Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:44 PM EDT

PDB ID	:	2B11 / pdb_00002b11
Title	:	Crystal structure of the protein-protein complex between F82W cytochrome c and cytochrome c peroxidase
Authors	:	Kang, S.A.; Crane, B.R.
Deposited on	:	2005-09-15
Resolution	:	2.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

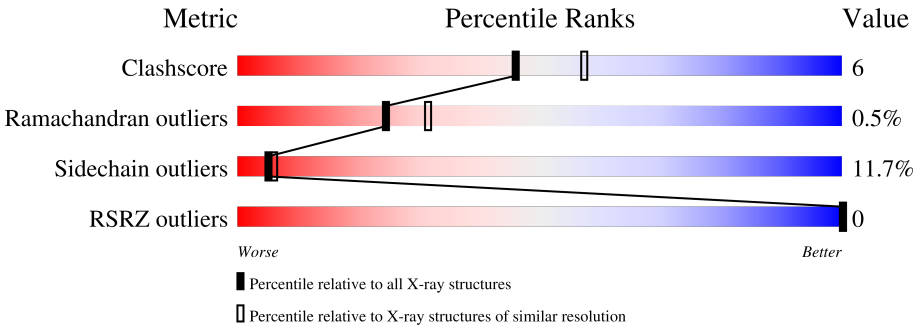
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	294	80% 16% •
1	C	294	82% 15% •
2	B	108	69% 29% •
2	D	108	76% 19% 5% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZNH	A	1001	X	-	-	-
3	ZNH	B	1101	X	-	-	-
4	HEC	C	1201	X	-	-	-
4	HEC	D	1301	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7111 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 Cytochrome c peroxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2370	1512	395	457	6			
1	C	294	Total	C	N	O	S	0	0	0
			2370	1512	395	457	6			

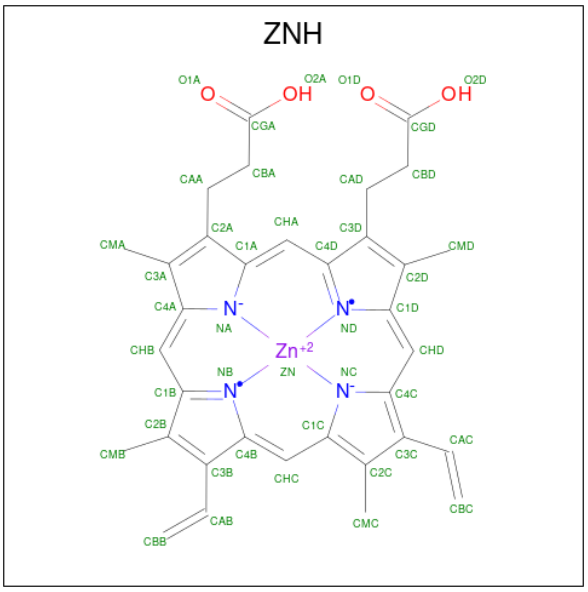
- Molecule 2 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			850	536	152	157	5			
2	D	108	Total	C	N	O	S	0	0	0
			850	536	152	157	5			

There are 2 discrepancies between the modelled and reference sequences:

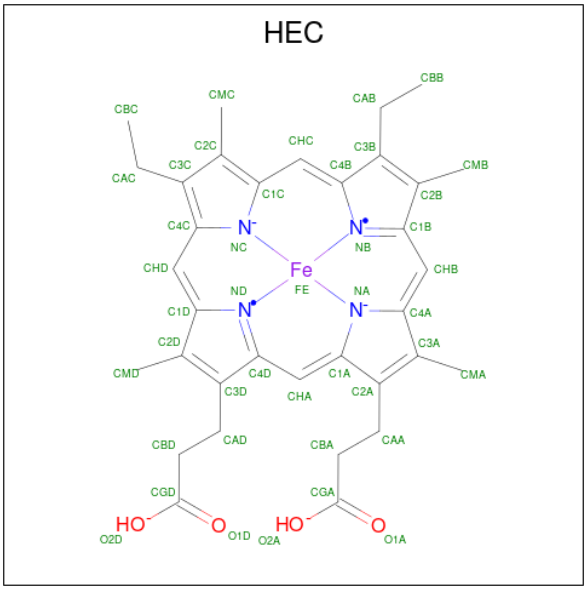
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	TRP	PHE	engineered mutation	UNP P00044
D	882	TRP	PHE	engineered mutation	UNP P00044

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING ZN (CCD ID: ZNH) (formula: $C_{34}H_{32}N_4O_4Zn$).



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

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	70	Total O 70 70	0	0
5	C	152	Total O 152 152	0	0
5	D	29	Total O 29 29	0	0

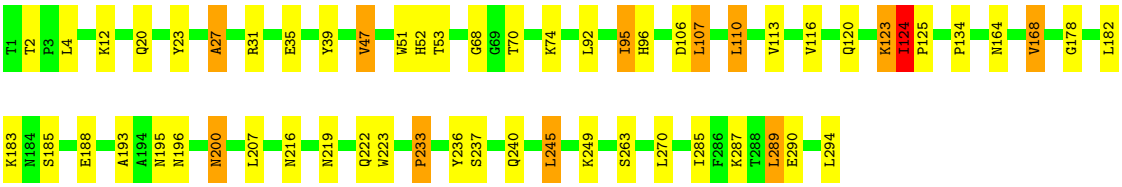
3 Residue-property plots (i)

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: Cytochrome c peroxidase, mitochondrial

Chain A:

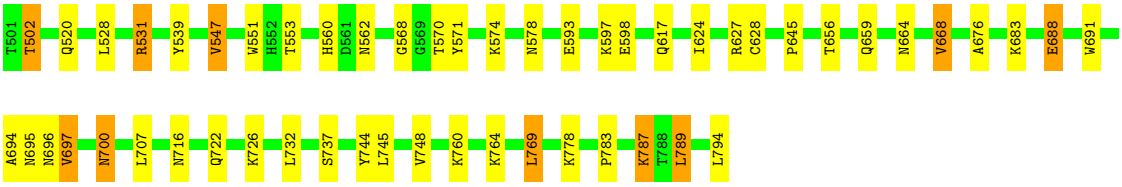




• Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain C:





• Molecule 2: Cytochrome c iso-1

Chain B:





• Molecule 2: Cytochrome c iso-1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.88Å 117.86Å 88.47Å 90.00° 104.23° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.30) 90.3 (30.00-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.293 0.249 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7111	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: ZNH, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.77	3/2437 (0.1%)	1.18	13/3301 (0.4%)
1	C	0.77	3/2437 (0.1%)	1.14	8/3301 (0.2%)
2	B	0.81	1/869 (0.1%)	1.24	7/1163 (0.6%)
2	D	0.81	1/869 (0.1%)	1.24	8/1163 (0.7%)
All	All	0.78	8/6612 (0.1%)	1.18	36/8928 (0.4%)

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	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	CYS	CB-SG	-12.07	1.41	1.81
2	B	402	CYS	CB-SG	-11.47	1.43	1.81
1	C	553	THR	CB-OG1	6.49	1.54	1.43
1	A	27	ALA	CA-CB	-6.40	1.43	1.53
1	A	53	THR	CB-OG1	6.38	1.53	1.43
1	C	547	VAL	CA-CB	5.06	1.61	1.54
1	C	502	THR	CA-CB	5.06	1.61	1.53
1	A	47	VAL	CA-CB	5.03	1.61	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	LYS	N-CA-C	8.75	122.94	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	828	VAL	N-CA-C	-7.92	102.37	111.00
2	D	870	ASN	CA-C-N	7.89	127.81	119.05
2	D	870	ASN	C-N-CA	7.89	127.81	119.05
2	B	318	HIS	N-CA-C	6.47	120.05	109.24
1	A	70	THR	N-CA-C	6.46	120.87	113.19
2	D	844	GLU	N-CA-C	6.29	119.33	109.96
1	C	695	ASN	N-CA-C	6.06	119.93	112.54
1	A	39	TYR	N-CA-C	5.96	120.50	113.23
1	C	539	TYR	N-CA-C	5.86	120.38	113.23
1	A	27	ALA	N-CA-C	5.79	117.59	111.28
2	D	831	ASN	N-CA-C	-5.60	101.56	109.96
2	B	370	ASN	CA-C-N	5.59	125.06	119.24
2	B	370	ASN	C-N-CA	5.59	125.06	119.24
1	A	134	PRO	N-CA-C	5.53	119.23	111.33
2	D	798	PHE	N-CA-C	-5.53	102.30	110.48
1	C	568	GLY	N-CA-C	5.50	120.72	114.67
1	C	676	ALA	N-CA-C	-5.48	106.44	113.01
1	A	185	SER	N-CA-C	5.37	120.84	113.97
1	A	68	GLY	N-CA-C	5.35	120.25	113.24
2	B	359	TRP	N-CA-C	5.35	117.19	108.63
2	D	815	LEU	N-CA-C	5.31	118.55	111.75
1	C	560	HIS	N-CA-C	5.30	117.05	111.28
1	C	570	THR	N-CA-C	5.29	119.22	112.87
2	B	328	VAL	N-CA-C	-5.27	104.50	111.09
2	D	849	THR	N-CA-C	-5.26	101.95	110.32
2	B	342	GLN	N-CA-C	5.23	120.30	113.30
1	A	92	LEU	N-CA-C	5.19	117.84	111.82
1	C	688	GLU	N-CA-C	5.18	117.86	108.69
1	A	96	HIS	N-CA-C	-5.15	105.74	112.23
1	A	124	ILE	N-CA-C	5.14	113.58	107.73
1	A	263	SER	N-CA-C	5.13	116.87	111.28
1	A	178	GLY	N-CA-C	5.09	121.06	111.80
1	C	645	PRO	N-CA-C	5.04	120.09	111.68
2	B	349	THR	N-CA-C	-5.03	103.08	110.52
1	A	23	TYR	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	571	TYR	Sidechain

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	2370	0	2246	27	0
1	C	2370	0	2243	25	0
2	B	850	0	847	10	0
2	D	850	0	847	8	0
3	A	43	0	30	0	0
3	B	43	0	28	1	0
4	C	43	0	32	3	0
4	D	43	0	28	3	0
5	A	248	0	0	12	0
5	B	70	0	0	3	0
5	C	152	0	0	10	0
5	D	29	0	0	3	0
All	All	7111	0	6301	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (75) 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:27:ALA:HB2	5:A:1842:HOH:O	1.60	1.02
1:C:617:GLN:HE21	1:C:624:ILE:H	1.20	0.85
2:B:313:ARG:HH21	2:B:313:ARG:HG2	1.43	0.83
2:B:380:MET:HE3	5:B:1840:HOH:O	1.79	0.82
1:C:520:GLN:HE22	1:C:787:LYS:H	1.26	0.80
1:A:95:ILE:HD11	1:A:107:LEU:HD21	1.64	0.79
1:A:233:PRO:HA	5:A:1763:HOH:O	1.83	0.78
1:A:236:TYR:HB3	5:A:1763:HOH:O	1.83	0.78
1:A:20:GLN:HE22	1:A:287:LYS:H	1.29	0.77
1:A:188:GLU:H	1:A:222:GLN:HE22	1.33	0.73
1:C:531:ARG:HG3	1:C:531:ARG:HH21	1.55	0.70
1:C:716:ASN:HD22	1:C:722:GLN:HE21	1.41	0.69
1:C:688:GLU:H	1:C:722:GLN:HE22	1.39	0.67
1:C:732:LEU:HD11	5:C:1878:HOH:O	1.95	0.66
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:TRP:CG	5:B:1840:HOH:O	2.49	0.66
1:C:789:LEU:HG	1:C:794:LEU:HD22	1.80	0.63
1:C:716:ASN:HD22	1:C:722:GLN:NE2	1.98	0.61
2:B:391:ARG:O	2:B:395:ILE:HG12	2.02	0.59
1:C:598:GLU:HG2	5:C:1860:HOH:O	2.03	0.57
1:A:196:ASN:OD1	5:A:1833:HOH:O	2.18	0.56
2:D:864:MET:HE1	4:D:1301:HEC:HMA3	1.88	0.56
1:A:106:ASP:O	1:A:110:LEU:HB2	2.04	0.56
1:C:694:ALA:HB1	1:C:697:VAL:HG13	1.87	0.55
4:D:1301:HEC:HHA	5:D:1426:HOH:O	2.06	0.55
2:B:371:PRO:HG2	2:B:382:TRP:HD1	1.71	0.54
1:A:200:ASN:H	1:A:200:ASN:HD22	1.55	0.54
1:A:193:ALA:HB3	5:A:1841:HOH:O	2.08	0.54
1:C:617:GLN:NE2	1:C:624:ILE:H	1.98	0.53
1:C:691:TRP:HZ2	5:C:1878:HOH:O	1.91	0.53
5:A:1841:HOH:O	3:B:1101:ZNH:HBC2	2.09	0.53
2:B:355:LYS:HZ3	2:B:357:VAL:HG11	1.75	0.51
2:B:313:ARG:HG2	2:B:313:ARG:NH2	2.19	0.51
4:C:1201:HEC:C1A	5:C:1878:HOH:O	2.58	0.51
1:C:664:ASN:O	1:C:668:VAL:HG13	2.10	0.51
1:C:656:THR:HG22	5:C:1409:HOH:O	2.12	0.50
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.59	0.49
1:C:744:TYR:O	1:C:748:VAL:HG23	2.13	0.49
2:B:399:LYS:O	2:B:403:GLU:OXT	2.31	0.49
1:A:164:ASN:O	1:A:168:VAL:HG13	2.14	0.48
1:C:691:TRP:CZ2	5:C:1878:HOH:O	2.55	0.48
1:C:531:ARG:HH12	1:C:794:LEU:HB3	1.79	0.47
1:C:628:CYS:N	5:C:1481:HOH:O	2.46	0.47
2:D:871:PRO:HG2	2:D:882:TRP:HD1	1.78	0.47
1:A:116:VAL:HG21	5:A:1776:HOH:O	2.14	0.47
1:A:289:LEU:HG	1:A:294:LEU:HD12	1.96	0.47
2:D:799:LYS:HB3	2:D:800:ALA:H	1.60	0.47
1:A:123:LYS:HG2	1:A:285:ILE:HG23	1.97	0.45
1:A:113:VAL:HG22	1:A:124:ILE:HD12	1.98	0.45
1:A:183:LYS:HG2	5:A:1452:HOH:O	2.17	0.45
1:C:794:LEU:HD12	1:C:794:LEU:N	2.31	0.45
2:D:864:MET:HE1	4:D:1301:HEC:CMA	2.47	0.45
1:C:700:ASN:H	1:C:700:ASN:HD22	1.65	0.45
1:A:223:TRP:NE1	5:A:1763:HOH:O	2.51	0.44
2:D:797:GLU:HG3	2:D:862:ASN:ND2	2.32	0.44
1:C:531:ARG:NH1	1:C:794:LEU:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:CB	5:A:1842:HOH:O	2.40	0.44
2:B:313:ARG:HB3	2:B:382:TRP:CH2	2.53	0.43
4:C:1201:HEC:C4A	5:C:1878:HOH:O	2.66	0.43
1:C:627:ARG:HH11	1:C:783:PRO:HD3	1.82	0.43
4:C:1201:HEC:C2A	5:C:1878:HOH:O	2.66	0.43
1:A:237:SER:HA	1:A:240:GLN:HE21	1.83	0.43
2:D:868:LEU:HA	5:D:1448:HOH:O	2.19	0.43
2:D:871:PRO:HG3	5:D:1448:HOH:O	2.18	0.43
1:A:113:VAL:HG13	1:A:124:ILE:HG23	2.01	0.42
1:C:783:PRO:HG2	5:C:1678:HOH:O	2.18	0.42
2:D:891:ARG:O	2:D:895:ILE:HG13	2.20	0.42
2:B:361:GLU:O	5:B:1891:HOH:O	2.22	0.42
1:A:124:ILE:HA	1:A:125:PRO:HD3	1.89	0.42
1:C:531:ARG:HG3	1:C:531:ARG:NH2	2.30	0.42
1:A:236:TYR:HA	5:A:1419:HOH:O	2.19	0.42
1:A:223:TRP:CD1	5:A:1763:HOH:O	2.74	0.41
1:A:245:LEU:HD22	1:A:249:LYS:HE2	2.02	0.40
1:A:200:ASN:HD22	1:A:200:ASN:N	2.18	0.40
1:C:551:TRP:HE3	1:C:769:LEU:HD11	1.87	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	292/294 (99%)	281 (96%)	11 (4%)	0	100 100
1	C	292/294 (99%)	284 (97%)	8 (3%)	0	100 100
2	B	106/108 (98%)	99 (93%)	5 (5%)	2 (2%)	6 5
2	D	106/108 (98%)	98 (92%)	6 (6%)	2 (2%)	6 5
All	All	796/804 (99%)	762 (96%)	30 (4%)	4 (0%)	24 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	856	ASN
2	B	299	LYS
2	B	300	ALA
2	D	799	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	252/253 (100%)	227 (90%)	25 (10%)	7	9
1	C	252/253 (100%)	227 (90%)	25 (10%)	7	9
2	B	89/89 (100%)	72 (81%)	17 (19%)	1	1
2	D	89/89 (100%)	76 (85%)	13 (15%)	3	3
All	All	682/684 (100%)	602 (88%)	80 (12%)	5	6

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	LEU
1	A	12	LYS
1	A	31	ARG
1	A	35	GLU
1	A	47	VAL
1	A	51	TRP
1	A	52	HIS
1	A	95	ILE
1	A	107	LEU
1	A	110	LEU
1	A	120	GLN
1	A	123	LYS
1	A	124	ILE
1	A	168	VAL
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	200	ASN
1	A	207	LEU
1	A	219	ASN
1	A	233	PRO
1	A	245	LEU
1	A	270	LEU
1	A	289	LEU
1	A	290	GLU
2	B	298	PHE
2	B	305	LYS
2	B	309	LEU
2	B	311	LYS
2	B	313	ARG
2	B	316	GLN
2	B	327	LYS
2	B	344	GLU
2	B	358	LEU
2	B	369	THR
2	B	373	LYS
2	B	379	LYS
2	B	380	MET
2	B	387	LYS
2	B	389	LYS
2	B	399	LYS
2	B	400	LYS
1	C	502	THR
1	C	528	LEU
1	C	531	ARG
1	C	547	VAL
1	C	562	ASN
1	C	574	LYS
1	C	578	ASN
1	C	593	GLU
1	C	597	LYS
1	C	659	GLN
1	C	668	VAL
1	C	683	LYS
1	C	696	ASN
1	C	697	VAL
1	C	700	ASN
1	C	707	LEU

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Mol	Chain	Res	Type
1	C	726	LYS
1	C	737	SER
1	C	745	LEU
1	C	760	LYS
1	C	764	LYS
1	C	769	LEU
1	C	778	LYS
1	C	787	LYS
1	C	789	LEU
2	D	797	GLU
2	D	798	PHE
2	D	799	LYS
2	D	805	LYS
2	D	809	LEU
2	D	815	LEU
2	D	821	GLU
2	D	822	LYS
2	D	864	MET
2	D	872	LYS
2	D	873	LYS
2	D	880	MET
2	D	895	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	82	ASN
1	A	141	ASN
1	A	181	HIS
1	A	200	ASN
1	A	222	GLN
1	A	240	GLN
1	A	255	GLN
1	A	292	GLN
2	B	356	ASN
2	B	362	ASN
1	C	520	GLN
1	C	524	ASN
1	C	562	ASN
1	C	617	GLN

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Mol	Chain	Res	Type
1	C	695	ASN
1	C	696	ASN
1	C	700	ASN
1	C	705	ASN
1	C	708	ASN
1	C	722	GLN
1	C	753	ASN
1	C	755	GLN
1	C	792	GLN
2	D	816	GLN
2	D	833	HIS
2	D	852	ASN
2	D	856	ASN
2	D	862	ASN

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)

4 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	$\#\|Z\|>2$
4	HEC	C	1201	1	50,50,50	1.61	11 (22%)	68,82,82	2.01	14 (20%)
4	HEC	D	1301	2	50,50,50	1.88	12 (24%)	68,82,82	1.83	12 (17%)
3	ZNH	B	1101	2	50,50,50	1.35	7 (14%)	65,82,82	1.24	3 (4%)
3	ZNH	A	1001	1	50,50,50	1.26	5 (10%)	65,82,82	1.46	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	C	1201	1	1/1/3/7	8/14/54/54	-
4	HEC	D	1301	2	1/1/3/7	4/14/54/54	-
3	ZNH	B	1101	2	1/1/3/9	6/14/54/54	-
3	ZNH	A	1001	1	1/1/3/9	2/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	HEC	FE-NC	5.42	2.13	1.95
3	B	1101	ZNH	CHC-C4B	4.25	1.47	1.38
4	D	1301	HEC	FE-ND	3.87	2.06	1.94
4	D	1301	HEC	CAB-C3B	-3.74	1.41	1.51
4	D	1301	HEC	CAC-C3C	-3.64	1.41	1.51
4	C	1201	HEC	CAC-C3C	-3.51	1.42	1.51
4	C	1201	HEC	FE-NC	3.39	2.06	1.95
4	D	1301	HEC	CBC-CAC	-3.28	1.37	1.51
4	C	1201	HEC	FE-ND	3.27	2.05	1.94
4	D	1301	HEC	CBB-CAB	-3.22	1.37	1.51
4	D	1301	HEC	C4D-C3D	3.20	1.50	1.45
4	C	1201	HEC	FE-NA	3.10	2.05	1.95
4	C	1201	HEC	C1C-NC	-3.09	1.33	1.39
4	C	1201	HEC	CAB-C3B	-3.03	1.43	1.51
4	D	1301	HEC	FE-NB	2.98	2.04	1.94
3	A	1001	ZNH	C4B-NB	2.90	1.44	1.38
4	D	1301	HEC	C4A-NA	-2.79	1.34	1.39
4	C	1201	HEC	FE-NB	2.78	2.03	1.94
4	C	1201	HEC	CMC-C2C	2.74	1.56	1.50
3	A	1001	ZNH	CMC-C2C	2.74	1.56	1.50
4	C	1201	HEC	CBC-CAC	-2.71	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	HEC	FE-NA	2.61	2.03	1.95
4	D	1301	HEC	C1C-NC	-2.50	1.34	1.39
3	B	1101	ZNH	CAC-C3C	-2.49	1.40	1.47
3	A	1001	ZNH	CMD-C2D	2.39	1.55	1.50
4	C	1201	HEC	CBB-CAB	-2.39	1.41	1.51
3	A	1001	ZNH	C4A-C3A	-2.27	1.40	1.45
3	B	1101	ZNH	ZN-NA	2.25	2.11	2.03
3	B	1101	ZNH	CMC-C2C	2.22	1.55	1.50
3	B	1101	ZNH	C3C-C4C	2.22	1.49	1.42
4	D	1301	HEC	C1A-NA	-2.19	1.35	1.39
3	A	1001	ZNH	C1D-C2D	2.13	1.48	1.44
3	B	1101	ZNH	CHC-C1C	2.09	1.44	1.39
3	B	1101	ZNH	CAB-C3B	-2.05	1.41	1.47
4	C	1201	HEC	CMD-C2D	2.02	1.54	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1201	HEC	CBC-CAC-C3C	8.20	134.64	112.42
4	C	1201	HEC	CBB-CAB-C3B	7.93	133.93	112.42
4	D	1301	HEC	CBB-CAB-C3B	6.64	130.43	112.42
4	D	1301	HEC	CBC-CAC-C3C	5.20	126.52	112.42
3	A	1001	ZNH	C4B-C3B-C2B	-4.77	102.89	107.28
3	B	1101	ZNH	C1A-CHA-C4D	4.02	134.56	126.02
3	A	1001	ZNH	C3B-C2B-C1B	3.70	109.19	106.41
4	D	1301	HEC	CHA-C4D-C3D	3.69	130.15	124.77
4	D	1301	HEC	C1A-CHA-C4D	3.65	133.77	126.02
4	D	1301	HEC	CHA-C4D-ND	-3.48	120.68	124.42
4	C	1201	HEC	CHC-C4B-NB	-3.37	120.20	124.37
4	D	1301	HEC	CAD-C3D-C4D	3.27	130.40	124.70
3	B	1101	ZNH	C2C-C1C-NC	3.24	113.09	109.02
3	A	1001	ZNH	CMB-C2B-C1B	-3.11	120.17	125.03
4	C	1201	HEC	CHA-C1A-C2A	3.07	129.71	124.86
4	C	1201	HEC	C3B-C4B-NB	2.92	113.38	110.17
4	C	1201	HEC	CAC-C3C-C2C	2.88	131.45	126.89
4	D	1301	HEC	CAB-C3B-C2B	2.84	132.78	127.56
4	D	1301	HEC	CHB-C1B-NB	-2.72	121.49	124.42
4	D	1301	HEC	CHA-C1A-NA	-2.55	121.68	124.45
4	C	1201	HEC	CHA-C1A-NA	-2.53	121.70	124.45
4	C	1201	HEC	C2D-C1D-ND	2.51	112.72	109.84
4	C	1201	HEC	CAB-C3B-C2B	2.45	132.06	127.56
4	D	1301	HEC	CAD-C3D-C2D	-2.43	123.31	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1301	HEC	C1C-CHC-C4B	2.42	131.94	126.25
3	A	1001	ZNH	C4B-NB-C1B	-2.41	103.27	106.47
4	C	1201	HEC	C4B-C3B-C2B	-2.34	103.48	106.89
3	B	1101	ZNH	CHA-C1A-NA	-2.32	120.99	124.82
3	A	1001	ZNH	CAD-C3D-C4D	2.30	128.70	124.70
4	C	1201	HEC	C3C-C4C-NC	2.24	112.64	110.15
4	C	1201	HEC	C4C-C3C-C2C	-2.20	103.46	106.87
4	C	1201	HEC	CMB-C2B-C1B	-2.14	121.69	125.03
3	A	1001	ZNH	CBA-CAA-C2A	2.14	118.44	112.53
4	D	1301	HEC	C4C-C3C-C2C	-2.10	103.62	106.87
4	C	1201	HEC	O2D-CGD-CBD	2.09	120.61	114.00
3	A	1001	ZNH	CHC-C4B-NB	-2.09	122.05	124.75
3	A	1001	ZNH	O2D-CGD-CBD	2.01	120.34	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1001	ZNH	NA
3	B	1101	ZNH	NA
4	C	1201	HEC	NA
4	D	1301	HEC	NA

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1101	ZNH	C2C-C3C-CAC-CBC
3	B	1101	ZNH	C4C-C3C-CAC-CBC
4	C	1201	HEC	C2C-C3C-CAC-CBC
4	C	1201	HEC	C4B-C3B-CAB-CBB
4	D	1301	HEC	C4B-C3B-CAB-CBB
4	C	1201	HEC	C4C-C3C-CAC-CBC
4	C	1201	HEC	C2B-C3B-CAB-CBB
4	D	1301	HEC	C2B-C3B-CAB-CBB
4	C	1201	HEC	CAD-CBD-CGD-O2D
3	A	1001	ZNH	CAA-CBA-CGA-O2A
4	C	1201	HEC	CAD-CBD-CGD-O1D
4	C	1201	HEC	CAA-CBA-CGA-O2A
4	C	1201	HEC	CAA-CBA-CGA-O1A
3	A	1001	ZNH	CAA-CBA-CGA-O1A
3	B	1101	ZNH	C4B-C3B-CAB-CBB
4	D	1301	HEC	CAA-CBA-CGA-O2A
3	B	1101	ZNH	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	D	1301	HEC	CAA-CBA-CGA-O1A
3	B	1101	ZNH	C2B-C3B-CAB-CBB
3	B	1101	ZNH	CAA-CBA-CGA-O1A

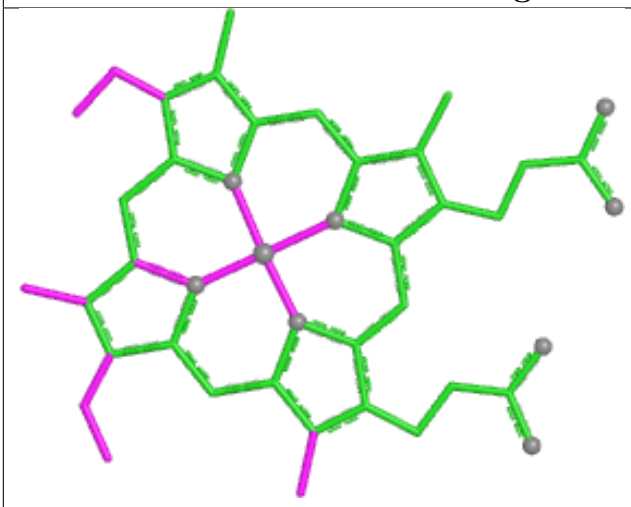
There are no ring outliers.

3 monomers are involved in 7 short contacts:

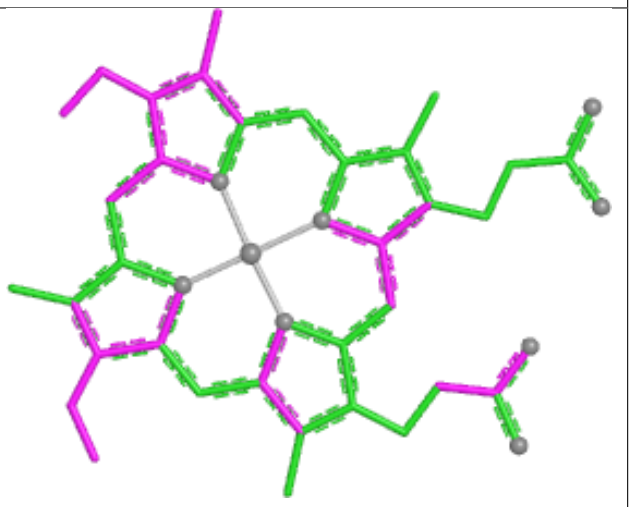
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1201	HEC	3	0
4	D	1301	HEC	3	0
3	B	1101	ZNH	1	0

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.

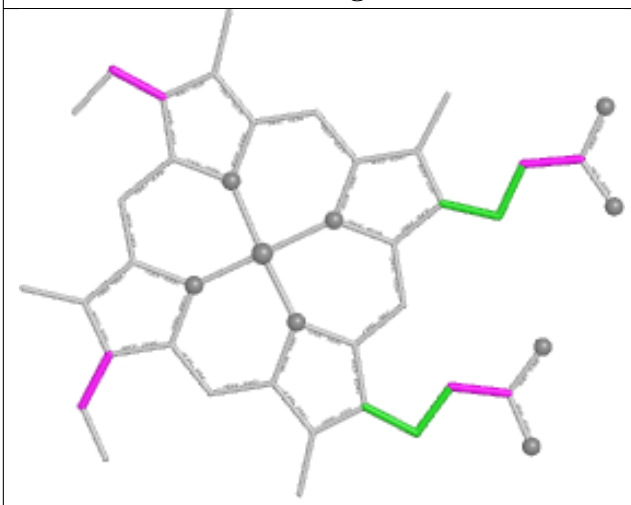
Ligand HEC C 1201



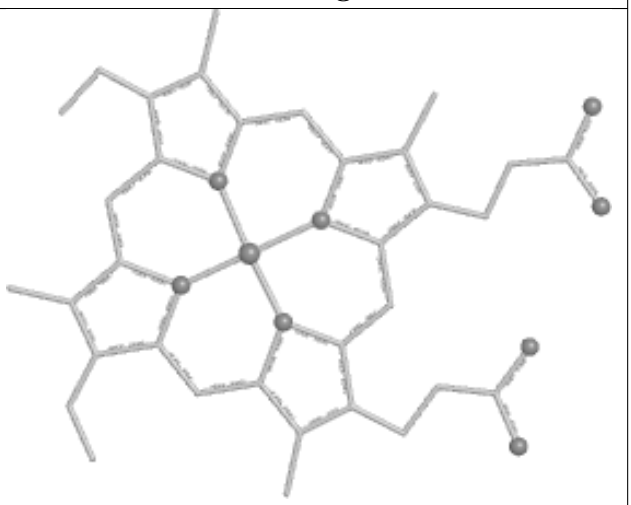
Bond lengths



Bond angles

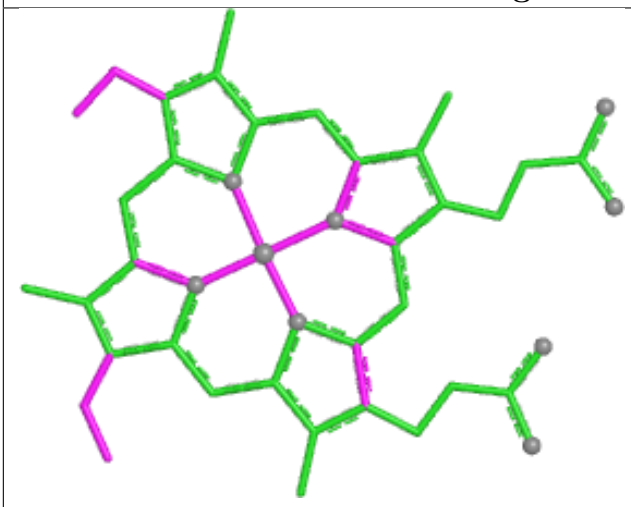


Torsions

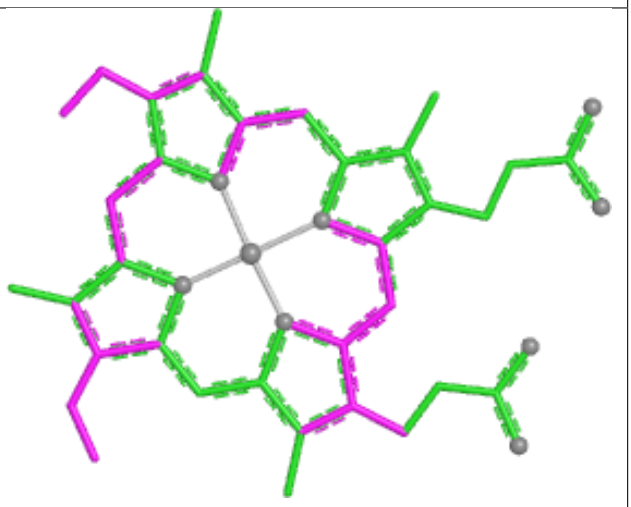


Rings

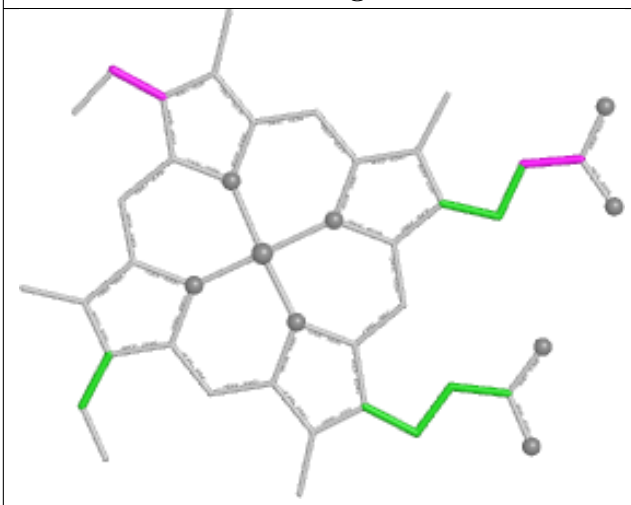
Ligand HEC D 1301



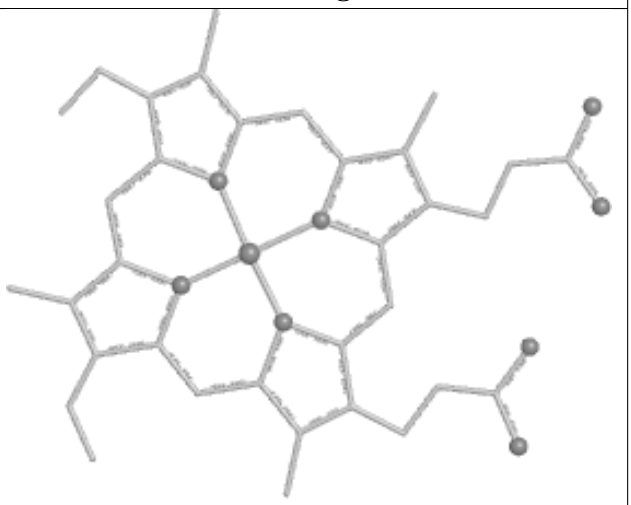
Bond lengths



Bond angles

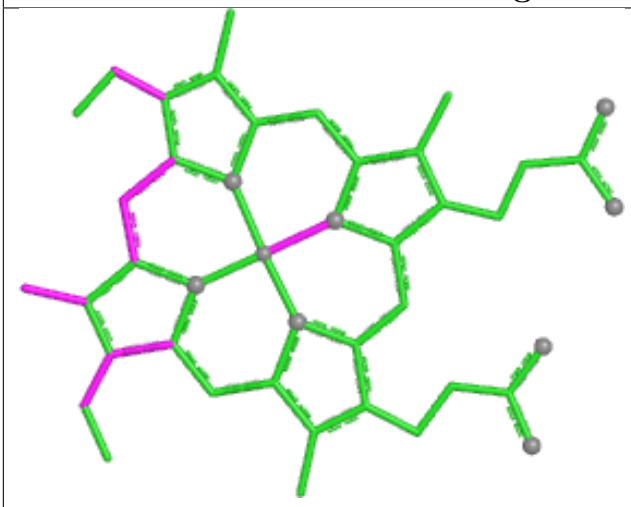


Torsions

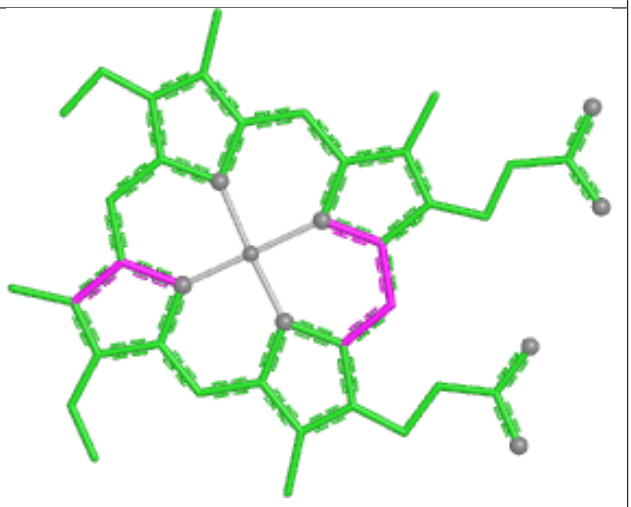


Rings

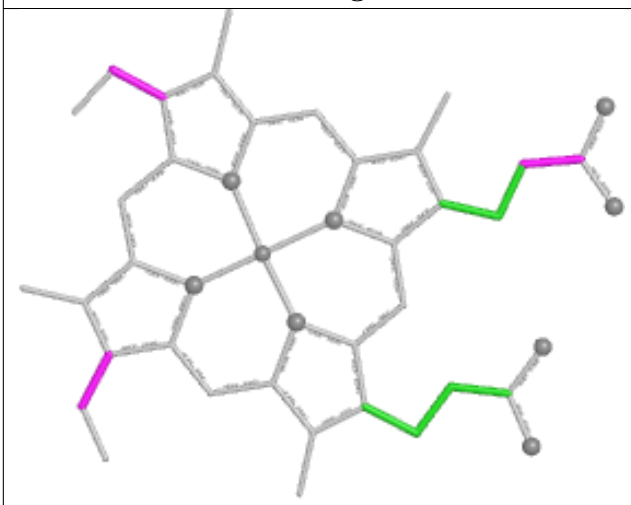
Ligand ZNH B 1101



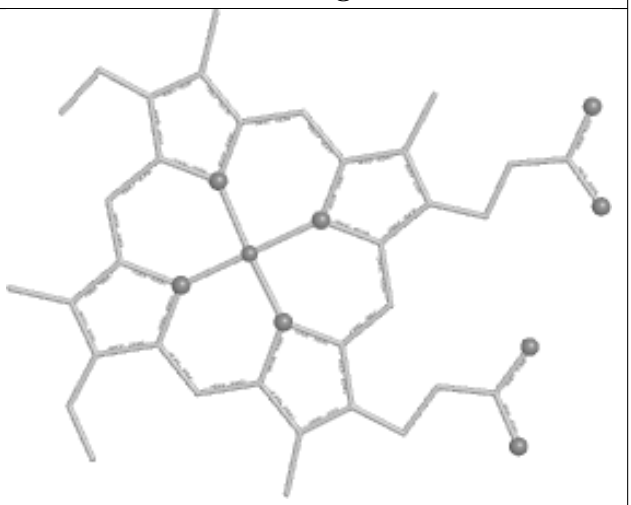
Bond lengths



Bond angles

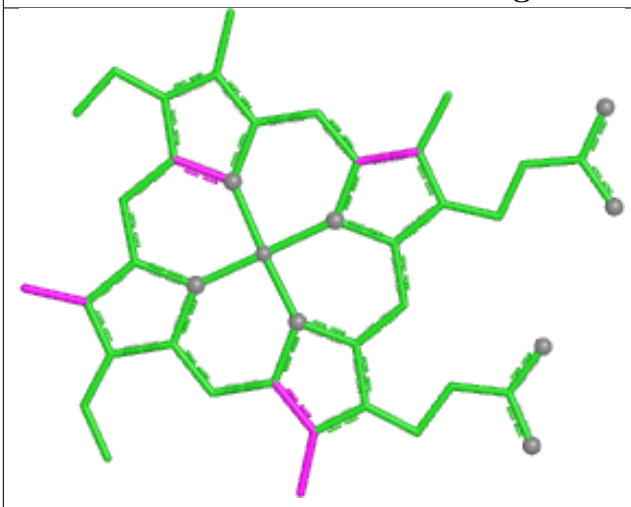


Torsions

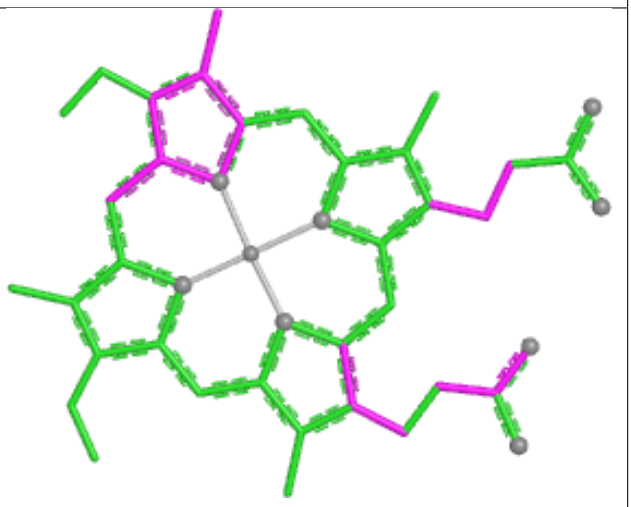


Rings

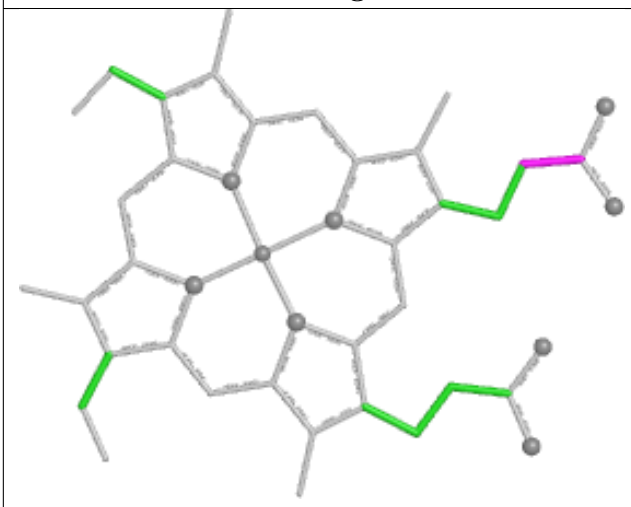
Ligand ZNH A 1001



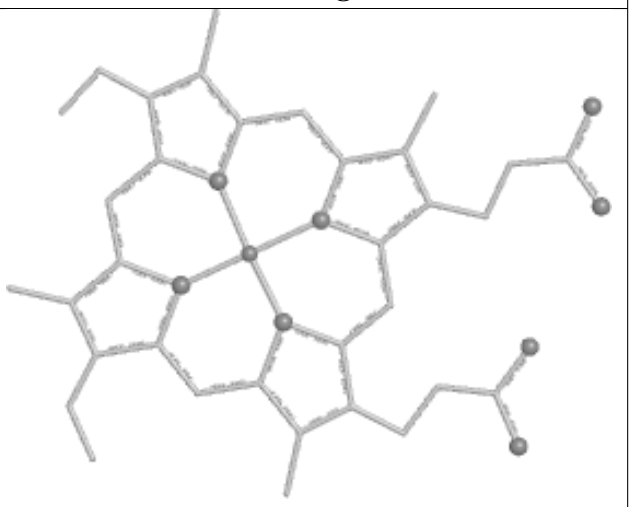
Bond lengths



Bond angles



Torsions



Rings

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	A	294/294 (100%)	-0.99	0	100	100	13, 33, 54, 105	0
1	C	294/294 (100%)	-0.98	0	100	100	12, 33, 54, 109	0
2	B	108/108 (100%)	-0.80	0	100	100	28, 50, 83, 113	0
2	D	108/108 (100%)	-0.62	0	100	100	30, 64, 85, 108	0
All	All	804/804 (100%)	-0.91	0	100	100	12, 37, 76, 113	0

There are no RSRZ outliers to report.

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

There are no oligosaccharides in this entry.

6.4 Ligands

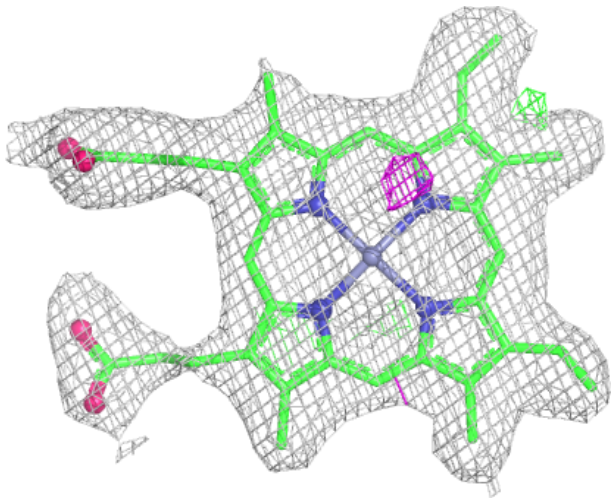
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

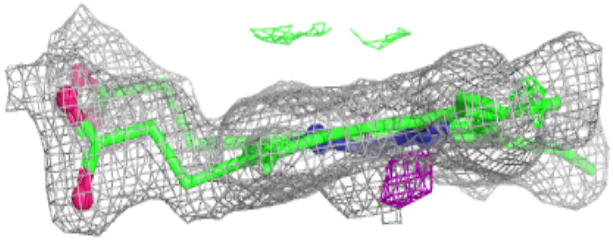
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZNH	A	1001	43/43	0.99	0.04	5,17,33,45	0
3	ZNH	B	1101	43/43	0.99	0.04	24,34,44,45	0
4	HEC	C	1201	43/43	0.99	0.03	2,13,27,32	0
4	HEC	D	1301	43/43	0.99	0.05	26,39,47,53	0

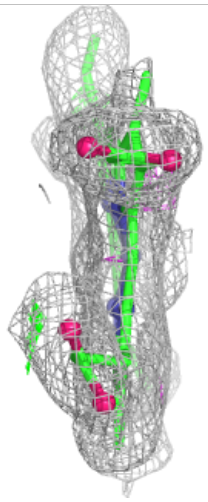
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZNH A 1001:

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

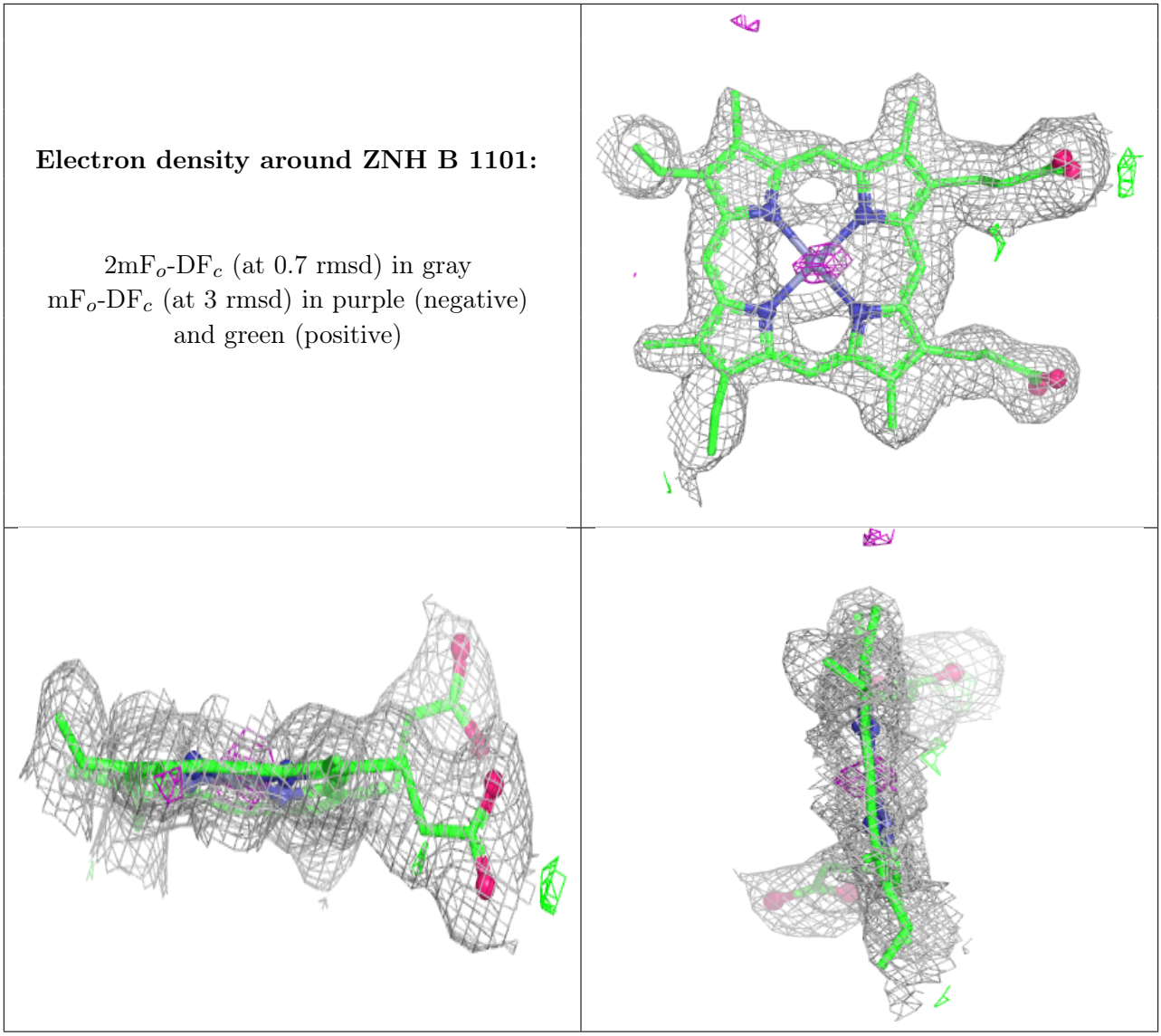






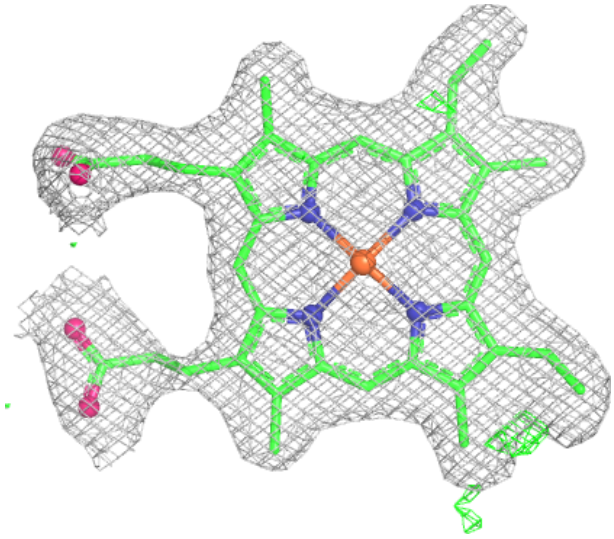
Electron density around ZNH B 1101:

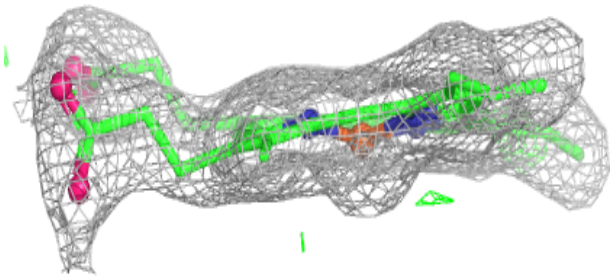
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

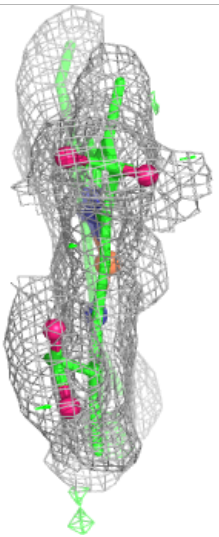


Electron density around HEC C 1201:

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

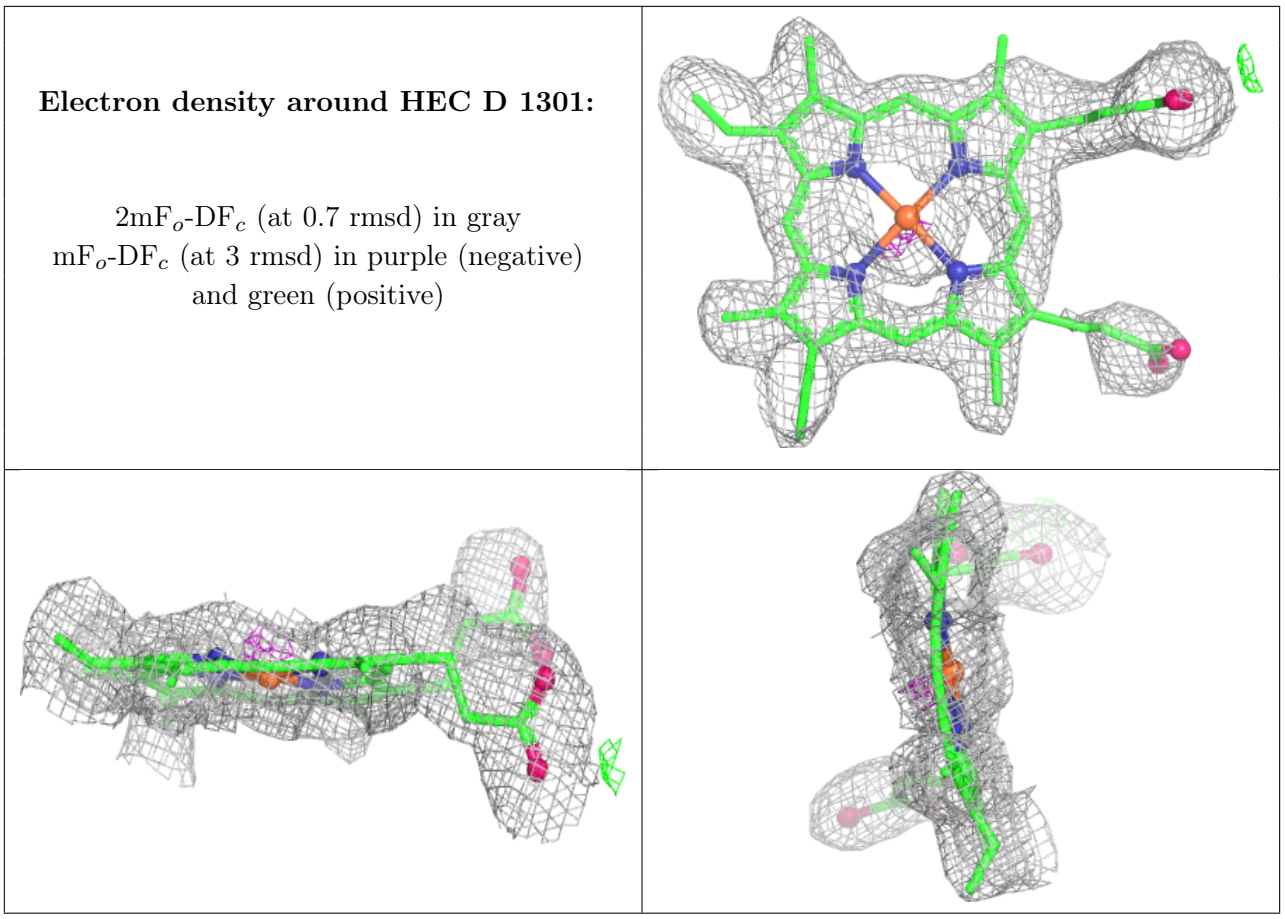






Electron density around HEC D 1301:

$2mF_o$-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

There are no such residues in this entry.