Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 08:27 am BST

PDB ID	:	4AX3 / pdb_00004ax3
Title	:	Structure of three-domain heme-Cu nitrite reductase from Ralstonia pickettii at 1.6 A resolution
Authors	:	Antonyuk, S.V.; Cong, H.; Eady, R.R.; Hasnain, S.S.
Deposited on	:	2012-06-07
Resolution	:	1.60 Å(reported)

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

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

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

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

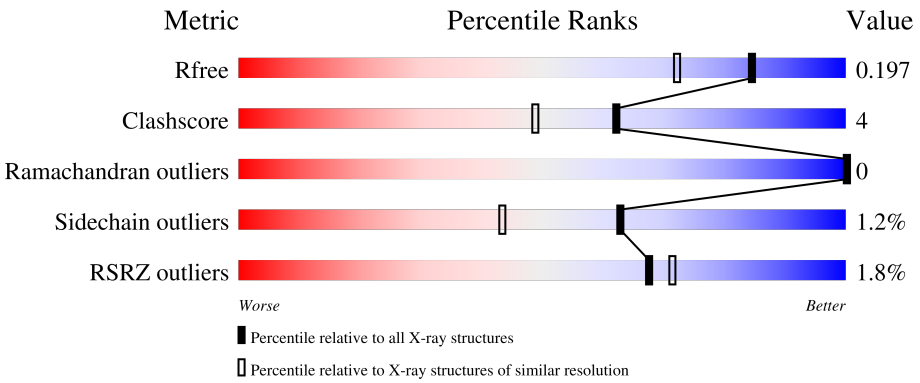
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	4% 90% 7% •
1	B	468	% 89% 8% •
1	C	468	% 89% 8% •
1	D	468	% 89% 9% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	A	600	X	-	-	-
3	HEC	B	600	X	-	-	-
3	HEC	C	600	X	-	-	-
3	HEC	D	600	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16795 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.

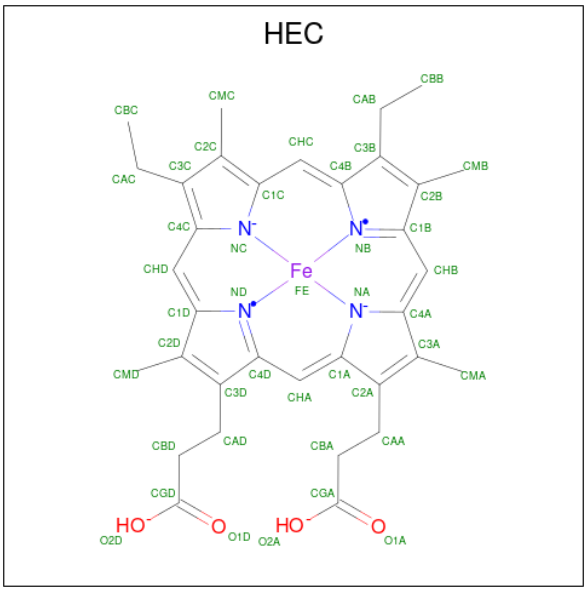
- Molecule 1 is a protein called COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3551	2270	610	655	16	0	21	0
1	B	455	3543	2260	607	661	15	0	21	0
1	C	455	3547	2264	603	664	16	0	22	0
1	D	457	3495	2225	603	652	15	0	9	0

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

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



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

- Molecule 4 is water.

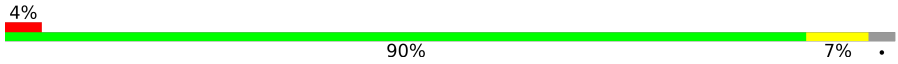
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	629	Total	O	0	7
			636	636		
4	B	633	Total	O	0	2
			635	635		
4	C	697	Total	O	0	0
			697	697		
4	D	511	Total	O	0	0
			511	511		

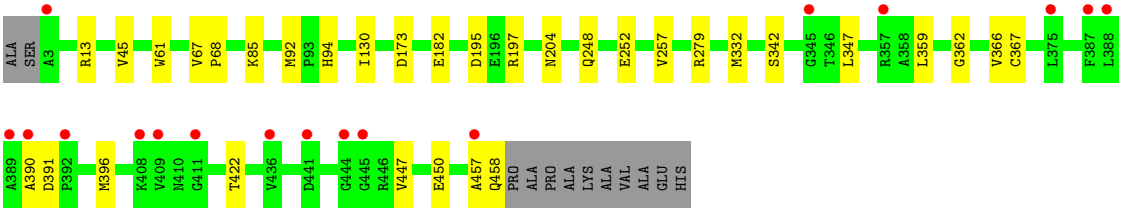
3 Residue-property plots (i)

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: COPPER-CONTAINING NITRITE REDUCTASE

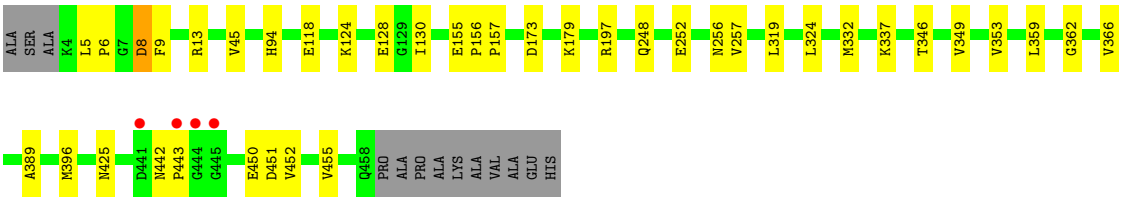
Chain A:





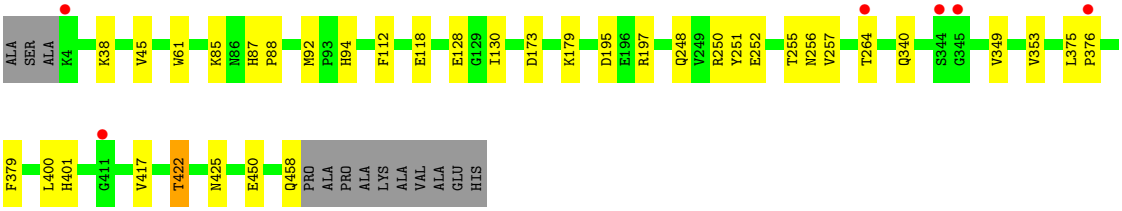
• Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE

Chain B:



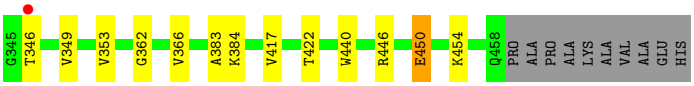
• Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE

Chain C:



• Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE

Chain D:


G345
T346
V349
V353
G362
V366
A383
K384
V417
T422
W440
R446
E450
K454
Q458
PRO
ALA
PRO
ALA
LYS
ALA
VAL
ALA
GLU
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	185.81Å 185.81Å 185.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60 25.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-1.60) 99.8 (25.00-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.194 0.168 , 0.197	Depositor DCC
R_{free} test set	14067 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16795	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1891e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CU, 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	0.85	0/3700	0.90	1/5026 (0.0%)
1	B	0.82	0/3687	0.90	6/5009 (0.1%)
1	C	0.92	0/3698	0.94	2/5022 (0.0%)
1	D	0.80	0/3607	0.86	0/4898
All	All	0.85	0/14692	0.90	9/19955 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	379	PHE	CA-C-N	-5.51	114.70	120.38
1	C	379	PHE	C-N-CA	-5.51	114.70	120.38
1	B	155	GLU	CA-C-N	-5.22	115.01	120.38
1	B	155	GLU	C-N-CA	-5.22	115.01	120.38
1	B	8[A]	ASP	CA-C-N	5.19	130.70	122.60
1	B	8[A]	ASP	C-N-CA	5.19	130.70	122.60
1	B	8[B]	ASP	CA-C-N	5.19	130.70	122.60
1	B	8[B]	ASP	C-N-CA	5.19	130.70	122.60
1	A	67	VAL	CA-C-O	5.07	122.58	119.94

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	3551	0	3578	26	0
1	B	3543	0	3544	31	0
1	C	3547	0	3556	34	0
1	D	3495	0	3477	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	0	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	A	636	0	0	5	0
4	B	635	0	0	4	0
4	C	697	0	0	12	1
4	D	511	0	0	7	0
All	All	16795	0	14275	117	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (117) 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:367:CYS:SG	3:A:600:HEC:CAC	2.03	1.47
1:B:396:MET:HE2	1:B:455:VAL:HG21	1.30	1.11
1:B:396:MET:HE2	1:B:455:VAL:CG2	1.98	0.94
1:B:362:GLY:O	1:B:366[B]:VAL:HG13	1.74	0.88
1:A:396:MET:HE2	1:A:447:VAL:HG13	1.53	0.88
1:C:264[B]:THR:HG23	1:C:264[B]:THR:O	1.73	0.88
1:D:279[A]:ARG:CZ	4:D:2362:HOH:O	2.23	0.86
1:C:85[B]:LYS:HE2	1:C:118[B]:GLU:OE2	1.75	0.86
1:C:195[B]:ASP:OD2	1:C:197[B]:ARG:HD2	1.76	0.84
1:B:396:MET:HE3	1:B:452:VAL:HA	1.60	0.81
1:B:396:MET:CE	1:B:455:VAL:CG2	2.60	0.79
1:C:400:LEU:O	1:C:422[B]:THR:HG22	1.85	0.74
1:C:197[A]:ARG:HD3	4:C:2392:HOH:O	1.85	0.74
1:B:396:MET:CE	1:B:455:VAL:HG21	2.15	0.73
1:B:396:MET:HE1	1:B:451:ASP:O	1.89	0.72
1:A:85[B]:LYS:HG3	4:A:2073:HOH:O	1.90	0.68
1:D:83:HIS:ND1	4:D:2157:HOH:O	2.25	0.68
1:C:85[B]:LYS:HE2	1:C:118[B]:GLU:CD	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:CYS:SG	3:A:600:HEC:CBC	2.79	0.68
1:A:248[B]:GLN:HG3	1:A:257:VAL:CG1	2.23	0.67
1:A:279[B]:ARG:CZ	4:A:2477:HOH:O	2.43	0.67
1:B:248:GLN:HG3	1:B:257:VAL:CG1	2.24	0.67
1:A:396:MET:HE2	1:A:447:VAL:CG1	2.26	0.66
1:A:367:CYS:SG	3:A:600:HEC:C3C	2.84	0.64
1:D:248[B]:GLN:CG	1:D:257:VAL:CG1	2.76	0.64
1:B:396:MET:CE	1:B:452:VAL:HA	2.28	0.62
1:C:179:LYS:HE2	1:C:425:ASN:ND2	2.16	0.60
1:C:255:THR:HG21	4:C:2468:HOH:O	2.01	0.60
1:C:85[B]:LYS:CE	1:C:118[B]:GLU:OE2	2.49	0.60
1:D:248[B]:GLN:HG3	1:D:257:VAL:CG1	2.33	0.59
1:A:182[A]:GLU:OE1	4:A:2347:HOH:O	2.16	0.59
1:B:118:GLU:HG2	4:B:2206:HOH:O	2.03	0.58
1:D:195[B]:ASP:OD2	1:D:197:ARG:HD2	2.03	0.58
1:A:279[B]:ARG:NH1	4:A:2477:HOH:O	2.36	0.58
1:C:45:VAL:HG11	1:C:94:HIS:CD2	2.39	0.57
1:D:349:VAL:HG23	1:D:446:ARG:HH21	1.69	0.57
1:B:9:PHE:CE2	1:B:157[B]:PRO:HG3	2.41	0.56
1:A:457:ALA:O	1:A:458:GLN:HB2	2.07	0.54
1:B:118:GLU:CG	4:B:2206:HOH:O	2.56	0.54
1:A:332[A]:MET:HE1	1:A:359:LEU:HD23	1.90	0.53
1:C:340[B]:GLN:NE2	4:C:2565:HOH:O	2.41	0.53
1:D:349:VAL:O	1:D:353:VAL:HG23	2.09	0.53
1:B:256:ASN:ND2	4:B:2434:HOH:O	2.37	0.52
1:C:130:ILE:O	1:C:252:GLU:HA	2.09	0.52
1:C:450[B]:GLU:HG3	4:C:2351:HOH:O	2.09	0.52
1:D:45:VAL:HG11	1:D:94:HIS:CD2	2.45	0.52
1:C:197[A]:ARG:CG	4:C:2392:HOH:O	2.58	0.52
1:A:85[B]:LYS:CG	4:A:2073:HOH:O	2.56	0.51
1:D:366:VAL:HG11	4:D:2447:HOH:O	2.10	0.51
1:D:197:ARG:HD3	4:D:2284:HOH:O	2.10	0.51
1:A:362:GLY:O	1:A:366[B]:VAL:HG23	2.11	0.50
1:B:442:ASN:HB3	1:B:443:PRO:HD2	1.92	0.50
1:D:446:ARG:HD2	4:D:2504:HOH:O	2.11	0.50
1:C:195[B]:ASP:HB3	1:C:197[B]:ARG:HG3	1.92	0.50
1:B:8[B]:ASP:CG	1:B:124[B]:LYS:HZ3	2.20	0.50
1:B:332:MET:HE1	1:B:359:LEU:HD23	1.94	0.50
1:C:256:ASN:ND2	4:C:2469:HOH:O	2.43	0.49
1:B:389:ALA:HB3	1:C:376:PRO:HG2	1.95	0.49
1:C:38:LYS:NZ	4:C:2121:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179[B]:LYS:HE2	1:B:425:ASN:OD1	2.12	0.49
1:B:362:GLY:O	1:B:366[A]:VAL:HG12	2.13	0.48
1:D:248[B]:GLN:CD	1:D:257:VAL:HG11	2.38	0.48
1:C:61:TRP:CH2	1:C:92[B]:MET:HG3	2.49	0.47
1:A:130:ILE:O	1:A:252:GLU:HA	2.15	0.47
1:A:248[B]:GLN:HG3	1:A:257:VAL:HG13	1.97	0.47
1:B:130:ILE:O	1:B:252:GLU:HA	2.15	0.46
1:D:130:ILE:O	1:D:252:GLU:HA	2.15	0.46
1:B:128[A]:GLU:HG3	1:B:156:PRO:HA	1.97	0.46
1:C:128[A]:GLU:OE2	1:C:250:ARG:NH1	2.42	0.46
1:C:248[B]:GLN:HG3	1:C:257:VAL:CG1	2.46	0.46
1:C:401:HIS:HE1	4:C:2629:HOH:O	2.00	0.45
1:C:458:GLN:C	4:C:2695:HOH:O	2.60	0.45
1:B:396:MET:HE1	1:B:455:VAL:CG2	2.47	0.45
1:A:68:PRO:HD3	1:A:204:ASN:HA	1.99	0.44
1:B:396:MET:HE1	1:B:455:VAL:HG23	1.97	0.44
1:B:128[A]:GLU:HG3	1:B:156:PRO:CA	2.48	0.44
1:C:112:PHE:HB2	4:C:2239:HOH:O	2.18	0.44
1:C:195[B]:ASP:OD2	1:C:197[B]:ARG:CD	2.59	0.43
1:A:248[B]:GLN:CG	1:A:257:VAL:CG1	2.95	0.43
1:A:390:ALA:O	1:D:440:TRP:HA	2.18	0.43
1:A:45:VAL:HG11	1:A:94:HIS:CD2	2.53	0.43
1:B:349:VAL:O	1:B:353:VAL:HG23	2.19	0.43
1:D:118:GLU:HG2	4:D:2157:HOH:O	2.17	0.43
1:D:344:SER:HB2	1:D:346:THR:HG22	2.01	0.43
1:D:82:PHE:O	1:D:120:GLN:HA	2.19	0.43
1:D:450:GLU:CD	1:D:450:GLU:H	2.27	0.43
1:A:61:TRP:CH2	1:A:92[A]:MET:HG3	2.54	0.42
1:C:85[B]:LYS:HG2	1:C:118[B]:GLU:CG	2.48	0.42
1:D:61:TRP:CH2	1:D:92:MET:HG3	2.53	0.42
1:A:248[B]:GLN:CG	1:A:257:VAL:HG13	2.48	0.42
1:D:68:PRO:HD3	1:D:204:ASN:HA	2.01	0.42
1:D:292:PHE:O	1:D:296:ASN:HB2	2.18	0.42
1:B:319:LEU:HD21	1:B:324:LEU:HD13	2.02	0.42
1:D:91[A]:LYS:NZ	4:D:2164:HOH:O	2.52	0.42
1:D:362:GLY:O	1:D:366:VAL:HG12	2.19	0.42
1:C:85[B]:LYS:CG	1:C:118[B]:GLU:CD	2.93	0.42
1:B:5:LEU:O	1:B:8[A]:ASP:HB2	2.20	0.41
1:D:302:ILE:HD11	1:D:324:LEU:HD21	2.01	0.41
1:C:85[B]:LYS:HG2	1:C:118[B]:GLU:CD	2.45	0.41
1:C:85[B]:LYS:HG3	4:C:2126:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422[B]:THR:HG21	4:C:2654:HOH:O	2.20	0.41
1:C:349:VAL:O	1:C:353:VAL:HG23	2.20	0.41
1:A:195[A]:ASP:HB3	1:A:197[A]:ARG:HG3	2.02	0.41
1:A:390:ALA:O	1:A:391:ASP:HB2	2.21	0.41
1:A:342:SER:OG	1:A:347:LEU:HD22	2.21	0.41
1:B:45:VAL:HG11	1:B:94:HIS:CD2	2.56	0.41
1:B:197[B]:ARG:NH2	4:B:2370:HOH:O	2.45	0.41
1:D:31:VAL:HG21	1:D:75:ARG:HB2	2.03	0.41
1:D:383:ALA:O	1:D:384:LYS:C	2.64	0.41
1:A:457:ALA:O	1:A:458:GLN:CB	2.69	0.40
1:C:87:HIS:CG	1:C:88:PRO:HD2	2.57	0.40
1:B:5:LEU:HB3	1:B:6:PRO:HD2	2.04	0.40
1:D:248[B]:GLN:CG	1:D:257:VAL:HG11	2.52	0.40
1:B:13[B]:ARG:HE	1:B:13[B]:ARG:HB2	1.72	0.40
1:D:218:ALA:HB3	1:D:305:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2392:HOH:O	4:C:2392:HOH:O[6_456]	1.81	0.39

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	475/468 (102%)	465 (98%)	10 (2%)	0	100	100
1	B	474/468 (101%)	466 (98%)	8 (2%)	0	100	100
1	C	475/468 (102%)	468 (98%)	7 (2%)	0	100	100
1	D	464/468 (99%)	458 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1888/1872 (101%)	1857 (98%)	31 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	384/371 (104%)	379 (99%)	5 (1%)	61 40
1	B	383/371 (103%)	378 (99%)	5 (1%)	61 40
1	C	385/371 (104%)	380 (99%)	5 (1%)	61 40
1	D	373/371 (100%)	368 (99%)	5 (1%)	61 40
All	All	1525/1484 (103%)	1505 (99%)	20 (1%)	63 40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	ARG
1	A	13[B]	ARG
1	A	173	ASP
1	A	422	THR
1	A	450	GLU
1	B	173	ASP
1	B	337[A]	LYS
1	B	337[B]	LYS
1	B	346	THR
1	B	450	GLU
1	C	173	ASP
1	C	375	LEU
1	C	417	VAL
1	C	422[A]	THR
1	C	422[B]	THR
1	D	173	ASP
1	D	417	VAL

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Mol	Chain	Res	Type
1	D	422	THR
1	D	450	GLU
1	D	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	296	ASN
1	A	350	GLN
1	B	248	GLN
1	B	296	ASN
1	B	350	GLN
1	B	354	GLN
1	B	412	GLN
1	C	296	ASN
1	C	404	ASN
1	C	425	ASN
1	C	438	ASN
1	D	350	GLN
1	D	352	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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	B	600	1	50,50,50	1.81	10 (20%)	68,82,82	2.10	17 (25%)
3	HEC	D	600	1	50,50,50	1.74	8 (16%)	68,82,82	1.76	16 (23%)
3	HEC	A	600	1	50,50,50	1.79	9 (18%)	68,82,82	1.93	19 (27%)
3	HEC	C	600	1	50,50,50	1.64	9 (18%)	68,82,82	1.86	19 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	600	1	1/1/3/7	8/14/54/54	-
3	HEC	D	600	1	1/1/3/7	8/14/54/54	-
3	HEC	A	600	1	1/1/3/7	8/14/54/54	-
3	HEC	C	600	1	1/1/3/7	8/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	HEC	C3D-C2D	7.08	1.51	1.36
3	B	600	HEC	C3D-C2D	6.83	1.51	1.36
3	D	600	HEC	C3D-C2D	6.81	1.51	1.36
3	C	600	HEC	C3D-C2D	6.45	1.50	1.36
3	D	600	HEC	FE-ND	3.73	2.06	1.94
3	A	600	HEC	CBC-CAC	-3.71	1.35	1.51
3	A	600	HEC	CBB-CAB	-3.55	1.35	1.51
3	B	600	HEC	CBB-CAB	-3.49	1.35	1.51
3	B	600	HEC	FE-NA	3.48	2.06	1.95
3	B	600	HEC	CBC-CAC	-3.46	1.36	1.51
3	A	600	HEC	FE-NA	3.41	2.06	1.95
3	D	600	HEC	CBB-CAB	-3.37	1.36	1.51
3	D	600	HEC	CBC-CAC	-3.36	1.36	1.51
3	B	600	HEC	FE-NC	3.35	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	HEC	FE-ND	3.11	2.04	1.94
3	D	600	HEC	FE-NB	3.09	2.04	1.94
3	A	600	HEC	FE-NC	3.05	2.05	1.95
3	C	600	HEC	CBB-CAB	-2.92	1.38	1.51
3	C	600	HEC	CMC-C2C	2.79	1.56	1.50
3	B	600	HEC	CMC-C2C	2.74	1.56	1.50
3	C	600	HEC	CBC-CAC	-2.73	1.39	1.51
3	C	600	HEC	FE-ND	2.72	2.03	1.94
3	C	600	HEC	FE-NC	2.67	2.04	1.95
3	C	600	HEC	FE-NA	2.60	2.03	1.95
3	B	600	HEC	CMB-C2B	2.52	1.56	1.50
3	D	600	HEC	FE-NA	2.51	2.03	1.95
3	A	600	HEC	CMC-C2C	2.49	1.56	1.50
3	A	600	HEC	CMB-C2B	2.30	1.55	1.50
3	C	600	HEC	C3C-C2C	-2.26	1.32	1.38
3	D	600	HEC	FE-NC	2.24	2.02	1.95
3	B	600	HEC	CAD-C3D	2.18	1.57	1.51
3	A	600	HEC	FE-ND	2.18	2.01	1.94
3	D	600	HEC	CMC-C2C	2.13	1.55	1.50
3	C	600	HEC	CMB-C2B	2.08	1.55	1.50
3	B	600	HEC	C3C-C2C	-2.04	1.33	1.38
3	A	600	HEC	C4A-NA	-2.01	1.35	1.39

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	HEC	C4A-NA-C1A	6.57	111.78	105.35
3	B	600	HEC	C4C-NC-C1C	6.36	111.58	105.35
3	C	600	HEC	C4C-NC-C1C	5.99	111.22	105.35
3	A	600	HEC	C4C-NC-C1C	5.88	111.10	105.35
3	A	600	HEC	C4A-NA-C1A	5.38	110.61	105.35
3	B	600	HEC	C2A-C1A-NA	-5.12	105.34	110.32
3	B	600	HEC	CHB-C4A-NA	4.80	129.64	124.44
3	A	600	HEC	C2A-C1A-NA	-4.79	105.67	110.32
3	B	600	HEC	C3C-C4C-NC	-4.47	105.15	110.15
3	D	600	HEC	C4C-NC-C1C	4.42	109.68	105.35
3	D	600	HEC	C1D-ND-C4D	4.36	109.58	105.07
3	C	600	HEC	C4A-NA-C1A	4.24	109.50	105.35
3	D	600	HEC	C4A-NA-C1A	4.21	109.47	105.35
3	B	600	HEC	CMD-C2D-C1D	3.98	131.10	125.04
3	C	600	HEC	C2A-C1A-NA	-3.97	106.46	110.32
3	C	600	HEC	C3C-C4C-NC	-3.94	105.75	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	HEC	CHB-C4A-NA	3.89	128.64	124.44
3	B	600	HEC	CAD-C3D-C4D	3.78	131.26	124.66
3	B	600	HEC	CHD-C4C-NC	3.72	130.69	123.85
3	A	600	HEC	CMD-C2D-C1D	3.47	130.32	125.04
3	D	600	HEC	C4B-NB-C1B	3.47	108.65	105.07
3	C	600	HEC	CMD-C2D-C1D	3.45	130.29	125.04
3	A	600	HEC	C3C-C4C-NC	-3.39	106.36	110.15
3	D	600	HEC	C2A-C1A-NA	-3.37	107.05	110.32
3	D	600	HEC	CMD-C2D-C1D	3.29	130.05	125.04
3	C	600	HEC	C2C-C1C-NC	-3.26	105.11	110.08
3	D	600	HEC	C3B-C4B-NB	-3.26	106.53	110.17
3	A	600	HEC	C1D-ND-C4D	3.22	108.40	105.07
3	C	600	HEC	C1D-C2D-C3D	-3.18	103.61	106.96
3	D	600	HEC	CHD-C4C-NC	3.15	129.65	123.85
3	A	600	HEC	CAD-C3D-C4D	3.10	130.07	124.66
3	A	600	HEC	CHB-C4A-NA	3.05	127.74	124.44
3	D	600	HEC	CAD-C3D-C4D	3.03	129.95	124.66
3	D	600	HEC	C3C-C4C-NC	-2.87	106.94	110.15
3	A	600	HEC	CBC-CAC-C3C	2.85	120.30	112.43
3	C	600	HEC	CHD-C4C-NC	2.71	128.83	123.85
3	B	600	HEC	CAD-C3D-C2D	-2.65	122.94	127.88
3	B	600	HEC	C1D-ND-C4D	2.59	107.75	105.07
3	A	600	HEC	C1D-C2D-C3D	-2.58	104.24	106.96
3	A	600	HEC	C2C-C1C-NC	-2.56	106.19	110.08
3	C	600	HEC	CAD-C3D-C4D	2.55	129.12	124.66
3	D	600	HEC	CAC-C3C-C4C	-2.48	121.47	124.92
3	B	600	HEC	C2C-C1C-NC	-2.48	106.31	110.08
3	D	600	HEC	CHB-C4A-NA	2.46	127.10	124.44
3	B	600	HEC	C3A-C4A-NA	-2.44	105.18	109.69
3	A	600	HEC	CHD-C4C-NC	2.39	128.24	123.85
3	A	600	HEC	O2A-CGA-CBA	2.37	121.65	114.03
3	D	600	HEC	C2C-C1C-NC	-2.34	106.51	110.08
3	D	600	HEC	CHA-C4D-ND	2.34	126.96	124.42
3	A	600	HEC	CAC-C3C-C4C	-2.31	121.72	124.92
3	A	600	HEC	CAC-C3C-C2C	2.30	130.54	126.86
3	A	600	HEC	CAD-C3D-C2D	-2.29	123.61	127.88
3	A	600	HEC	CMC-C2C-C1C	-2.28	121.89	125.37
3	D	600	HEC	CAC-C3C-C2C	2.28	130.52	126.86
3	B	600	HEC	O2A-CGA-CBA	2.28	121.36	114.03
3	C	600	HEC	O2A-CGA-CBA	2.27	121.31	114.03
3	C	600	HEC	C1C-C2C-C3C	2.21	109.41	106.83
3	C	600	HEC	O2A-CGA-O1A	-2.19	117.85	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	HEC	CAC-C3C-C4C	-2.15	121.93	124.92
3	C	600	HEC	C1A-C2A-C3A	2.15	109.93	107.13
3	A	600	HEC	O1D-CGD-CBD	-2.15	116.18	123.08
3	C	600	HEC	C1B-C2B-C3B	-2.13	104.71	106.96
3	C	600	HEC	CHA-C1A-NA	2.12	126.73	124.44
3	A	600	HEC	CHA-C1A-NA	2.12	126.73	124.44
3	B	600	HEC	C1D-C2D-C3D	-2.09	104.76	106.96
3	C	600	HEC	C4B-C3B-C2B	2.07	109.91	106.90
3	D	600	HEC	CAD-C3D-C2D	-2.06	124.03	127.88
3	B	600	HEC	CHC-C4B-NB	2.05	126.90	124.37
3	C	600	HEC	C2D-C1D-ND	2.05	112.26	109.84
3	C	600	HEC	CAD-C3D-C2D	-2.04	124.08	127.88
3	B	600	HEC	CHA-C1A-C2A	2.02	128.21	124.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	HEC	NA
3	B	600	HEC	NA
3	C	600	HEC	NA
3	D	600	HEC	NA

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	600	HEC	C2B-C3B-CAB-CBB
3	B	600	HEC	C2B-C3B-CAB-CBB
3	D	600	HEC	C2C-C3C-CAC-CBC
3	C	600	HEC	C2C-C3C-CAC-CBC
3	B	600	HEC	C2C-C3C-CAC-CBC
3	D	600	HEC	C4C-C3C-CAC-CBC
3	A	600	HEC	C2C-C3C-CAC-CBC
3	C	600	HEC	C4C-C3C-CAC-CBC
3	B	600	HEC	C4C-C3C-CAC-CBC
3	A	600	HEC	C4C-C3C-CAC-CBC
3	A	600	HEC	C2B-C3B-CAB-CBB
3	B	600	HEC	C4B-C3B-CAB-CBB
3	D	600	HEC	C4B-C3B-CAB-CBB
3	C	600	HEC	C2B-C3B-CAB-CBB
3	A	600	HEC	C4B-C3B-CAB-CBB
3	B	600	HEC	CAA-CBA-CGA-O1A
3	D	600	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	600	HEC	CAA-CBA-CGA-O1A
3	B	600	HEC	CAA-CBA-CGA-O2A
3	A	600	HEC	CAD-CBD-CGD-O1D
3	A	600	HEC	CAD-CBD-CGD-O2D
3	C	600	HEC	C4B-C3B-CAB-CBB
3	C	600	HEC	CAA-CBA-CGA-O2A
3	D	600	HEC	CAA-CBA-CGA-O2A
3	A	600	HEC	CAA-CBA-CGA-O1A
3	B	600	HEC	CAD-CBD-CGD-O1D
3	C	600	HEC	CAD-CBD-CGD-O1D
3	D	600	HEC	CAD-CBD-CGD-O2D
3	D	600	HEC	CAD-CBD-CGD-O1D
3	A	600	HEC	CAA-CBA-CGA-O2A
3	C	600	HEC	CAD-CBD-CGD-O2D
3	B	600	HEC	CAD-CBD-CGD-O2D

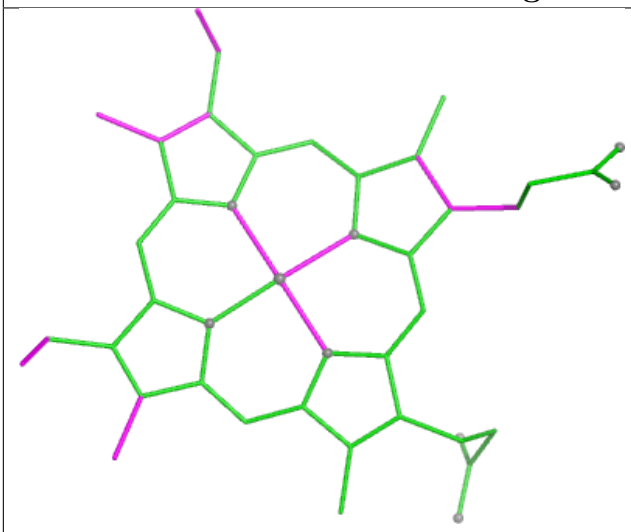
There are no ring outliers.

1 monomer is involved in 3 short contacts:

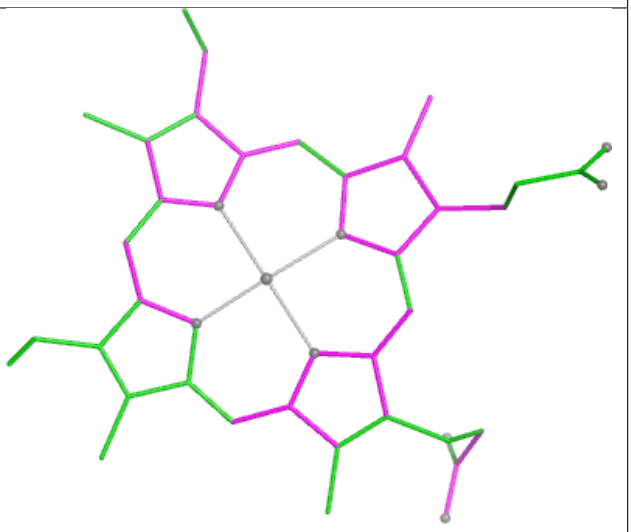
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	HEC	3	0

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.

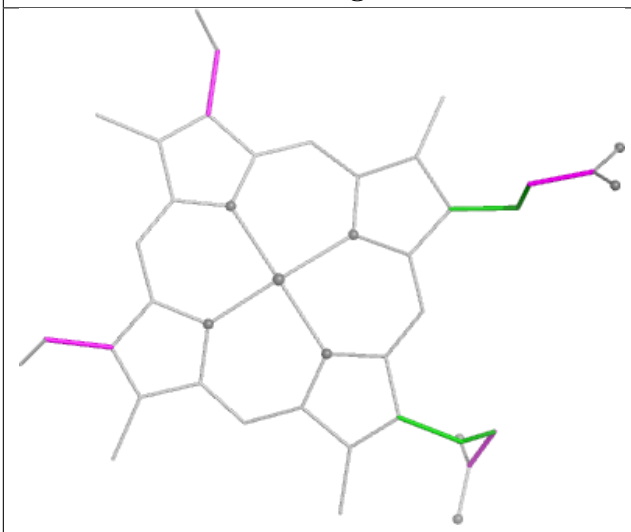
Ligand HEC B 600



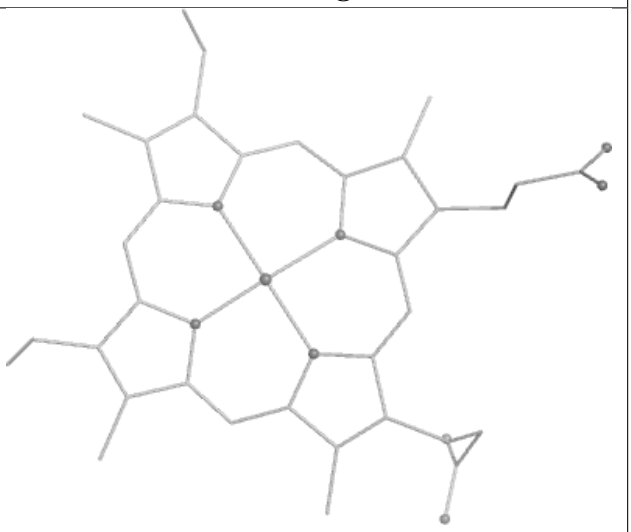
Bond lengths



Bond angles

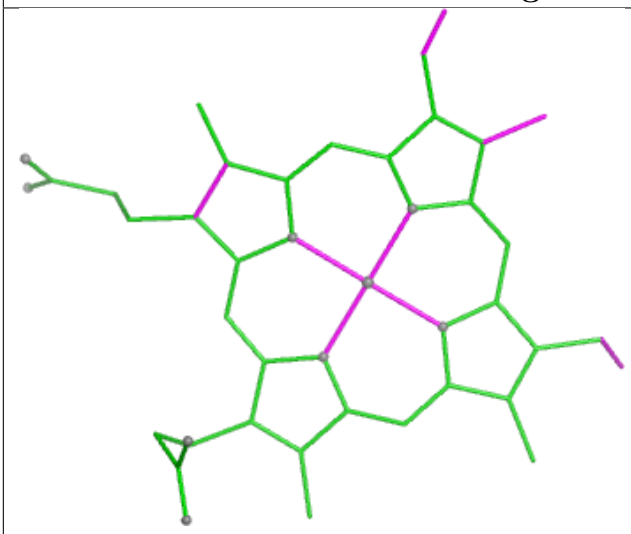


Torsions

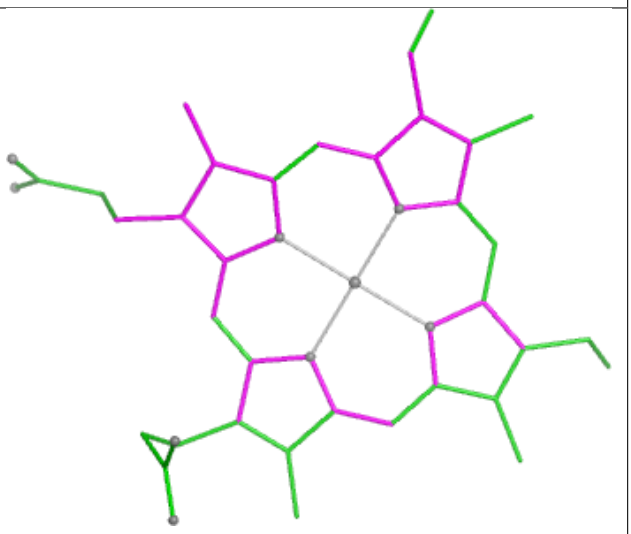


Rings

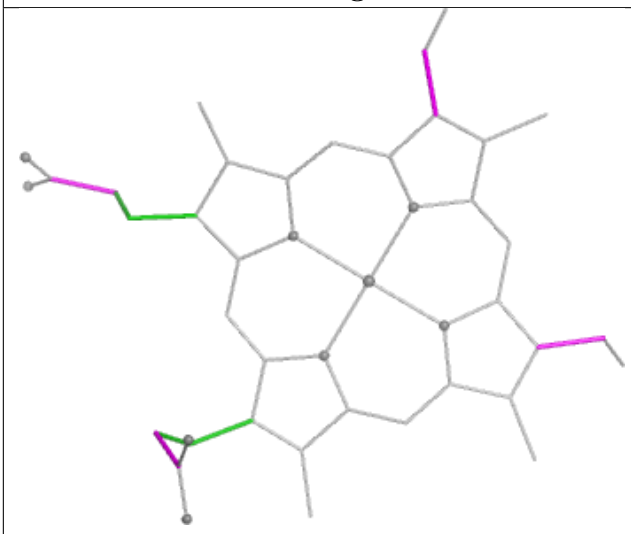
Ligand HEC D 600



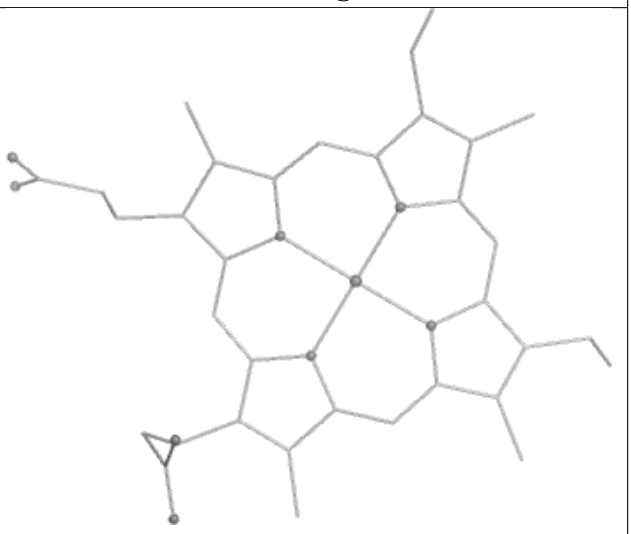
Bond lengths



Bond angles

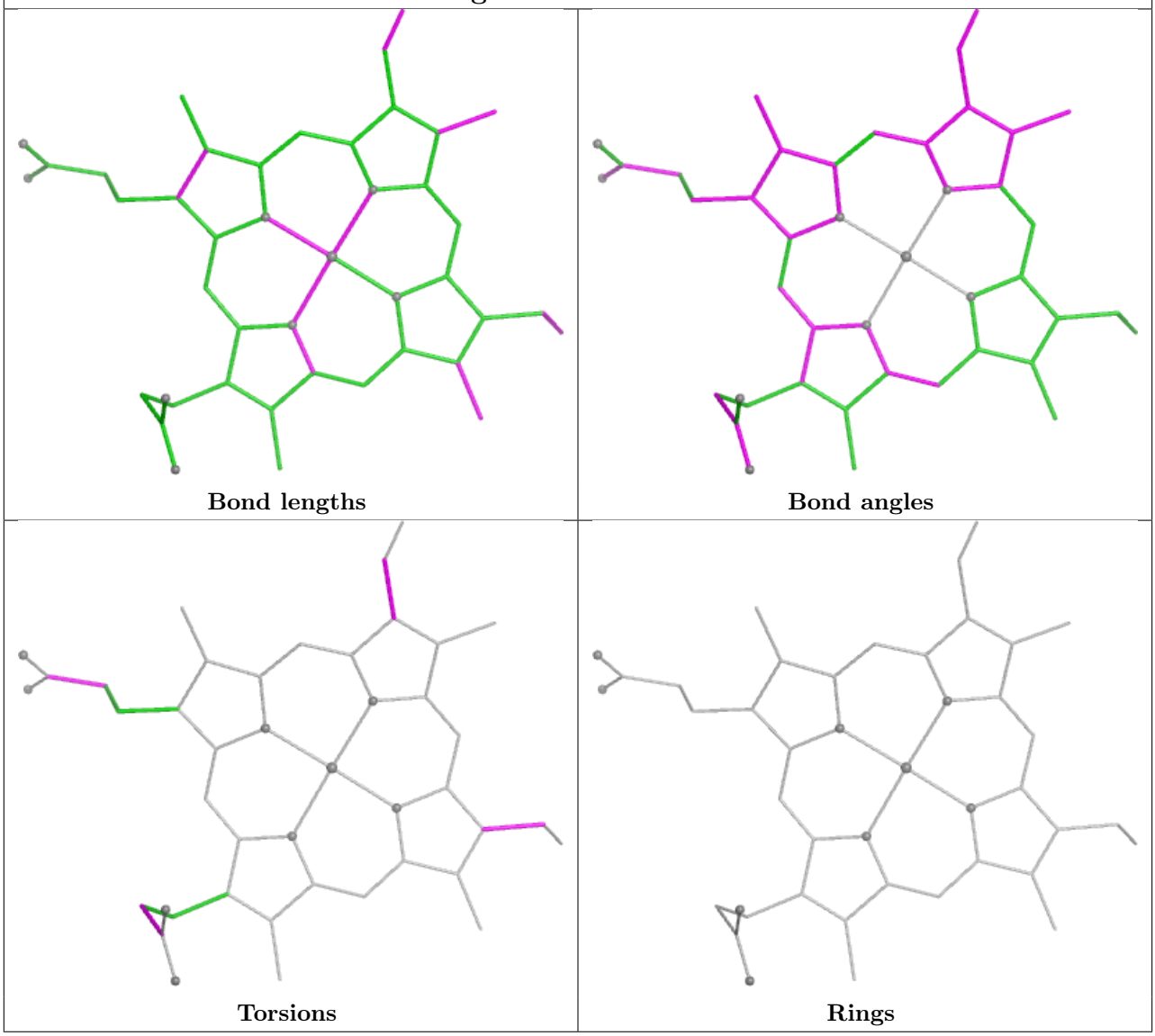


Torsions

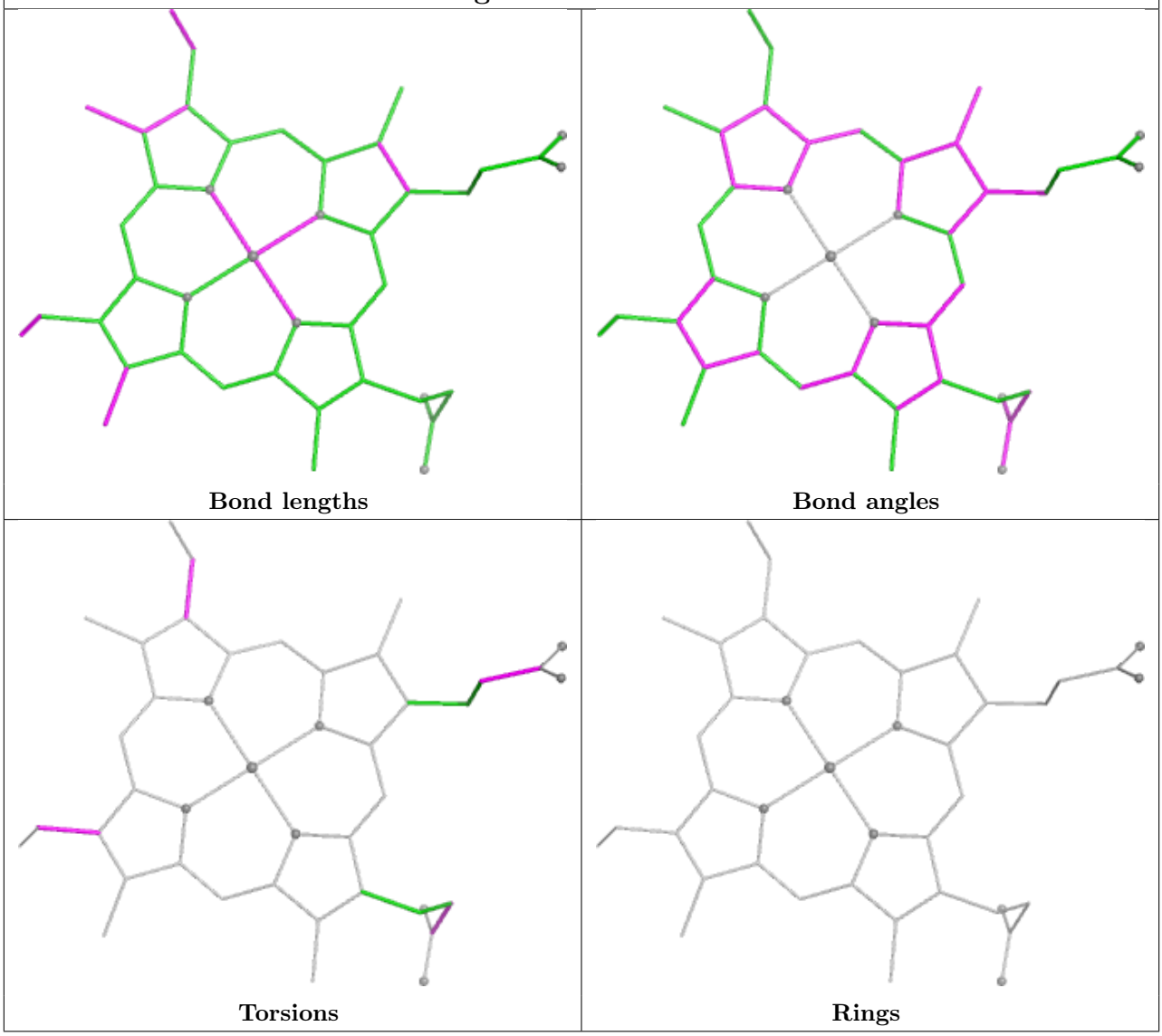


Rings

Ligand HEC A 600



Ligand HEC C 600



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	456/468 (97%)	-0.05	17 (3%)	45	47	8, 19, 45, 58	32 (7%)
1	B	455/468 (97%)	-0.24	4 (0%)	81	84	8, 18, 38, 50	29 (6%)
1	C	455/468 (97%)	-0.31	6 (1%)	75	79	9, 18, 32, 44	27 (5%)
1	D	457/468 (97%)	0.01	6 (1%)	75	79	13, 23, 41, 49	22 (4%)
All	All	1823/1872 (97%)	-0.15	33 (1%)	67	71	8, 20, 40, 58	110 (6%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	5.2
1	C	4	LYS	5.1
1	A	389	ALA	3.4
1	D	343	VAL	3.4
1	C	411	GLY	3.1
1	A	409	VAL	2.9
1	D	346	THR	2.8
1	A	392	PRO	2.7
1	A	441	ASP	2.5
1	B	441	ASP	2.5
1	D	3	ALA	2.4
1	B	443	PRO	2.4
1	D	340	GLN	2.4
1	A	390	ALA	2.4
1	A	387	PHE	2.4
1	A	445	GLY	2.3
1	C	344	SER	2.3
1	A	436	VAL	2.3
1	A	411	GLY	2.3
1	B	444	GLY	2.3
1	B	445	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	2.2
1	A	444	GLY	2.2
1	D	344	SER	2.2
1	A	357	ARG	2.1
1	A	345	GLY	2.1
1	C	345	GLY	2.1
1	C	264[A]	THR	2.1
1	A	375[A]	LEU	2.1
1	D	2	SER	2.0
1	C	376	PRO	2.0
1	A	457	ALA	2.0
1	A	408	LYS	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
3	HEC	A	600	43/43	0.95	0.09	23,29,33,38	0
3	HEC	B	600	43/43	0.96	0.08	20,24,27,29	0
3	HEC	D	600	43/43	0.97	0.07	22,26,28,29	0
2	CU	D	501	1/1	0.98	0.03	19,19,19,19	0
3	HEC	C	600	43/43	0.98	0.06	14,17,22,24	0
2	CU	A	501	1/1	0.98	0.03	18,18,18,18	0
2	CU	B	501	1/1	0.99	0.02	17,17,17,17	0
2	CU	C	501	1/1	0.99	0.02	14,14,14,14	0
2	CU	A	502	1/1	0.99	0.02	15,15,15,15	0
2	CU	D	502	1/1	0.99	0.02	19,19,19,19	0
2	CU	B	502	1/1	1.00	0.01	16,16,16,16	0

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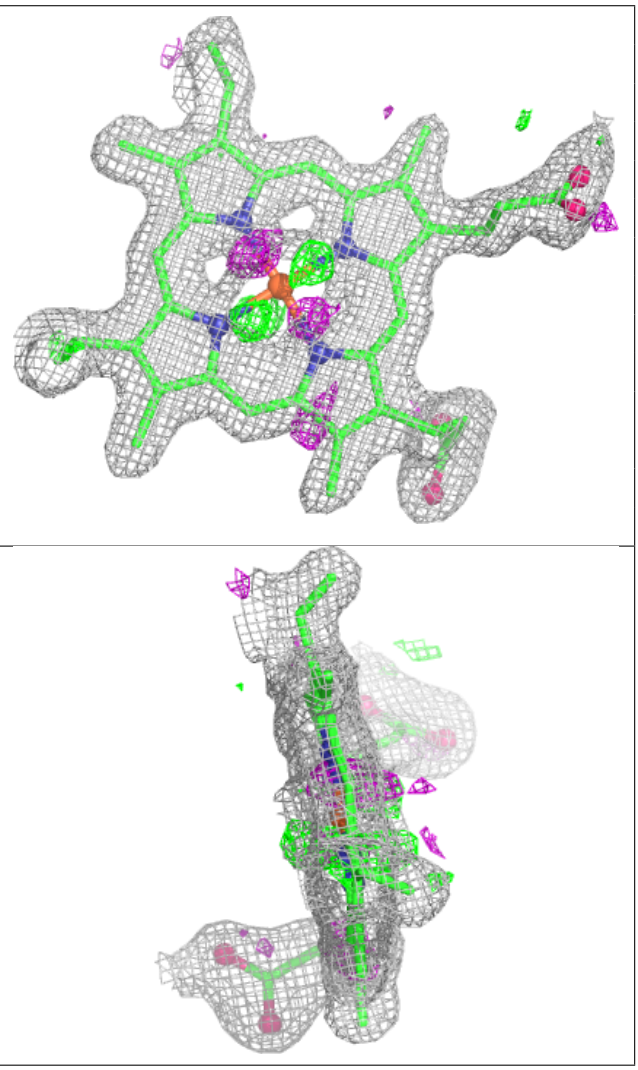
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	C	502	1/1	1.00	0.01	14,14,14,14	0

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.

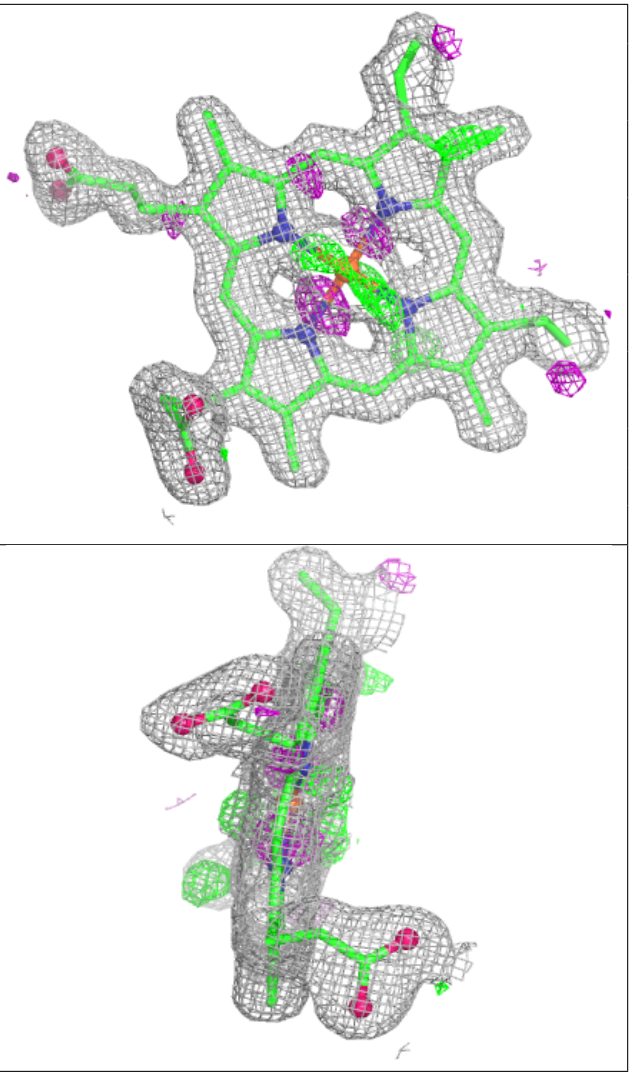
Electron density around HEC A 600:

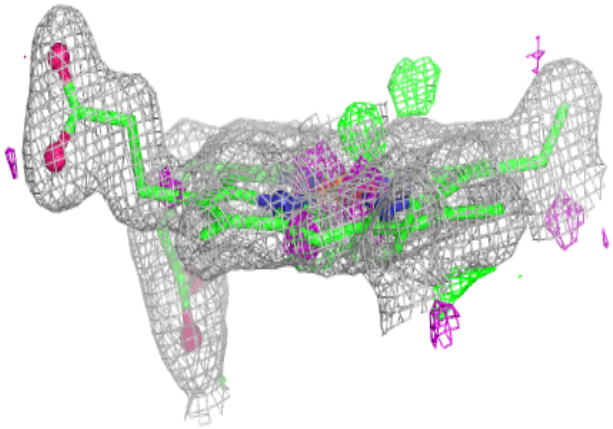
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC B 600:

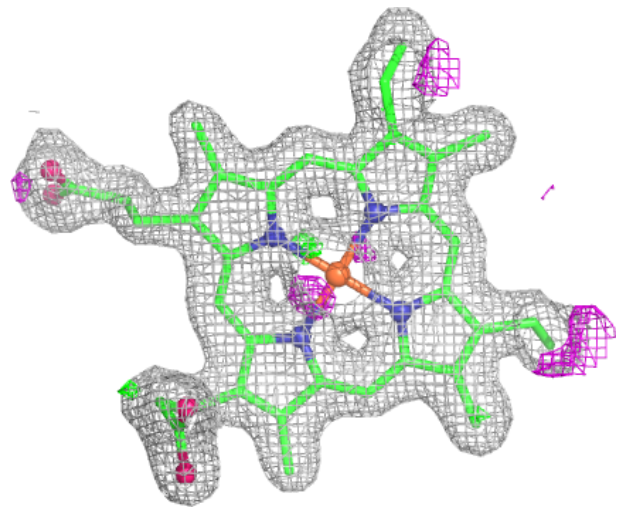
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

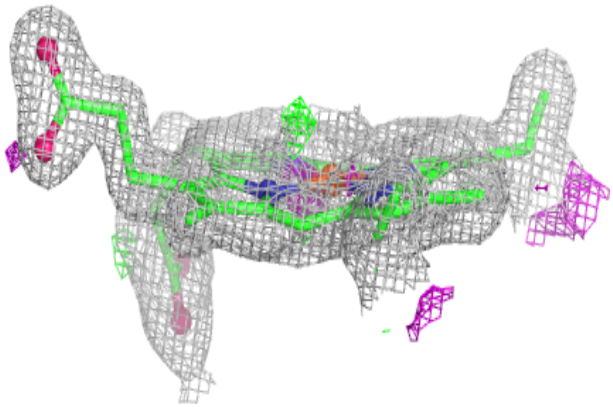


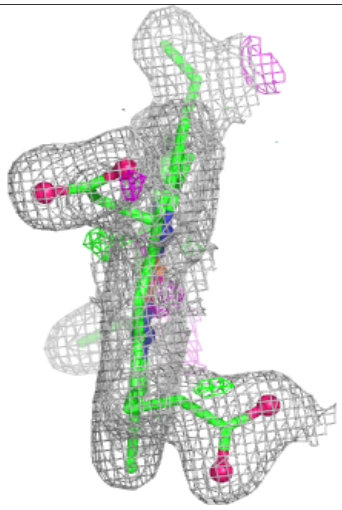


Electron density around HEC D 600:

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

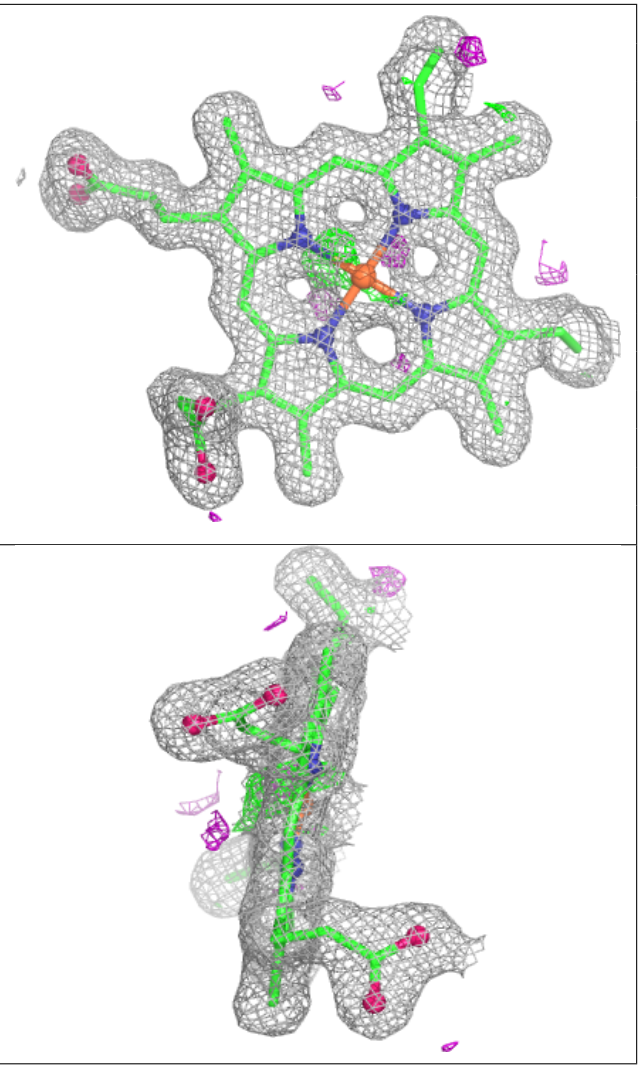






Electron density around HEC C 600:

$2mF_o$-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.