.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.170 , 0.201 0.163 , 0.196	Depositor DCC
R_{free} test set	3245 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: DHE, HEC, SO2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.46	0/4235	0.97	13/5762 (0.2%)
1	B	0.44	0/4313	0.96	14/5869 (0.2%)
All	All	0.45	0/8548	0.96	27/11631 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	361	ASN	N-CA-C	10.11	123.24	111.11
1	B	361	ASN	N-CA-C	8.52	121.64	111.33
1	A	390	GLY	N-CA-C	-7.98	96.18	110.86
1	B	390	GLY	N-CA-C	-7.90	96.32	110.86
1	A	360	ALA	N-CA-C	-7.31	95.00	108.24
1	A	263	TYR	N-CA-C	-6.98	102.75	112.45
1	B	360	ALA	N-CA-C	-6.88	95.78	108.24
1	A	244	SER	N-CA-C	6.66	120.02	109.50
1	B	438	LEU	N-CA-C	6.55	118.08	111.07
1	A	333	LEU	N-CA-C	6.25	118.15	109.15
1	B	173	LEU	N-CA-C	-6.20	100.31	109.11
1	B	244	SER	N-CA-C	6.06	119.08	109.50
1	B	332	ASN	N-CA-C	-6.02	100.56	109.11
1	A	438	LEU	N-CA-C	6.01	117.50	111.07
1	B	263	TYR	N-CA-C	-5.90	104.24	112.45
1	B	318	GLU	N-CA-C	5.88	118.47	111.71
1	A	318	GLU	N-CA-C	5.72	118.28	111.71
1	B	77	THR	N-CA-C	-5.69	104.69	111.69
1	B	100	TYR	N-CA-C	5.41	119.94	113.23
1	B	27	PRO	N-CA-C	5.36	119.73	111.21
1	A	332	ASN	N-CA-C	-5.30	101.07	108.54
1	A	258	ALA	N-CA-C	-5.24	101.10	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	MET	CA-C-N	5.20	125.11	119.85
1	A	106	MET	C-N-CA	5.20	125.11	119.85
1	A	317	LYS	N-CA-C	5.14	121.75	110.80
1	B	30	ASP	N-CA-C	5.08	118.58	112.38
1	B	446	LYS	N-CA-C	5.04	116.90	108.99

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	4133	0	3992	35	0
1	B	4210	0	4063	44	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	49	0	24	1	0
3	B	49	0	24	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	267	0	0	0	0
5	B	285	0	0	1	0
All	All	9085	0	8163	77	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 (77) 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:57:ALA:HB2	1:A:122:LEU:HD22	1.59	0.84
1:A:334:LYS:HE2	1:B:334:LYS:HE2	1.57	0.84
1:B:101:ALA:HB1	1:B:106:MET:O	1.82	0.79
1:A:101:ALA:HB1	1:A:106:MET:O	1.87	0.75
1:B:101:ALA:HB2	1:B:108:ASN:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:HB2	1:B:108:ASN:CA	2.18	0.73
1:B:26:GLU:HG3	1:B:68:CYS:SG	2.29	0.72
1:A:101:ALA:HB2	1:A:107:PRO:C	2.22	0.65
1:B:199:VAL:HA	1:B:215:GLY:HA2	1.77	0.64
1:A:222:MET:HE1	1:A:274:GLU:HA	1.82	0.62
1:B:116:SER:H	1:B:119:GLN:HE21	1.47	0.61
1:A:100:TYR:O	1:A:101:ALA:HB3	1.99	0.61
1:B:100:TYR:O	1:B:101:ALA:HB3	2.00	0.60
1:B:101:ALA:HB2	1:B:107:PRO:C	2.25	0.60
1:B:501:GLY:O	1:B:503:PRO:HD3	2.02	0.59
1:B:101:ALA:HB2	1:B:108:ASN:HA	1.84	0.58
1:A:101:ALA:HB2	1:A:108:ASN:CA	2.35	0.56
1:A:71:VAL:HG12	1:A:134:PRO:CG	2.36	0.56
1:A:101:ALA:HB2	1:A:108:ASN:N	2.21	0.56
1:B:71:VAL:CG1	1:B:134:PRO:HG2	2.36	0.56
1:B:74:LYS:HG2	1:B:296:PRO:HG3	1.88	0.54
1:B:222:MET:HE1	1:B:274:GLU:HA	1.89	0.54
1:A:101:ALA:HB2	1:A:108:ASN:HA	1.89	0.54
1:A:119:GLN:O	1:A:123:MET:HG2	2.07	0.54
1:A:43:PRO:HD2	1:A:46:VAL:HB	1.90	0.53
1:B:79:LYS:HG3	2:B:601:HEC:HAD2	1.91	0.53
1:B:53:GLN:HB3	1:B:122:LEU:HD21	1.91	0.52
1:B:31:ASN:O	1:B:34:GLN:HG2	2.10	0.52
1:B:253:TRP:CE3	1:B:256:LYS:HD2	2.46	0.51
1:B:55:ASN:O	1:B:59:LYS:HG3	2.11	0.51
1:B:27:PRO:HA	3:B:602:DHE:HAB2	1.92	0.50
1:A:61:TYR:CE1	1:A:65:CYS:HB2	2.46	0.50
1:A:527:GLN:HE21	1:A:527:GLN:HA	1.77	0.49
1:B:116:SER:H	1:B:119:GLN:NE2	2.10	0.49
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.77	0.48
1:A:304:LEU:HD21	1:A:348:GLY:HA2	1.95	0.48
1:A:61:TYR:HA	1:A:65:CYS:SG	2.53	0.48
1:B:35:GLN:HB3	5:B:721:HOH:O	2.12	0.48
1:B:43:PRO:HG3	1:B:87:ARG:CZ	2.44	0.48
1:A:369:ILE:HD13	1:A:376:LEU:HA	1.95	0.48
1:B:132:ALA:O	1:B:134:PRO:HD3	2.14	0.47
1:B:64:ARG:O	2:B:601:HEC:HMC3	2.15	0.47
1:A:123:MET:O	1:A:127:LEU:HG	2.16	0.46
1:B:43:PRO:HG3	1:B:87:ARG:NH2	2.31	0.46
1:B:156:PRO:HG3	1:B:160:MET:HE2	1.96	0.46
1:A:275:THR:O	1:A:276:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ALA:HA	1:A:43:PRO:HD3	1.81	0.45
1:A:198:ALA:HB3	1:A:216:ARG:HD3	1.99	0.45
1:A:438:LEU:HG	1:A:471:ALA:HB2	1.99	0.45
1:A:492:ILE:HB	1:A:505:VAL:HG21	1.99	0.45
1:B:33:ALA:CB	1:B:63:GLU:HG3	2.47	0.45
1:B:83:PRO:HG2	1:B:131:PRO:HD3	1.98	0.45
1:A:100:TYR:O	1:A:101:ALA:CB	2.63	0.45
1:A:71:VAL:HG12	1:A:134:PRO:HG3	1.98	0.45
1:A:134:PRO:HB2	1:A:264:TRP:CZ2	2.52	0.44
1:A:199:VAL:HA	1:A:215:GLY:HA2	1.99	0.44
1:B:33:ALA:O	1:B:59:LYS:HG2	2.18	0.43
1:B:102:SER:HB3	1:B:106:MET:HB3	2.00	0.43
1:A:201:ILE:HD13	3:A:602:DHE:O2A	2.18	0.43
1:B:393:ALA:HB1	1:B:447:THR:HG22	2.00	0.43
1:A:289:TYR:HE1	1:A:342:ARG:HG3	1.83	0.43
1:B:275:THR:O	1:B:276:LEU:HB2	2.19	0.43
1:A:531:LEU:HG	1:A:550:LEU:HD21	1.99	0.43
1:B:492:ILE:HB	1:B:505:VAL:HG21	2.00	0.43
1:B:369:ILE:HD13	1:B:376:LEU:HA	2.01	0.42
1:B:491:PRO:HB2	1:B:494:GLU:HB3	2.00	0.42
1:B:505:VAL:HA	1:B:520:SER:O	2.20	0.42
1:A:133:ALA:HA	1:A:134:PRO:HD3	1.89	0.42
1:B:412:ASP:HB3	1:B:439:GLY:HA2	2.00	0.41
1:A:268:TYR:CZ	1:A:282:GLN:HB2	2.56	0.41
1:B:108:ASN:HB2	1:B:111:THR:OG1	2.20	0.41
1:A:139:MET:HB2	1:B:292:GLN:HB2	2.01	0.41
1:A:181:LEU:HD12	1:A:191:THR:CG2	2.51	0.41
1:B:106:MET:HA	1:B:107:PRO:HD3	1.88	0.41
1:A:55:ASN:O	1:A:59:LYS:HG3	2.21	0.41
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.36	0.40
1:B:210:TYR:CD1	1:B:222:MET:HE2	2.56	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	530/567 (94%)	505 (95%)	21 (4%)	4 (1%)	16	11
1	B	540/567 (95%)	517 (96%)	20 (4%)	3 (1%)	21	17
All	All	1070/1134 (94%)	1022 (96%)	41 (4%)	7 (1%)	18	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ALA
1	A	507	GLN
1	B	507	GLN
1	A	174	ARG
1	B	174	ARG
1	A	76	ALA
1	B	317	LYS

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	440/470 (94%)	433 (98%)	7 (2%)	55	62
1	B	449/470 (96%)	444 (99%)	5 (1%)	65	73
All	All	889/940 (95%)	877 (99%)	12 (1%)	61	68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	CYS
1	A	97	PHE
1	A	122	LEU
1	A	125	ASN
1	A	160	MET
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	527	GLN
1	B	30	ASP
1	B	65	CYS
1	B	97	PHE
1	B	125	ASN
1	B	527	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	385	GLN
1	A	527	GLN
1	B	34	GLN
1	B	119	GLN
1	B	125	ASN
1	B	527	GLN

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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	A	601	1	50,50,50	0.87	0	68,82,82	1.16	5 (7%)
4	SO2	A	603	3	2,2,2	0.32	0	1,1,1	0.65	0
2	HEC	B	601	1	50,50,50	0.83	0	68,82,82	1.23	4 (5%)
4	SO2	B	603	3	2,2,2	0.24	0	1,1,1	0.67	0
3	DHE	A	602	1,4	52,56,56	1.89	8 (15%)	68,94,94	1.73	10 (14%)
3	DHE	B	602	1,4	52,56,56	1.95	9 (17%)	68,94,94	1.63	9 (13%)

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	B	601	1	1/1/3/7	6/14/54/54	-
3	DHE	B	602	1,4	1/1/15/19	6/20/108/108	-
3	DHE	A	602	1,4	1/1/15/19	6/20/108/108	-
2	HEC	A	601	1	1/1/3/7	4/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	CBD-CAD	-6.84	1.28	1.51
3	A	602	DHE	CBD-CAD	-6.43	1.29	1.51
3	B	602	DHE	FE-ND	4.20	2.09	1.95
3	B	602	DHE	FE-NB	4.17	2.07	1.94
3	A	602	DHE	FE-NB	4.14	2.07	1.94
3	A	602	DHE	FE-NC	4.13	2.07	1.94
3	B	602	DHE	FE-NC	4.12	2.07	1.94
3	B	602	DHE	CGC-C3C	4.09	1.61	1.54
3	A	602	DHE	FE-ND	4.01	2.08	1.95
3	B	602	DHE	FE-NA	3.98	2.08	1.95
3	A	602	DHE	CGB-C3B	3.97	1.61	1.54
3	A	602	DHE	FE-NA	3.86	2.07	1.95
3	B	602	DHE	CGB-C3B	3.70	1.61	1.54
3	A	602	DHE	CGC-C3C	3.46	1.60	1.54
3	A	602	DHE	CAB-C3B	-2.29	1.48	1.54
3	B	602	DHE	O2A-CGA	-2.12	1.23	1.30
3	B	602	DHE	CAC-C3C	-2.07	1.48	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	DHE	CBD-CAD-C3D	5.09	126.61	112.53
3	B	602	DHE	CBD-CAD-C3D	5.03	126.43	112.53
3	A	602	DHE	C1C-NC-C4C	5.02	111.15	105.21
3	A	602	DHE	C4B-NB-C1B	4.98	111.10	105.21
3	A	602	DHE	CAD-CBD-CGD	4.68	126.09	113.67
3	B	602	DHE	C4B-NB-C1B	4.40	110.41	105.21
3	B	602	DHE	C1C-NC-C4C	4.38	110.39	105.21
3	B	602	DHE	CAD-CBD-CGD	4.36	125.22	113.67
2	B	601	HEC	CAD-C3D-C4D	4.34	132.26	124.70
2	B	601	HEC	CBD-CAD-C3D	3.89	123.29	112.53
2	B	601	HEC	CAD-C3D-C2D	-3.63	121.06	127.87
3	A	602	DHE	C3B-C4B-CHC	3.60	125.64	122.44
2	A	601	HEC	CAD-C3D-C4D	3.29	130.43	124.70
2	A	601	HEC	CBD-CAD-C3D	3.25	121.53	112.53
3	B	602	DHE	C3B-C4B-CHC	2.97	125.08	122.44
2	A	601	HEC	CBB-CAB-C3B	2.83	120.10	112.42
3	A	602	DHE	CHB-C1B-NB	2.82	127.46	124.42
3	B	602	DHE	C1C-CHC-C4B	2.67	129.47	125.23
3	A	602	DHE	C1C-CHC-C4B	2.63	129.40	125.23
3	B	602	DHE	CHB-C1B-NB	2.56	127.18	124.42
3	A	602	DHE	C2A-C1A-NA	-2.51	107.90	110.32
2	A	601	HEC	CAC-C3C-C4C	2.45	128.28	124.91
3	B	602	DHE	C2A-C1A-NA	-2.41	108.00	110.32
2	A	601	HEC	CAD-C3D-C2D	-2.33	123.49	127.87
3	A	602	DHE	CAC-C3C-C2C	2.33	114.82	112.22
3	A	602	DHE	CHC-C1C-NC	2.20	126.79	124.42
2	B	601	HEC	CBC-CAC-C3C	2.14	118.22	112.42
3	B	602	DHE	CHC-C1C-NC	2.12	126.71	124.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	HEC	NA
2	B	601	HEC	NA
3	A	602	DHE	NA
3	B	602	DHE	NA

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	C2D-C3D-CAD-CBD
3	B	602	DHE	C4D-C3D-CAD-CBD
2	A	601	HEC	C4B-C3B-CAB-CBB
2	B	601	HEC	C2D-C3D-CAD-CBD
2	B	601	HEC	C4C-C3C-CAC-CBC
2	A	601	HEC	C2B-C3B-CAB-CBB
2	B	601	HEC	C4D-C3D-CAD-CBD
2	B	601	HEC	C2C-C3C-CAC-CBC
2	A	601	HEC	C2D-C3D-CAD-CBD
3	B	602	DHE	C3C-CAC-CBC-O2C
2	B	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4D-C3D-CAD-CBD
3	B	602	DHE	C3C-CAC-CBC-O1C
3	A	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3C-CAC-CBC-O1C
3	A	602	DHE	C3C-CAC-CBC-O2C
2	B	601	HEC	C4B-C3B-CAB-CBB
3	B	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3B-CAB-CBB-O1B
3	B	602	DHE	C3B-CAB-CBB-O1B

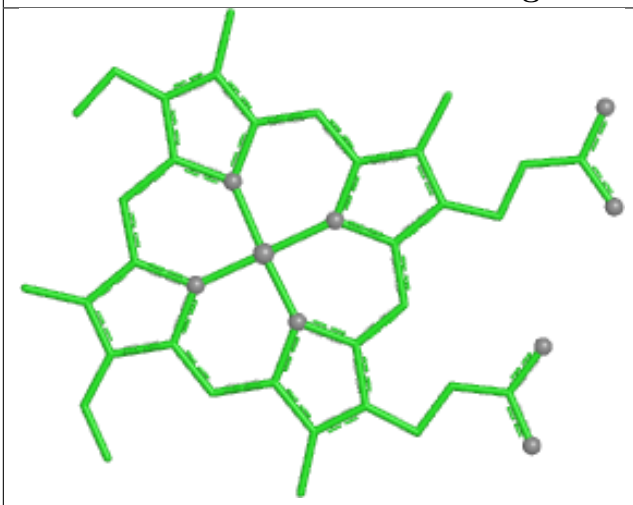
There are no ring outliers.

3 monomers are involved in 4 short contacts:

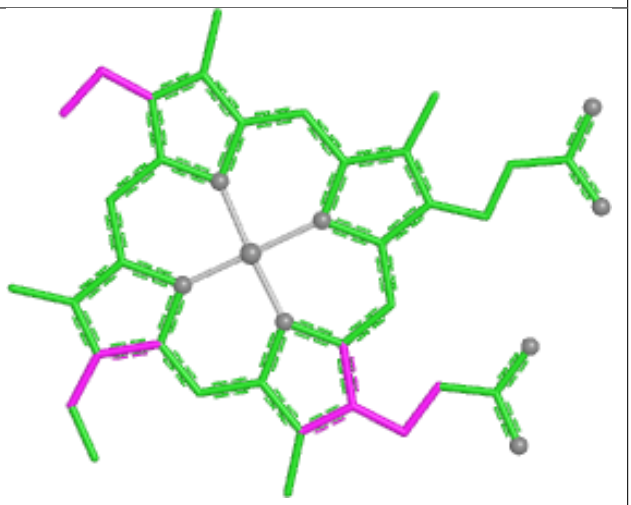
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEC	2	0
3	A	602	DHE	1	0
3	B	602	DHE	1	0

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.

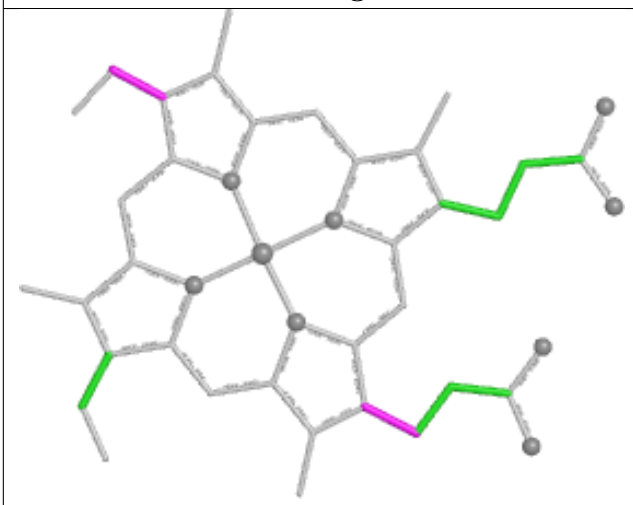
Ligand HEC A 601



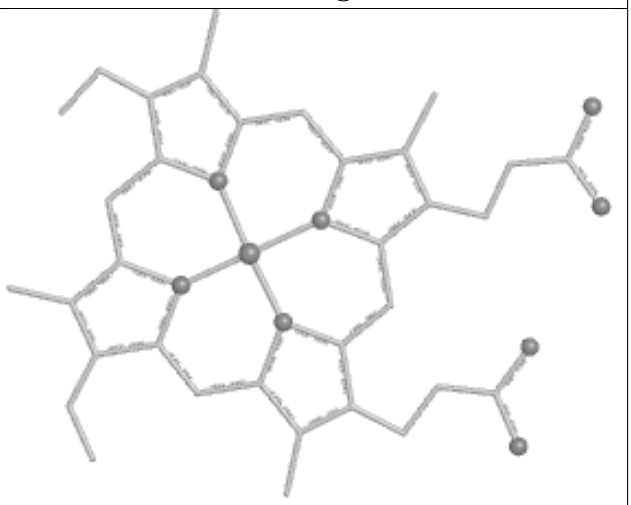
Bond lengths



Bond angles

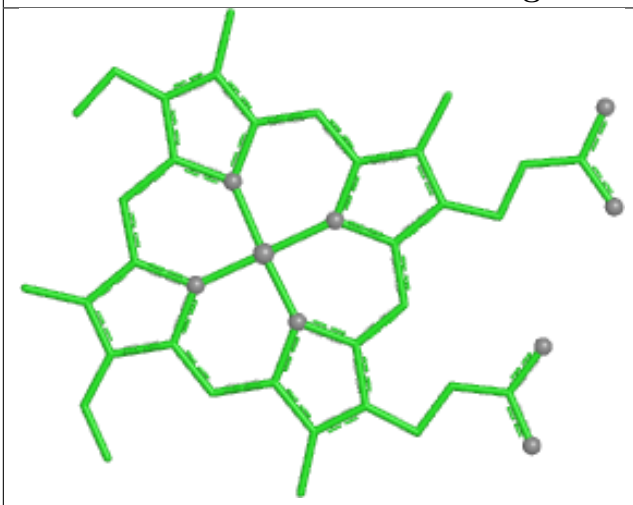


Torsions

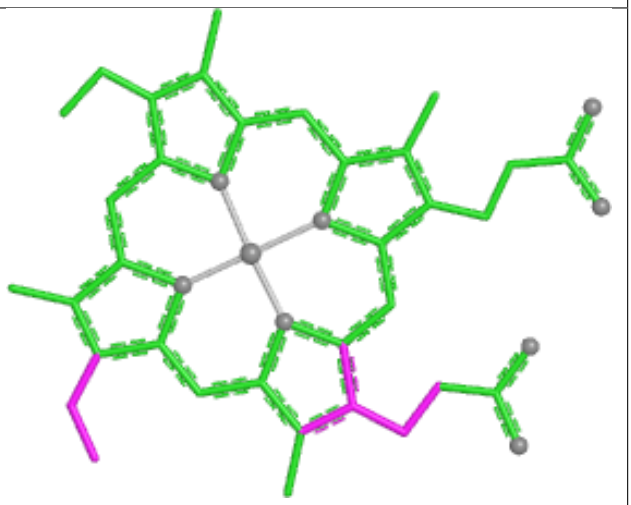


Rings

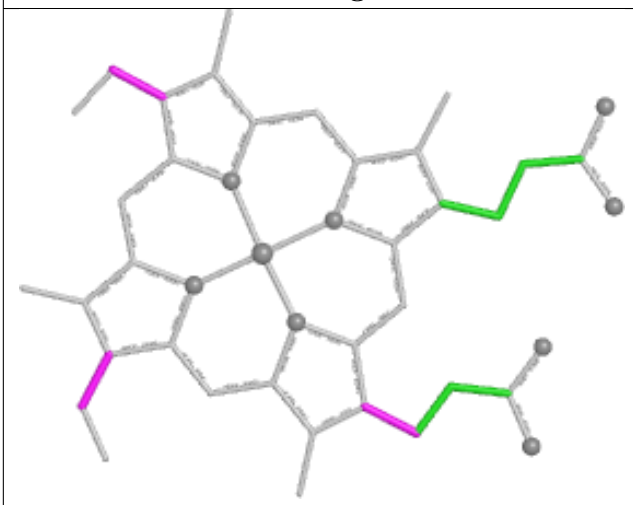
Ligand HEC B 601



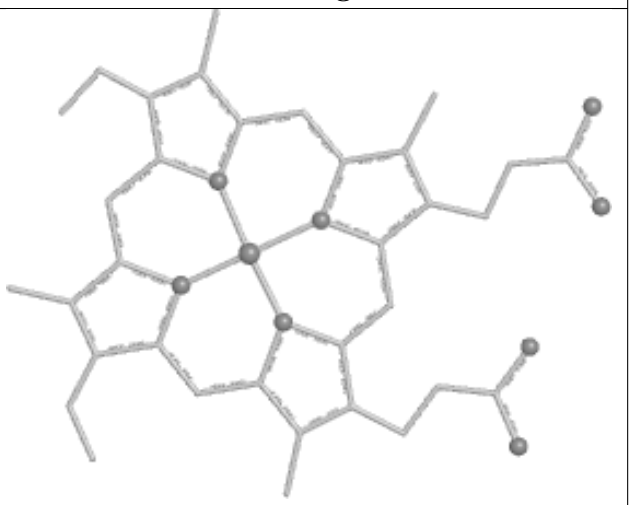
Bond lengths



Bond angles

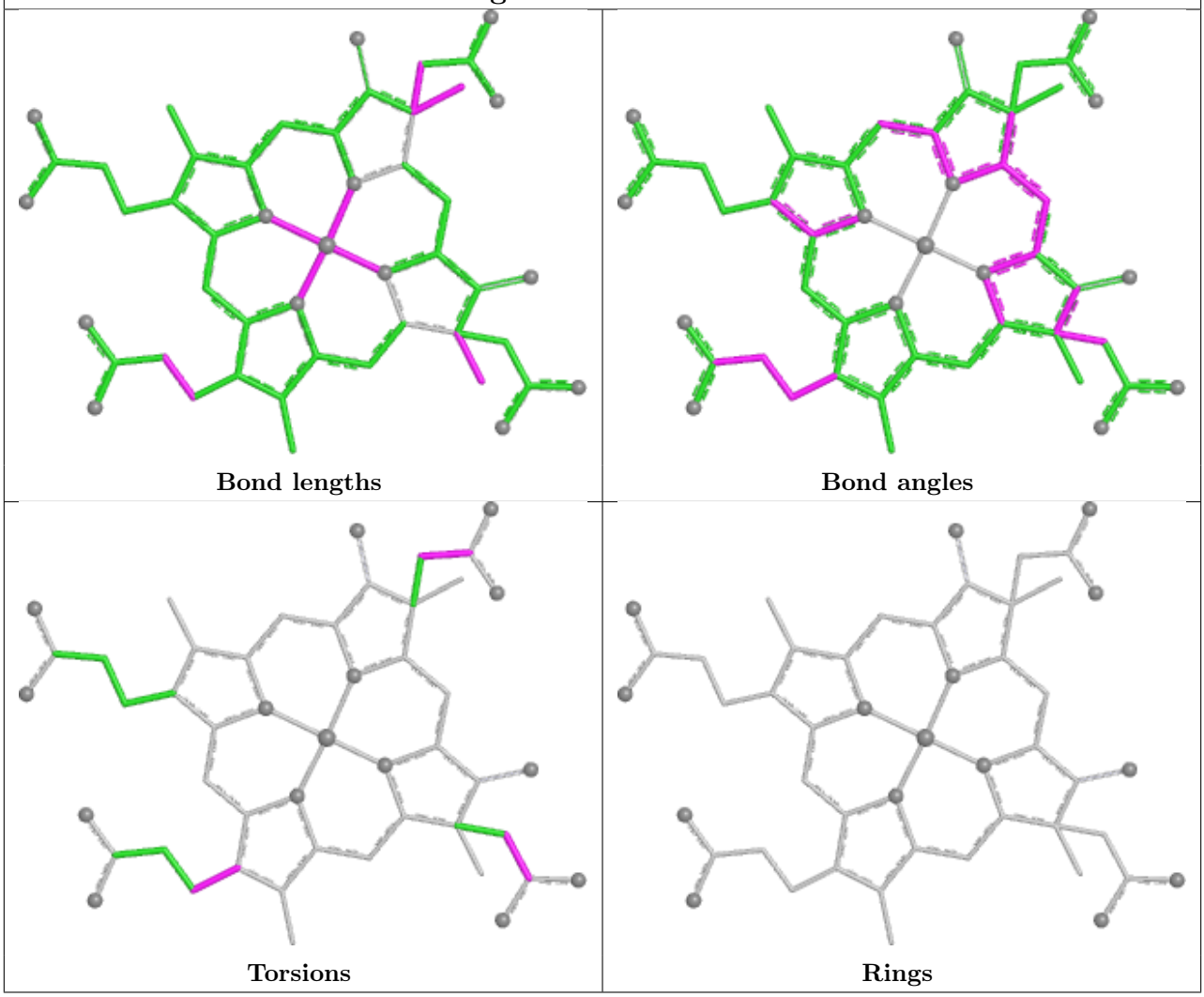


Torsions

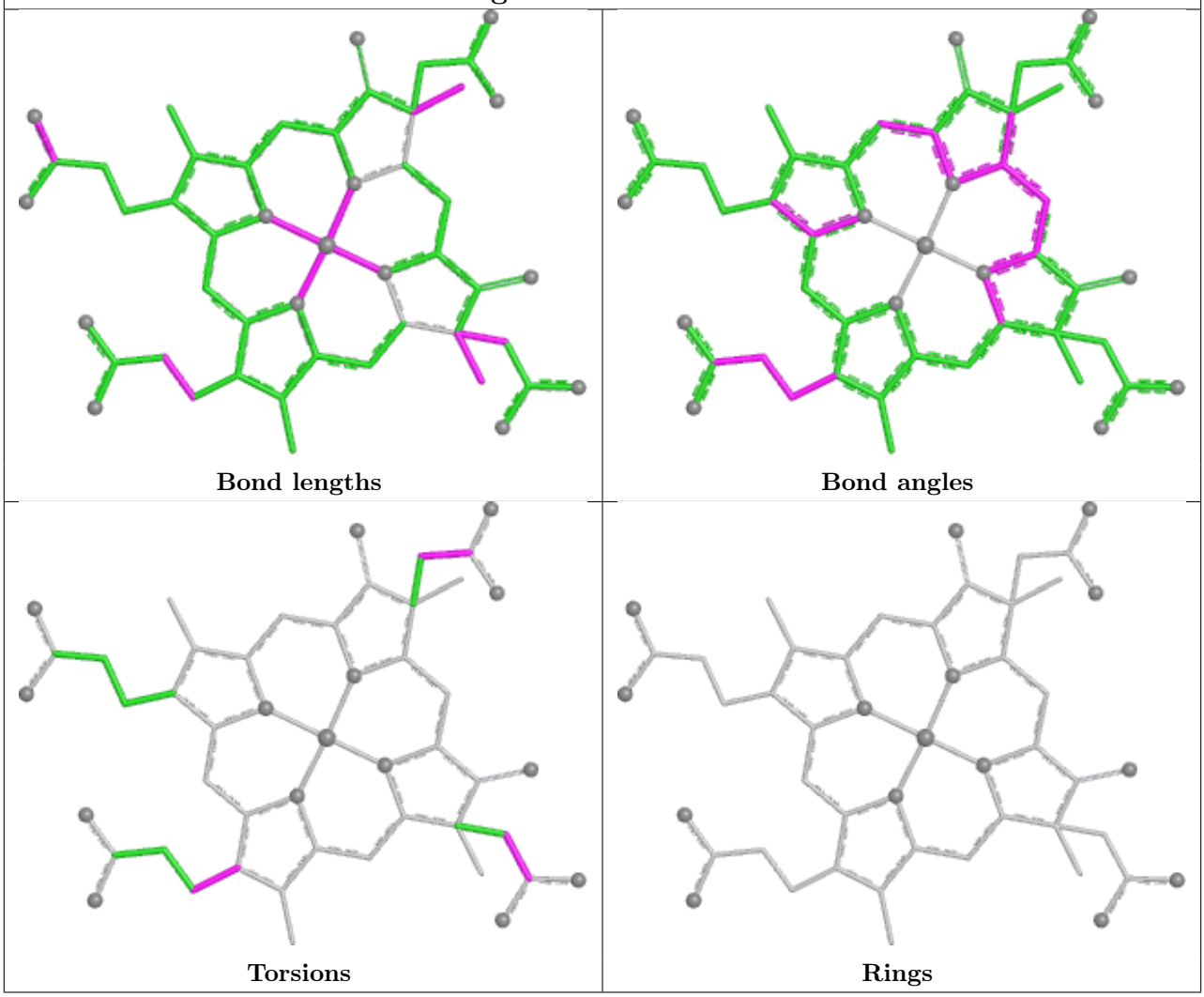


Rings

Ligand DHE A 602



Ligand DHE B 602



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	532/567 (93%)	-0.01	58 (10%)	10	9	12, 21, 44, 52	59 (11%)
1	B	542/567 (95%)	-0.24	16 (2%)	52	51	14, 24, 44, 52	0
All	All	1074/1134 (94%)	-0.13	74 (6%)	23	21	12, 22, 44, 52	59 (5%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ILE	6.9
1	A	62	PHE	5.2
1	A	97	PHE	4.8
1	A	71	VAL	4.6
1	A	105	GLY	4.5
1	A	108	ASN	4.3
1	A	117	ALA	4.0
1	A	93	TYR	3.9
1	A	501	GLY	3.9
1	A	116	SER	3.8
1	A	72	LEU	3.8
1	A	115	LEU	3.8
1	A	111	THR	3.7
1	A	88	ASP	3.7
1	A	160	MET	3.6
1	A	89	LEU	3.5
1	A	64	ARG	3.4
1	A	94	LEU	3.4
1	A	91	PHE	3.4
1	A	110	GLY	3.3
1	A	114	GLU	3.3
1	B	499	THR	3.3
1	A	134	PRO	3.3
1	B	103	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	THR	3.2
1	A	100	TYR	3.2
1	B	160	MET	3.2
1	A	104	ALA	3.1
1	A	85	LEU	3.1
1	A	101	ALA	3.0
1	B	502	GLN	3.0
1	A	66	ALA	3.0
1	A	68	CYS	2.9
1	A	113	GLY	2.9
1	A	70	GLY	2.9
1	A	133	ALA	2.8
1	A	90	GLY	2.8
1	B	480	GLY	2.8
1	B	33	ALA	2.8
1	A	120	VAL	2.8
1	A	103	PRO	2.7
1	A	65	CYS	2.7
1	A	82	THR	2.7
1	A	63	GLU	2.6
1	A	77	THR	2.6
1	A	102	SER	2.6
1	A	119	GLN	2.6
1	A	118	GLU	2.6
1	A	83	PRO	2.5
1	A	132	ALA	2.5
1	B	35	GLN	2.5
1	A	109	TRP	2.5
1	A	106	MET	2.4
1	A	69	HIS	2.4
1	A	86	THR	2.4
1	B	105	GLY	2.3
1	A	84	ASP	2.3
1	A	87	ARG	2.3
1	B	77	THR	2.3
1	B	132	ALA	2.3
1	A	197	TYR	2.3
1	A	124	ALA	2.2
1	A	61	TYR	2.2
1	B	104	ALA	2.2
1	A	96	SER	2.2
1	A	500	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	26	GLU	2.1
1	B	526	ASP	2.1
1	A	78	GLY	2.1
1	B	481	ASP	2.1
1	A	76	ALA	2.1
1	B	101	ALA	2.1
1	A	67	GLY	2.0
1	B	100	TYR	2.0

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)

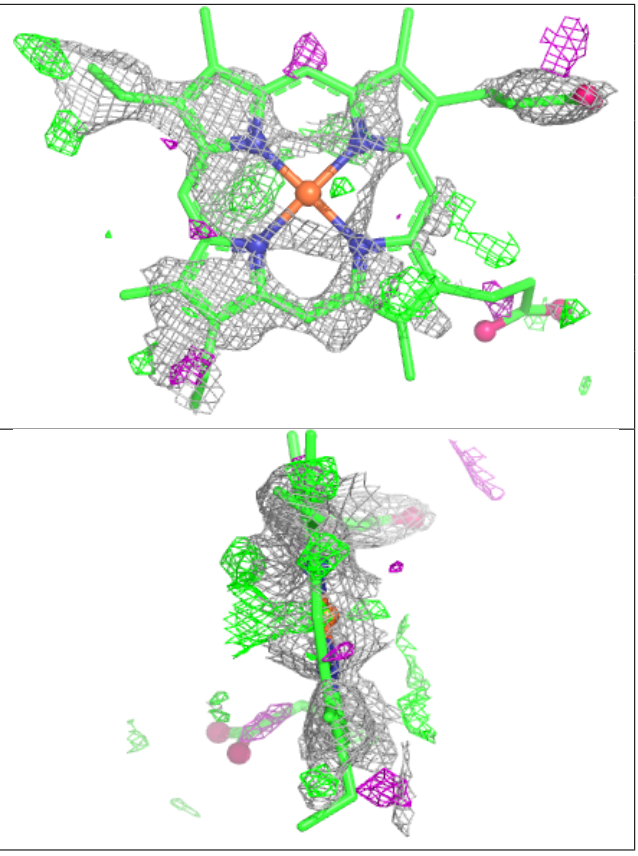
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	601	43/43	0.81	0.15	30,37,45,48	43
2	HEC	B	601	43/43	0.95	0.10	26,31,45,52	0
4	SO2	A	603	3/3	0.97	0.08	24,24,26,30	0
4	SO2	B	603	3/3	0.97	0.07	23,23,30,31	0
3	DHE	A	602	49/49	0.98	0.06	12,17,26,33	0
3	DHE	B	602	49/49	0.99	0.05	14,18,23,28	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.

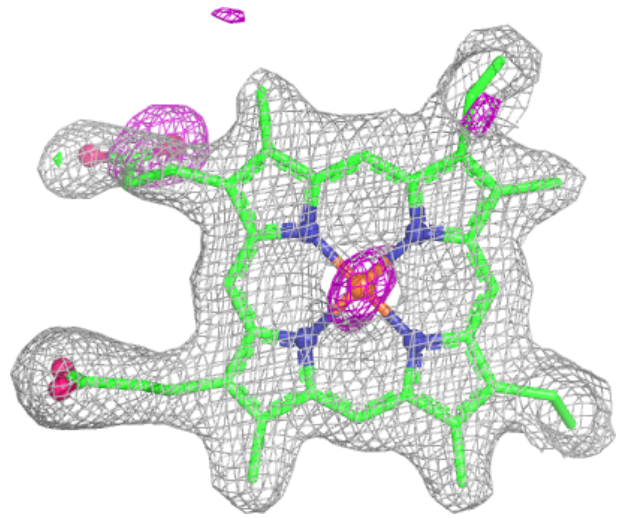
Electron density around HEC A 601:

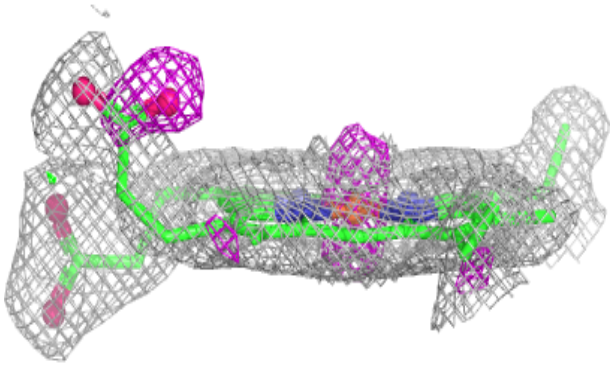
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

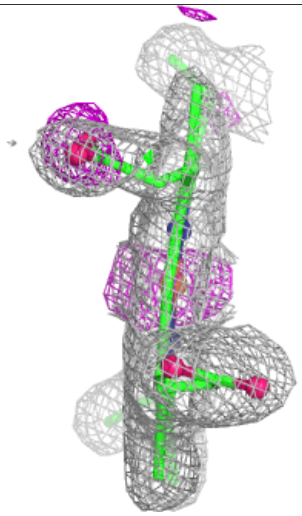


Electron density around HEC B 601:

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

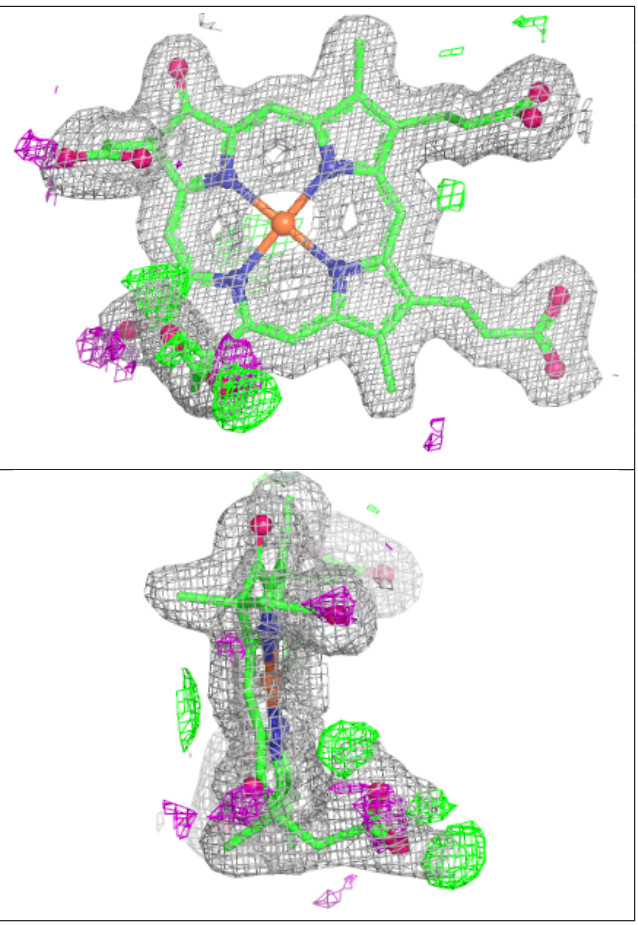






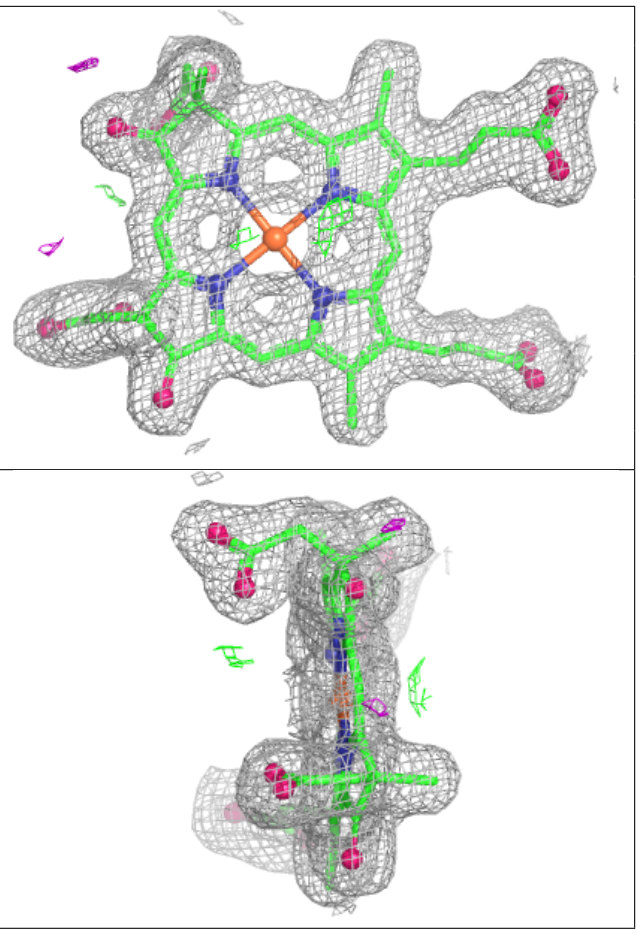
Electron density around DHE A 602:

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



Electron density around DHE B 602:

$2mF_o$-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.