Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 09:39 pm BST

PDB ID	:	4AAO / pdb_00004aao
Title	:	MacA-H93G
Authors	:	Seidel, J.
Deposited on	:	2011-12-05
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 (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:

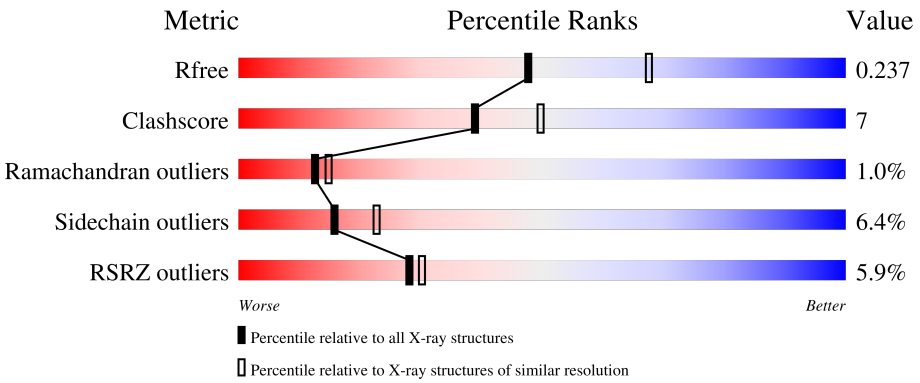
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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))
R_{free}	180053	6319 (2.30-2.30)
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	341	5% 73% 14% • 11%
1	B	341	6% 77% 9% • 11%

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	400	X	-	-	-
2	HEC	A	401	X	-	-	-
2	HEC	B	400	X	-	-	-
2	HEC	B	401	X	-	-	-
4	SO4	A	1352	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5078 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 C551 PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2278	1446	390	430	12	0	0	0
1	B	305	2269	1438	391	428	12	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	TRP	-	expression tag	UNP Q74FY6
A	7	SER	-	expression tag	UNP Q74FY6
A	8	HIS	-	expression tag	UNP Q74FY6
A	9	PRO	-	expression tag	UNP Q74FY6
A	10	GLN	-	expression tag	UNP Q74FY6
A	11	PHE	-	expression tag	UNP Q74FY6
A	12	GLU	-	expression tag	UNP Q74FY6
A	13	LYS	-	expression tag	UNP Q74FY6
A	14	GLY	-	expression tag	UNP Q74FY6
A	15	ALA	-	expression tag	UNP Q74FY6
A	16	GLU	-	expression tag	UNP Q74FY6
A	17	THR	-	expression tag	UNP Q74FY6
A	18	ALA	-	expression tag	UNP Q74FY6
A	19	VAL	-	expression tag	UNP Q74FY6
A	20	PRO	-	expression tag	UNP Q74FY6
A	21	ASN	-	expression tag	UNP Q74FY6
A	22	SER	-	expression tag	UNP Q74FY6
A	93	GLY	HIS	engineered mutation	UNP Q74FY6
B	6	TRP	-	expression tag	UNP Q74FY6
B	7	SER	-	expression tag	UNP Q74FY6
B	8	HIS	-	expression tag	UNP Q74FY6
B	9	PRO	-	expression tag	UNP Q74FY6
B	10	GLN	-	expression tag	UNP Q74FY6
B	11	PHE	-	expression tag	UNP Q74FY6
B	12	GLU	-	expression tag	UNP Q74FY6

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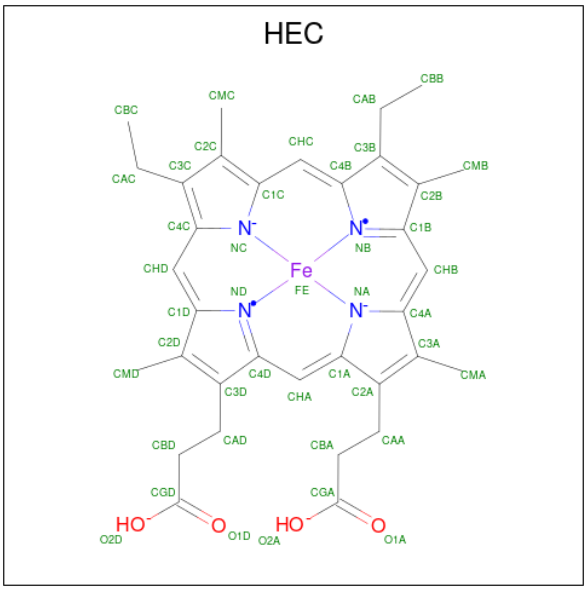
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LYS	-	expression tag	UNP Q74FY6
B	14	GLY	-	expression tag	UNP Q74FY6
B	15	ALA	-	expression tag	UNP Q74FY6
B	16	GLU	-	expression tag	UNP Q74FY6
B	17	THR	-	expression tag	UNP Q74FY6
B	18	ALA	-	expression tag	UNP Q74FY6
B	19	VAL	-	expression tag	UNP Q74FY6
B	20	PRO	-	expression tag	UNP Q74FY6
B	21	ASN	-	expression tag	UNP Q74FY6
B	22	SER	-	expression tag	UNP Q74FY6
B	93	GLY	HIS	engineered mutation	UNP Q74FY6

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

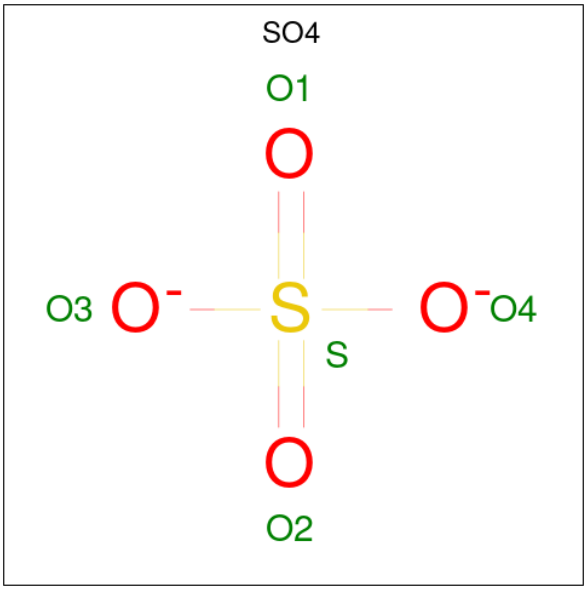


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0

- Molecule 5 is water.

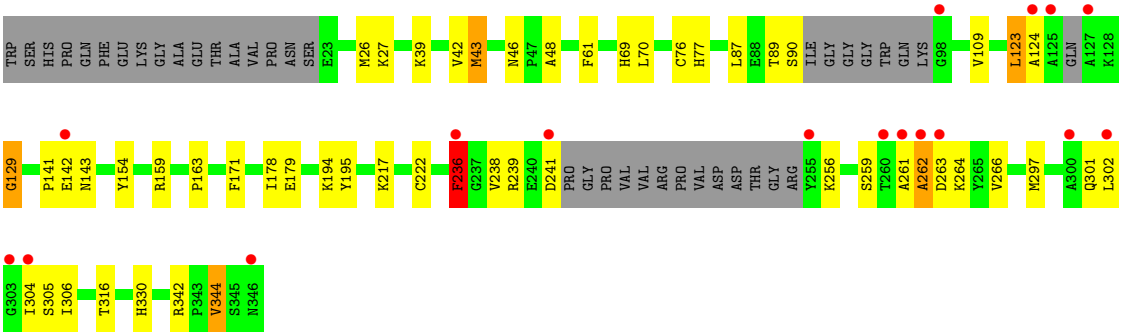
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	169	169	169	0	0
			Total	O		
5	B	133	133	133	0	0

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.

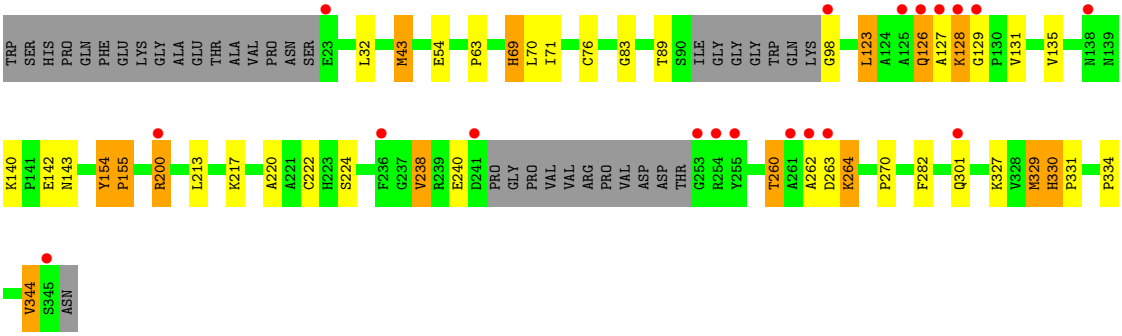
• Molecule 1: CYTOCHROME C551 PEROXIDASE

Chain A:



• Molecule 1: CYTOCHROME C551 PEROXIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.72Å 118.72Å 245.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	102.81 – 2.30 102.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.2 (102.81-2.30) 93.1 (102.81-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.6.0113	Depositor
R, R_{free}	0.190 , 0.241 0.184 , 0.237	Depositor DCC
R_{free} test set	2268 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5078	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: CA, HEC, SO4

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	1.28	4/2332 (0.2%)	1.22	20/3170 (0.6%)
1	B	1.21	4/2323 (0.2%)	1.21	10/3165 (0.3%)
All	All	1.24	8/4655 (0.2%)	1.22	30/6335 (0.5%)

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	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	HIS	CG-CD2	6.36	1.42	1.35
1	B	334	PRO	CA-C	6.13	1.56	1.52
1	A	77	HIS	CB-CG	5.94	1.58	1.50
1	A	266	VAL	CA-C	-5.39	1.46	1.52
1	B	54	GLU	C-O	-5.35	1.18	1.24
1	B	330	HIS	ND1-CE1	5.32	1.37	1.32
1	B	69	HIS	CG-CD2	5.08	1.41	1.35
1	A	42	VAL	CA-C	5.04	1.58	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	LYS	CA-C-N	6.62	128.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	LYS	C-N-CA	6.62	128.12	119.84
1	A	90	SER	N-CA-C	6.52	129.25	111.00
1	A	344	VAL	CB-CA-C	6.12	119.46	110.77
1	A	163	PRO	CA-C-N	-6.06	116.23	123.44
1	A	163	PRO	C-N-CA	-6.06	116.23	123.44
1	B	154	TYR	CA-C-N	-6.04	114.16	120.38
1	B	154	TYR	C-N-CA	-6.04	114.16	120.38
1	B	123	LEU	N-CA-C	-6.03	104.62	111.14
1	A	306	ILE	N-CA-C	5.97	117.28	108.45
1	A	236	PHE	CB-CA-C	-5.92	103.35	111.51
1	B	71	ILE	N-CA-C	5.91	116.44	108.17
1	A	259	SER	N-CA-C	5.87	117.44	108.52
1	A	129	GLY	CA-C-N	5.64	125.31	119.05
1	A	129	GLY	C-N-CA	5.64	125.31	119.05
1	A	48	ALA	N-CA-C	-5.61	100.54	109.96
1	A	171	PHE	N-CA-C	5.56	117.02	111.07
1	A	330	HIS	CA-C-N	-5.56	114.86	120.31
1	A	330	HIS	C-N-CA	-5.56	114.86	120.31
1	A	123	LEU	N-CA-C	-5.37	105.60	111.82
1	A	301	GLN	N-CA-C	5.27	118.81	112.38
1	B	344	VAL	CB-CA-C	5.17	118.62	111.38
1	A	46	ASN	CA-C-N	-5.13	114.44	119.99
1	A	46	ASN	C-N-CA	-5.13	114.44	119.99
1	B	83	GLY	N-CA-C	-5.08	108.24	115.30
1	B	98	GLY	CA-C-N	-5.07	114.52	119.99
1	B	98	GLY	C-N-CA	-5.07	114.52	119.99
1	A	154	TYR	CA-C-N	-5.05	115.17	120.38
1	A	154	TYR	C-N-CA	-5.05	115.17	120.38
1	A	61	PHE	N-CA-C	-5.02	106.57	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	THR	Peptide
1	B	89	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2278	0	2248	29	0
1	B	2269	0	2221	32	0
2	A	86	0	62	9	0
2	B	86	0	62	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	4	0
4	B	25	0	0	2	0
5	A	169	0	0	5	0
5	B	133	0	0	0	0
All	All	5078	0	4593	64	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 7.

All (64) 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:B:76:CYS:SG	2:B:400:HEC:CAC	2.06	1.41
1:A:76:CYS:SG	2:A:400:HEC:CAC	2.08	1.40
1:A:222:CYS:SG	2:A:401:HEC:CAC	2.23	1.27
1:B:76:CYS:SG	2:B:400:HEC:HAC	1.79	1.12
1:B:222:CYS:SG	2:B:401:HEC:CAC	2.38	1.10
1:A:76:CYS:SG	2:A:400:HEC:HAC	1.89	1.09
1:A:236:PHE:HE2	1:A:302:LEU:HD23	1.22	1.02
1:A:222:CYS:SG	2:A:401:HEC:HAC	2.05	0.93
1:B:76:CYS:HG	2:B:400:HEC:HAC	1.27	0.92
1:A:236:PHE:CE2	1:A:302:LEU:HD23	2.05	0.91
1:A:129:GLY:CA	4:A:1352:SO4:O4	2.24	0.86
1:A:129:GLY:HA3	4:A:1352:SO4:O4	1.82	0.80
1:A:236:PHE:HE2	1:A:302:LEU:CD2	1.97	0.77
1:A:236:PHE:CZ	1:A:302:LEU:HB3	2.21	0.75
1:A:76:CYS:SG	2:A:400:HEC:C3C	2.75	0.74
1:B:76:CYS:SG	2:B:400:HEC:C3C	2.76	0.73
1:B:76:CYS:SG	2:B:400:HEC:CBC	2.76	0.73
1:A:76:CYS:SG	2:A:400:HEC:CBC	2.76	0.72
1:A:43:MET:HE1	1:A:109:VAL:CG2	2.22	0.69
1:A:222:CYS:SG	2:A:401:HEC:C3C	2.82	0.68
1:B:126:GLN:HG3	1:B:128:LYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:CYS:SG	2:B:401:HEC:CBC	2.82	0.68
1:B:222:CYS:SG	2:B:401:HEC:C3C	2.84	0.65
1:A:236:PHE:CE2	1:A:302:LEU:HB3	2.33	0.64
1:B:200:ARG:HB3	1:B:200:ARG:HH11	1.64	0.62
1:B:200:ARG:HH11	1:B:200:ARG:CB	2.12	0.62
1:B:43:MET:HA	1:B:43:MET:HE2	1.81	0.61
1:A:43:MET:HE1	1:A:109:VAL:HG21	1.84	0.60
1:A:236:PHE:HZ	1:A:302:LEU:HB3	1.66	0.59
1:A:129:GLY:N	4:A:1352:SO4:O4	2.36	0.58
1:A:222:CYS:SG	2:A:401:HEC:CBC	2.91	0.57
1:A:297:MET:O	1:A:302:LEU:HD11	2.05	0.56
1:B:213:LEU:O	1:B:217:LYS:HG2	2.07	0.54
1:A:261:ALA:O	1:A:262:ALA:CB	2.56	0.53
1:B:238:VAL:HG21	1:B:282:PHE:CD2	2.44	0.53
1:B:263:ASP:O	1:B:264:LYS:CB	2.57	0.52
1:A:26:MET:HE2	1:A:195:TYR:O	2.10	0.51
1:B:127:ALA:O	1:B:128:LYS:CB	2.59	0.51
1:A:194:LYS:NZ	5:A:2118:HOH:O	2.43	0.50
2:B:401:HEC:HBC3	2:B:401:HEC:HMC3	1.93	0.50
1:B:222:CYS:SG	2:B:401:HEC:HBC3	2.51	0.50
1:B:131:VAL:O	1:B:135:VAL:HG23	2.13	0.49
1:A:159:ARG:HD3	5:A:2099:HOH:O	2.12	0.48
1:B:329:MET:HE2	1:B:329:MET:HA	1.96	0.48
1:A:316:THR:OG1	4:A:1353:SO4:O3	2.20	0.47
1:B:220:ALA:O	1:B:224:SER:HB3	2.15	0.46
2:B:401:HEC:HMB3	2:B:401:HEC:HBB3	1.98	0.46
1:A:342:ARG:NH2	5:A:2164:HOH:O	2.49	0.45
1:B:330:HIS:HD2	1:B:331:PRO:O	2.00	0.45
1:B:76:CYS:CB	2:B:400:HEC:C3C	2.95	0.44
1:B:129:GLY:HA3	4:B:1348:SO4:O2	2.17	0.44
1:B:260:THR:CG2	1:B:301:GLN:NE2	2.81	0.44
1:B:126:GLN:HG3	1:B:128:LYS:N	2.31	0.44
1:A:178:ILE:HG21	2:A:400:HEC:CMB	2.48	0.44
1:B:143:ASN:N	1:B:143:ASN:HD22	2.15	0.43
1:B:327:LYS:HE3	4:B:1350:SO4:O4	2.18	0.43
1:B:222:CYS:SG	2:B:401:HEC:HAC	2.48	0.43
1:B:76:CYS:HG	2:B:400:HEC:CAC	1.96	0.42
1:A:179:GLU:OE1	5:A:2109:HOH:O	2.22	0.42
1:B:63:PRO:O	1:B:69:HIS:HA	2.20	0.41
1:B:154:TYR:O	1:B:155:PRO:C	2.62	0.41
1:B:270:PRO:HG2	2:B:401:HEC:HBA1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:ND2	5:A:2084:HOH:O	2.50	0.40
2:B:400:HEC:HMC3	2:B:400:HEC:HBC3	2.02	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	295/341 (86%)	277 (94%)	15 (5%)	3 (1%)	12	15
1	B	299/341 (88%)	281 (94%)	15 (5%)	3 (1%)	12	15
All	All	594/682 (87%)	558 (94%)	30 (5%)	6 (1%)	12	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ALA
1	B	264	LYS
1	A	304	ILE
1	B	128	LYS
1	B	262	ALA
1	A	124	ALA

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	246/280 (88%)	228 (93%)	18 (7%)	13	18
1	B	242/280 (86%)	229 (95%)	13 (5%)	20	29
All	All	488/560 (87%)	457 (94%)	31 (6%)	16	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	39	LYS
1	A	43	MET
1	A	70	LEU
1	A	87	LEU
1	A	123	LEU
1	A	141	PRO
1	A	142	GLU
1	A	217	LYS
1	A	236	PHE
1	A	238	VAL
1	A	239	ARG
1	A	241	ASP
1	A	256	LYS
1	A	263	ASP
1	A	264	LYS
1	A	305	SER
1	A	344	VAL
1	B	32	LEU
1	B	43	MET
1	B	70	LEU
1	B	123	LEU
1	B	126	GLN
1	B	142	GLU
1	B	155	PRO
1	B	200	ARG
1	B	238	VAL
1	B	240	GLU
1	B	260	THR
1	B	329	MET
1	B	344	VAL

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	132	GLN
1	A	138	ASN
1	B	132	GLN
1	B	138	ASN
1	B	143	ASN
1	B	301	GLN
1	B	330	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	SO4	A	1351	-	4,4,4	0.54	0	6,6,6	0.42	0
2	HEC	A	400	1	50,50,50	2.21	14 (28%)	68,82,82	2.66	24 (35%)
2	HEC	B	401	1	50,50,50	2.26	13 (26%)	68,82,82	2.35	17 (25%)
4	SO4	A	1350	-	4,4,4	0.60	0	6,6,6	0.55	0
4	SO4	B	1348	-	4,4,4	0.55	0	6,6,6	0.30	0
4	SO4	A	1354	-	4,4,4	0.41	0	6,6,6	0.85	0
4	SO4	B	1349	-	4,4,4	0.57	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	A	401	1	50,50,50	2.26	12 (24%)	68,82,82	2.38	19 (27%)
4	SO4	A	1349	-	4,4,4	0.44	0	6,6,6	0.43	0
2	HEC	B	400	1	50,50,50	2.12	13 (26%)	68,82,82	2.43	20 (29%)
4	SO4	B	1352	-	4,4,4	0.35	0	6,6,6	0.39	0
4	SO4	B	1351	-	4,4,4	0.42	0	6,6,6	0.35	0
4	SO4	A	1353	-	4,4,4	0.55	0	6,6,6	0.75	0
4	SO4	B	1350	-	4,4,4	0.56	0	6,6,6	0.92	0
4	SO4	A	1352	-	4,4,4	0.59	0	6,6,6	0.55	0

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	A	401	1	1/1/3/7	2/14/54/54	-
2	HEC	A	400	1	1/1/3/7	6/14/54/54	-
2	HEC	B	401	1	1/1/3/7	4/14/54/54	-
2	HEC	B	400	1	1/1/3/7	7/14/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEC	FE-NB	10.33	2.26	1.94
2	B	401	HEC	FE-NB	9.87	2.25	1.94
2	A	400	HEC	FE-NB	9.46	2.24	1.94
2	B	400	HEC	FE-NB	9.45	2.24	1.94
2	A	401	HEC	C4B-NB	-4.68	1.32	1.40
2	B	400	HEC	C4B-NB	-4.64	1.32	1.40
2	B	401	HEC	C4B-NB	-4.64	1.32	1.40
2	A	401	HEC	FE-NC	4.36	2.09	1.95
2	A	400	HEC	C4B-NB	-4.35	1.32	1.40
2	A	401	HEC	CBC-CAC	-3.99	1.33	1.51
2	B	401	HEC	FE-NC	3.86	2.08	1.95
2	A	400	HEC	C1B-NB	-3.64	1.31	1.38
2	B	401	HEC	C1B-NB	-3.51	1.31	1.38
2	B	401	HEC	CBC-CAC	-3.48	1.36	1.51
2	A	400	HEC	FE-NC	3.46	2.06	1.95
2	B	400	HEC	CBC-CAC	-3.42	1.36	1.51
2	A	400	HEC	C1D-ND	-3.39	1.34	1.40
2	A	401	HEC	CBB-CAB	-3.29	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEC	CBB-CAB	-3.25	1.37	1.51
2	A	400	HEC	CBC-CAC	-3.24	1.37	1.51
2	B	400	HEC	FE-NC	3.03	2.05	1.95
2	B	400	HEC	C1A-C2A	-3.01	1.39	1.45
2	A	400	HEC	CBB-CAB	-2.93	1.38	1.51
2	B	400	HEC	C1B-NB	-2.82	1.33	1.38
2	B	400	HEC	C4C-NC	-2.76	1.34	1.39
2	A	400	HEC	C4C-NC	-2.71	1.34	1.39
2	B	400	HEC	C1D-ND	-2.66	1.35	1.40
2	B	401	HEC	C1D-ND	-2.64	1.35	1.40
2	A	400	HEC	C1C-NC	-2.51	1.34	1.39
2	B	400	HEC	CBB-CAB	-2.48	1.40	1.51
2	A	401	HEC	C4A-C3A	-2.47	1.40	1.45
2	B	401	HEC	C4C-NC	-2.45	1.35	1.39
2	A	400	HEC	C4A-C3A	-2.45	1.40	1.45
2	A	400	HEC	CAB-C3B	-2.44	1.44	1.51
2	B	400	HEC	CMA-C3A	2.41	1.55	1.50
2	A	400	HEC	C4D-C3D	2.36	1.49	1.45
2	B	401	HEC	C4D-C3D	2.28	1.49	1.45
2	B	401	HEC	C4D-ND	-2.27	1.34	1.38
2	A	401	HEC	CHC-C4B	2.25	1.43	1.38
2	A	401	HEC	FE-NA	2.24	2.02	1.95
2	B	400	HEC	C4A-C3A	-2.18	1.41	1.45
2	B	401	HEC	CHD-C4C	-2.17	1.34	1.39
2	B	400	HEC	O2A-CGA	-2.13	1.23	1.30
2	A	401	HEC	C1D-C2D	2.11	1.48	1.44
2	B	400	HEC	C4D-C3D	2.10	1.48	1.45
2	A	400	HEC	CBA-CGA	2.10	1.55	1.50
2	B	401	HEC	C1C-NC	-2.09	1.35	1.39
2	A	401	HEC	C1B-NB	-2.05	1.34	1.38
2	A	401	HEC	CHB-C1B	2.03	1.43	1.39
2	A	401	HEC	CHB-C4A	2.03	1.42	1.38
2	B	401	HEC	O1D-CGD	2.02	1.28	1.22
2	A	400	HEC	CMA-C3A	2.00	1.55	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HEC	C4B-NB-C1B	12.11	117.58	105.07
2	A	400	HEC	C4B-NB-C1B	11.63	117.08	105.07
2	B	400	HEC	C4B-NB-C1B	11.13	116.56	105.07
2	A	401	HEC	C4B-NB-C1B	10.63	116.06	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	HEC	C3B-C4B-NB	-6.78	102.61	110.17
2	B	400	HEC	C3B-C4B-NB	-6.24	103.21	110.17
2	B	401	HEC	C3B-C4B-NB	-5.88	103.62	110.17
2	A	401	HEC	C3B-C4B-NB	-5.86	103.64	110.17
2	A	401	HEC	CHA-C4D-ND	4.86	129.70	124.42
2	A	401	HEC	C4C-NC-C1C	4.73	109.98	105.35
2	A	400	HEC	C4C-NC-C1C	4.71	109.96	105.35
2	A	401	HEC	C2B-C1B-NB	-4.70	104.25	109.88
2	A	400	HEC	CHA-C4D-ND	4.65	129.47	124.42
2	B	401	HEC	C2B-C1B-NB	-4.55	104.44	109.88
2	A	401	HEC	CHC-C4B-NB	4.49	129.91	124.37
2	A	400	HEC	C2A-C1A-NA	-4.48	105.96	110.32
2	B	400	HEC	C4C-NC-C1C	4.36	109.62	105.35
2	B	400	HEC	CHC-C4B-NB	4.33	129.71	124.37
2	B	400	HEC	C2B-C1B-NB	-4.30	104.73	109.88
2	B	400	HEC	CHB-C4A-NA	4.16	128.94	124.44
2	A	400	HEC	CHC-C4B-NB	4.15	129.50	124.37
2	B	401	HEC	CHC-C4B-NB	4.05	129.37	124.37
2	A	401	HEC	CHA-C4D-C3D	-4.04	118.90	124.84
2	A	400	HEC	O2D-CGD-O1D	-3.98	113.39	123.30
2	A	400	HEC	C2B-C1B-NB	-3.94	105.16	109.88
2	B	400	HEC	CBC-CAC-C3C	3.87	123.11	112.43
2	B	401	HEC	C4C-NC-C1C	3.78	109.05	105.35
2	B	401	HEC	C4A-NA-C1A	3.70	108.97	105.35
2	B	401	HEC	C2D-C1D-ND	3.56	114.06	109.84
2	A	400	HEC	O2D-CGD-CBD	3.53	125.36	114.03
2	A	400	HEC	CHB-C4A-NA	3.48	128.20	124.44
2	B	400	HEC	C4A-NA-C1A	3.42	108.69	105.35
2	A	400	HEC	C4A-NA-C1A	3.35	108.63	105.35
2	B	401	HEC	CBC-CAC-C3C	3.34	121.65	112.43
2	A	401	HEC	CHB-C4A-NA	3.33	128.04	124.44
2	A	400	HEC	CHA-C4D-C3D	-3.30	119.99	124.84
2	A	400	HEC	C1A-CHA-C4D	-3.25	119.05	126.06
2	A	400	HEC	CHD-C1D-ND	3.25	128.38	124.37
2	B	401	HEC	C1D-C2D-C3D	-3.17	103.63	106.96
2	A	400	HEC	CBD-CAD-C3D	-3.14	103.90	112.63
2	B	400	HEC	CHA-C4D-C3D	-3.14	120.23	124.84
2	A	400	HEC	CHA-C1A-NA	3.09	127.78	124.44
2	B	400	HEC	CBA-CAA-C2A	-3.08	104.07	112.63
2	A	401	HEC	CHB-C1B-C2B	2.99	129.65	124.98
2	A	400	HEC	CBC-CAC-C3C	2.91	120.44	112.43
2	A	401	HEC	C1A-CHA-C4D	-2.89	119.83	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEC	CBC-CAC-C3C	2.86	120.32	112.43
2	B	400	HEC	CBD-CAD-C3D	-2.83	104.75	112.63
2	A	400	HEC	CHB-C1B-NB	2.82	127.48	124.42
2	B	401	HEC	CBD-CAD-C3D	-2.79	104.87	112.63
2	B	400	HEC	CHA-C4D-ND	2.79	127.45	124.42
2	B	401	HEC	CHD-C1D-C2D	-2.79	118.99	126.73
2	B	400	HEC	CHD-C1D-ND	2.77	127.79	124.37
2	A	400	HEC	CHD-C1D-C2D	-2.72	119.17	126.73
2	B	400	HEC	CHB-C1B-NB	2.66	127.31	124.42
2	A	401	HEC	C4C-CHD-C1D	-2.62	120.12	126.34
2	B	401	HEC	CAC-C3C-C2C	2.59	131.00	126.86
2	A	400	HEC	C4C-CHD-C1D	-2.56	120.25	126.34
2	B	400	HEC	CAD-C3D-C4D	2.50	129.03	124.66
2	A	400	HEC	CAC-C3C-C2C	2.49	130.85	126.86
2	A	400	HEC	CBA-CAA-C2A	-2.47	105.77	112.63
2	A	401	HEC	CHD-C1D-ND	2.45	127.39	124.37
2	B	400	HEC	C2A-C1A-NA	-2.43	107.96	110.32
2	B	401	HEC	CHB-C1B-NB	2.38	127.00	124.42
2	A	401	HEC	C4A-NA-C1A	2.38	107.67	105.35
2	A	401	HEC	CHD-C1D-C2D	-2.36	120.19	126.73
2	A	401	HEC	CMD-C2D-C1D	2.30	128.55	125.04
2	A	401	HEC	CAC-C3C-C2C	2.30	130.55	126.86
2	B	400	HEC	C4C-CHD-C1D	-2.27	120.96	126.34
2	B	401	HEC	C2A-C1A-NA	-2.25	108.14	110.32
2	B	401	HEC	CHB-C1B-C2B	2.22	128.45	124.98
2	B	400	HEC	C3C-C4C-NC	-2.21	107.68	110.15
2	A	400	HEC	C2D-C1D-ND	2.20	112.45	109.84
2	B	400	HEC	CHD-C1D-C2D	-2.18	120.69	126.73
2	B	400	HEC	C1A-CHA-C4D	-2.16	121.39	126.06
2	B	401	HEC	O2A-CGA-CBA	2.14	120.91	114.03
2	A	401	HEC	O2A-CGA-CBA	2.14	120.91	114.03
2	A	401	HEC	C1D-C2D-C3D	-2.08	104.77	106.96
2	B	401	HEC	CBA-CAA-C2A	-2.03	106.99	112.63
2	A	400	HEC	CAA-CBA-CGA	-2.03	109.25	113.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400	HEC	NA
2	A	401	HEC	NA
2	B	400	HEC	NA
2	B	401	HEC	NA

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	HEC	C2C-C3C-CAC-CBC
2	B	401	HEC	C4C-C3C-CAC-CBC
2	A	401	HEC	C2C-C3C-CAC-CBC
2	A	400	HEC	C2C-C3C-CAC-CBC
2	B	400	HEC	C2C-C3C-CAC-CBC
2	A	401	HEC	C4C-C3C-CAC-CBC
2	A	400	HEC	C4C-C3C-CAC-CBC
2	B	400	HEC	C4C-C3C-CAC-CBC
2	B	401	HEC	C2B-C3B-CAB-CBB
2	A	400	HEC	CAA-CBA-CGA-O1A
2	B	400	HEC	CAA-CBA-CGA-O1A
2	A	400	HEC	CAA-CBA-CGA-O2A
2	B	400	HEC	CAA-CBA-CGA-O2A
2	B	400	HEC	CAD-CBD-CGD-O2D
2	A	400	HEC	CAD-CBD-CGD-O2D
2	B	401	HEC	C4B-C3B-CAB-CBB
2	B	400	HEC	CAD-CBD-CGD-O1D
2	A	400	HEC	CAD-CBD-CGD-O1D
2	B	400	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

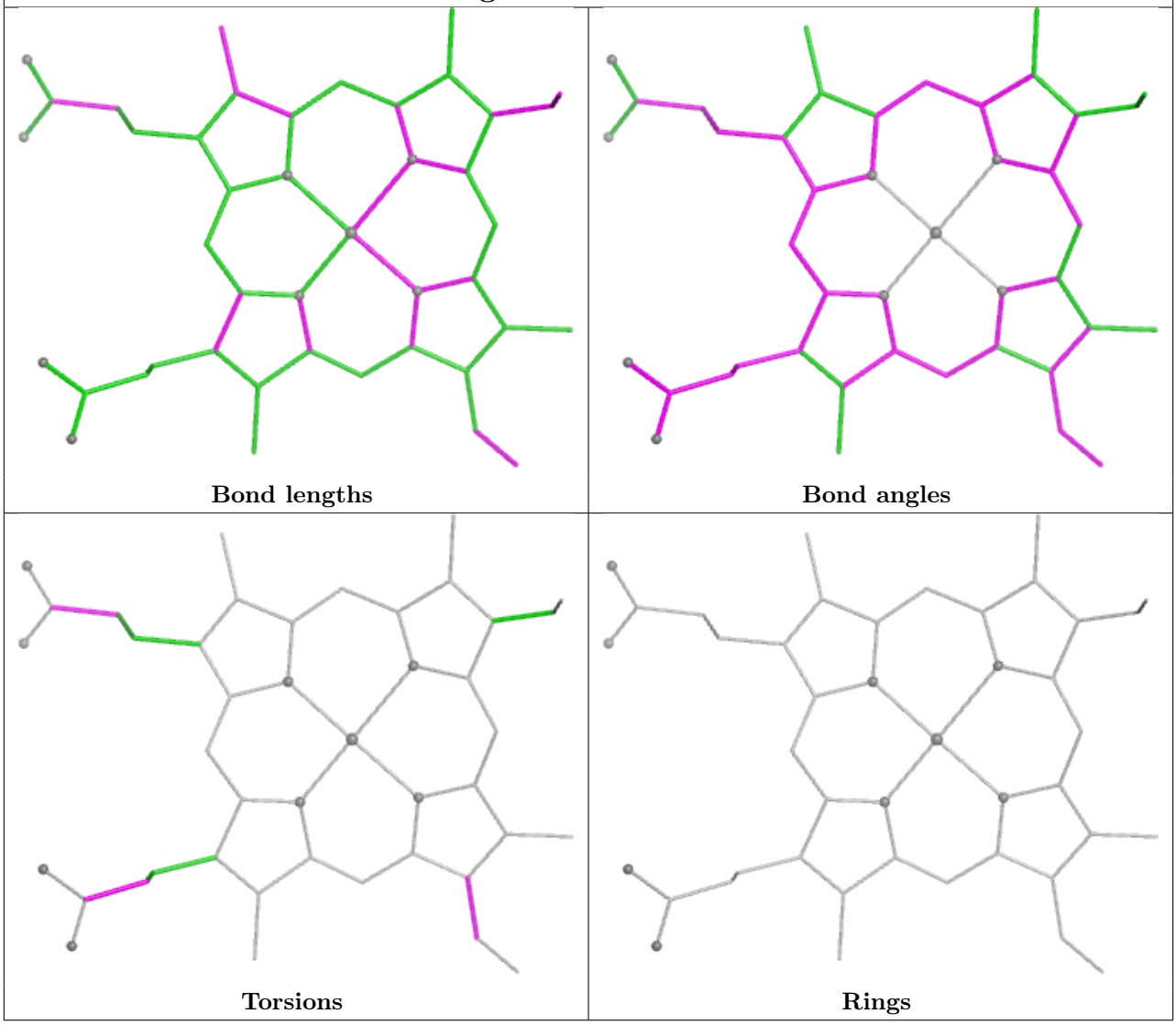
8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	HEC	5	0
2	B	401	HEC	8	0
4	B	1348	SO4	1	0
2	A	401	HEC	4	0
2	B	400	HEC	8	0
4	A	1353	SO4	1	0
4	B	1350	SO4	1	0
4	A	1352	SO4	3	0

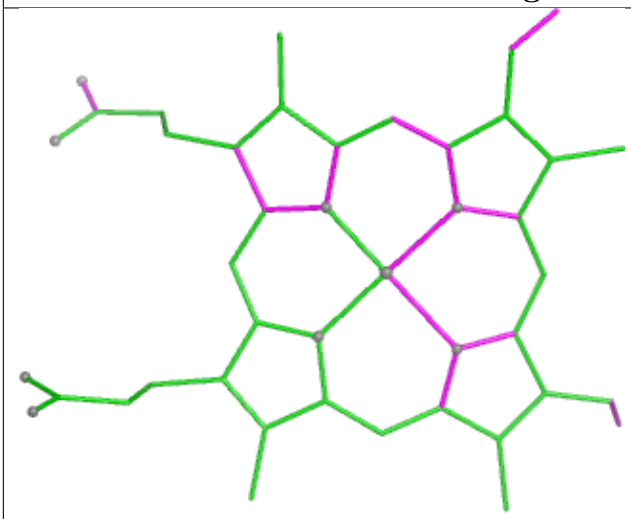
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

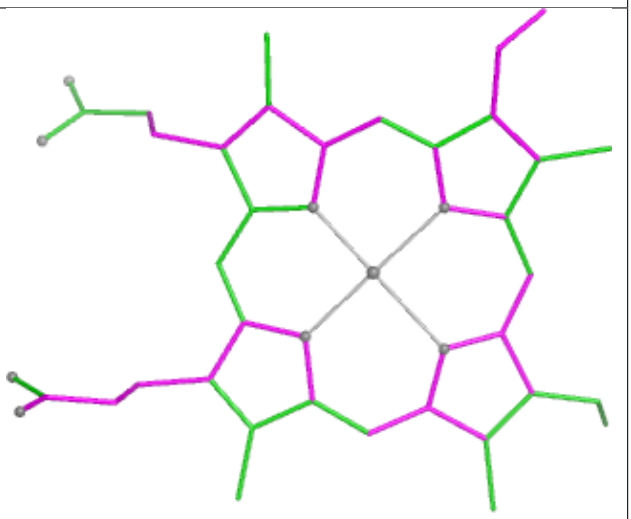
Ligand HEC A 400



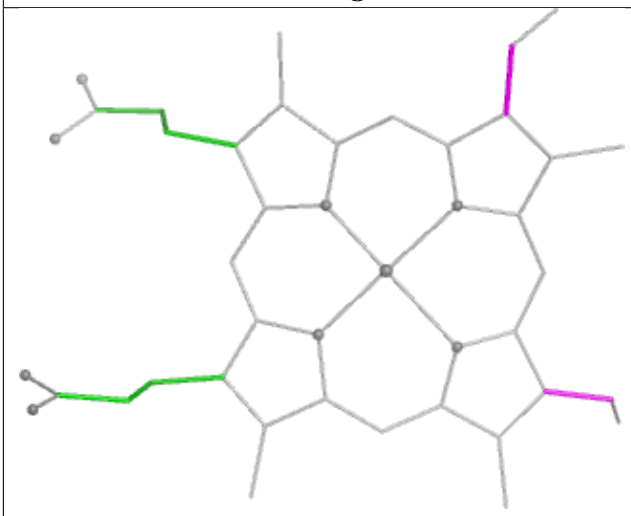
Ligand HEC B 401



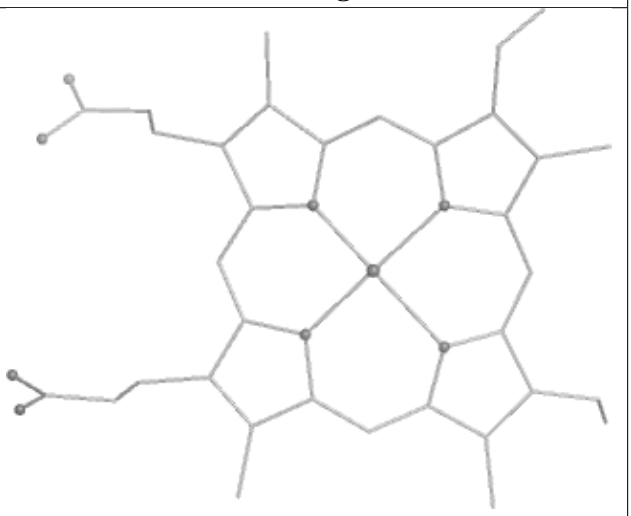
Bond lengths



Bond angles

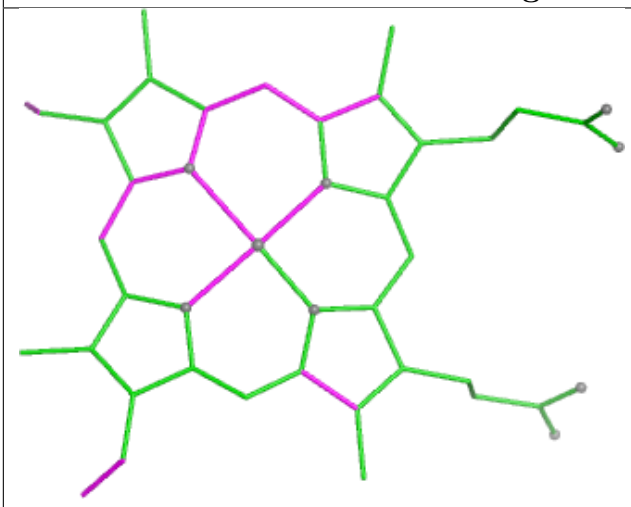


Torsions

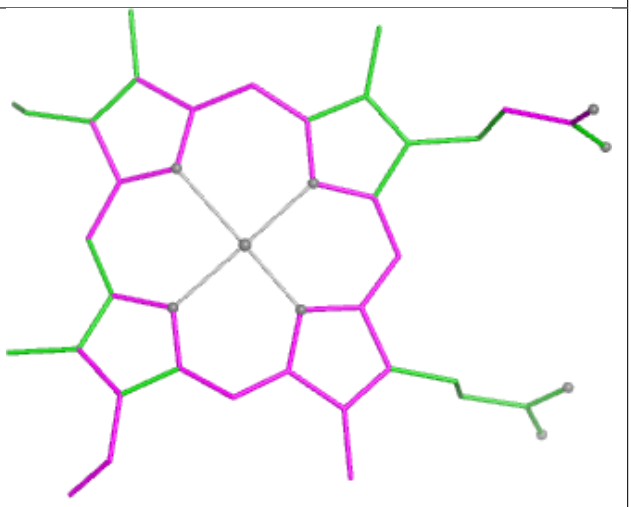


Rings

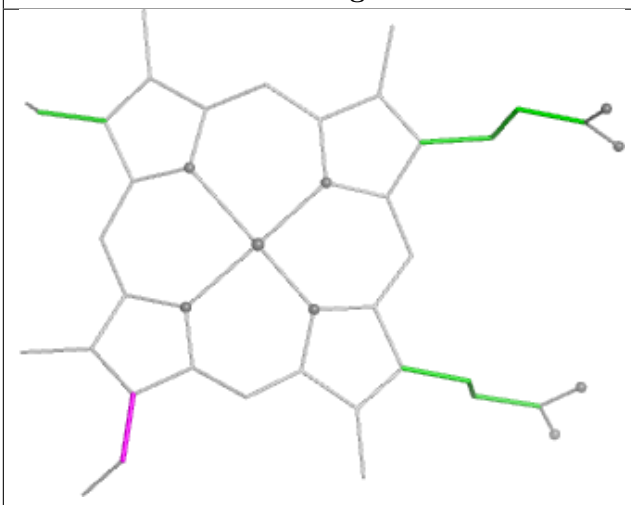
Ligand HEC A 401



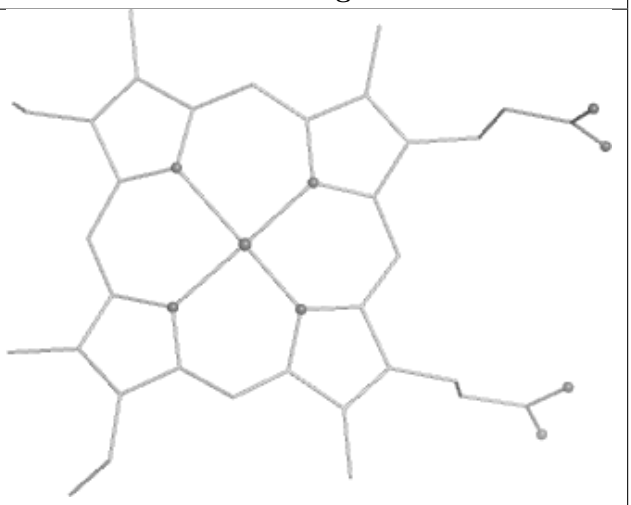
Bond lengths



Bond angles

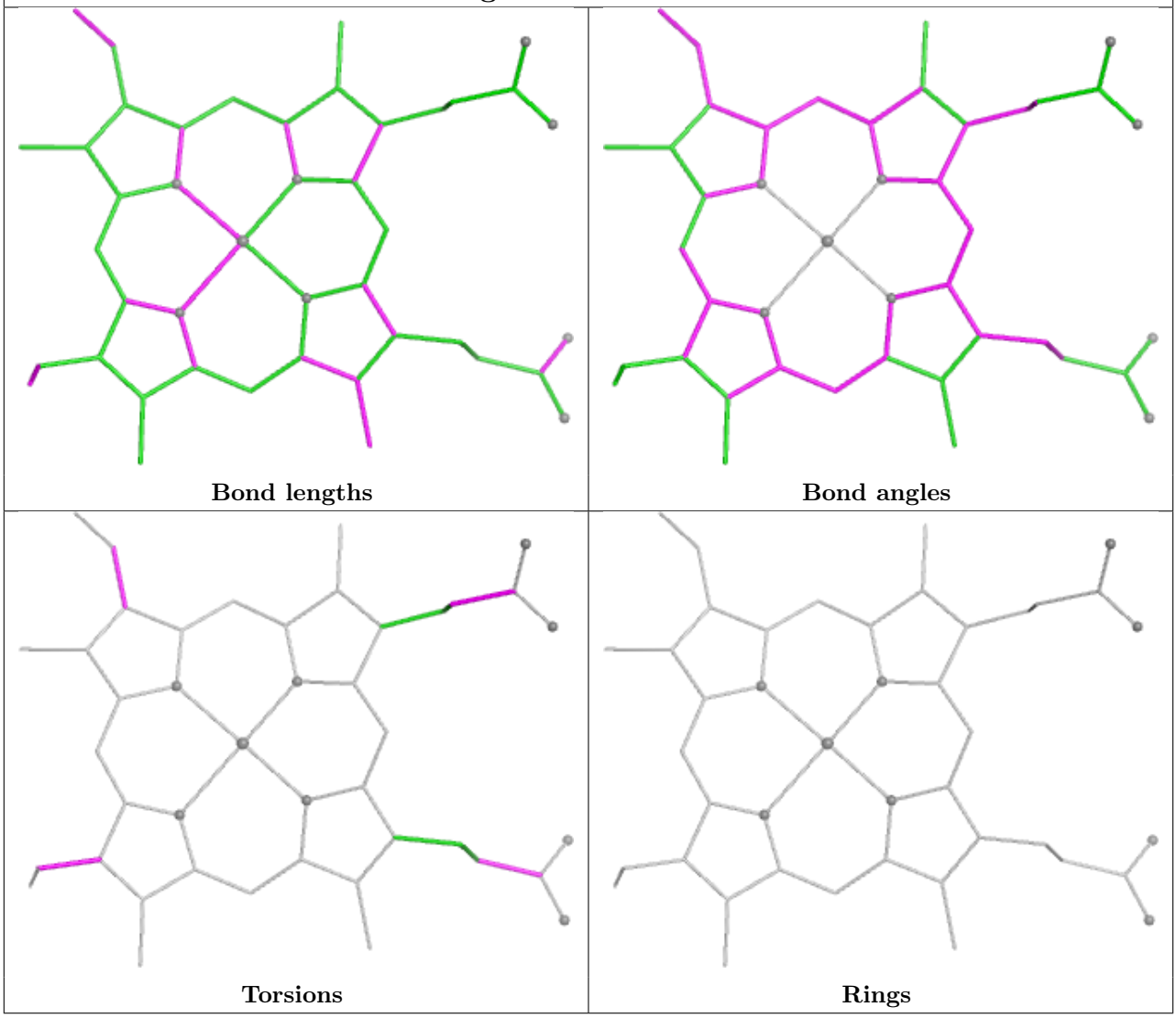


Torsions



Rings

Ligand HEC B 400



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	303/341 (88%)	-0.12	17 (5%)	30	32	19, 34, 66, 94	0
1	B	305/341 (89%)	-0.01	19 (6%)	26	28	19, 37, 69, 98	0
All	All	608/682 (89%)	-0.07	36 (5%)	28	30	19, 36, 69, 98	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ALA	7.8
1	B	127	ALA	7.4
1	B	253	GLY	6.5
1	A	262	ALA	5.0
1	A	303	GLY	4.9
1	A	260	THR	4.7
1	A	261	ALA	4.2
1	A	127	ALA	4.1
1	A	302	LEU	4.1
1	B	125	ALA	4.1
1	A	125	ALA	4.0
1	B	23	GLU	4.0
1	B	254	ARG	3.9
1	B	236	PHE	3.8
1	A	236	PHE	3.5
1	A	346	ASN	3.5
1	B	138	ASN	3.5
1	A	255	TYR	3.5
1	B	126	GLN	3.3
1	B	98	GLY	3.2
1	A	304	ILE	3.2
1	B	261	ALA	3.1
1	A	142	GLU	2.9
1	A	263	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	263	ASP	2.9
1	B	255	TYR	2.6
1	B	345	SER	2.6
1	B	128	LYS	2.6
1	B	301	GLN	2.5
1	A	300	ALA	2.4
1	B	129	GLY	2.3
1	B	200	ARG	2.2
1	A	98	GLY	2.2
1	A	241	ASP	2.1
1	A	124	ALA	2.0
1	B	241	ASP	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
4	SO4	B	1349	5/5	0.66	0.15	79,98,104,110	0
4	SO4	B	1348	5/5	0.69	0.18	84,97,101,108	0
4	SO4	A	1351	5/5	0.70	0.14	76,82,101,105	0
4	SO4	B	1350	5/5	0.70	0.18	58,74,80,89	0
4	SO4	A	1354	5/5	0.75	0.18	82,83,98,102	0
4	SO4	A	1353	5/5	0.78	0.13	74,75,89,91	0
4	SO4	A	1352	5/5	0.80	0.14	76,78,88,95	0
4	SO4	A	1350	5/5	0.82	0.12	67,83,89,98	0
4	SO4	B	1351	5/5	0.83	0.13	84,96,108,109	0
4	SO4	B	1352	5/5	0.85	0.08	79,80,85,90	0
4	SO4	A	1349	5/5	0.89	0.15	65,72,76,77	0

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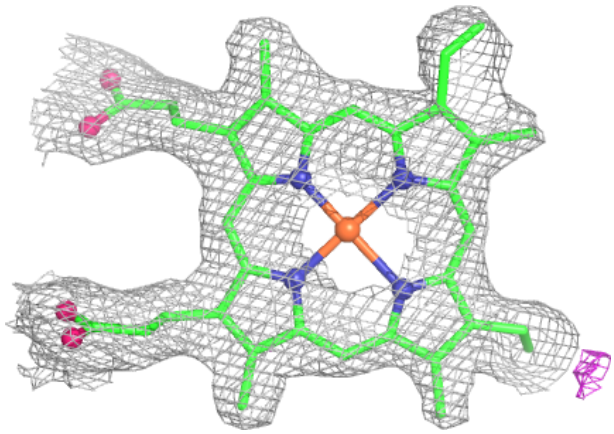
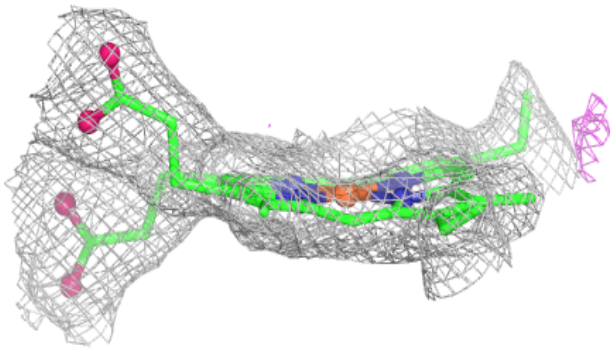
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	B	401	43/43	0.98	0.06	27,32,38,41	0
2	HEC	A	400	43/43	0.99	0.06	20,23,30,34	0
2	HEC	A	401	43/43	0.99	0.06	22,32,36,39	0
2	HEC	B	400	43/43	0.99	0.05	22,25,32,35	0
3	CA	B	402	1/1	1.00	0.01	27,27,27,27	0
3	CA	A	402	1/1	1.00	0.01	28,28,28,28	0

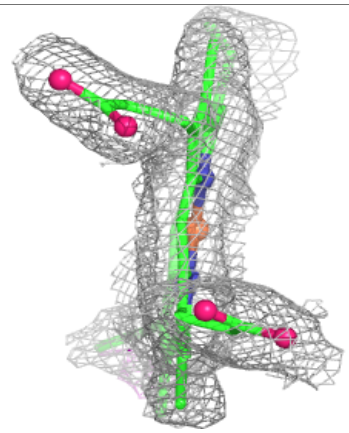
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC B 401:

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

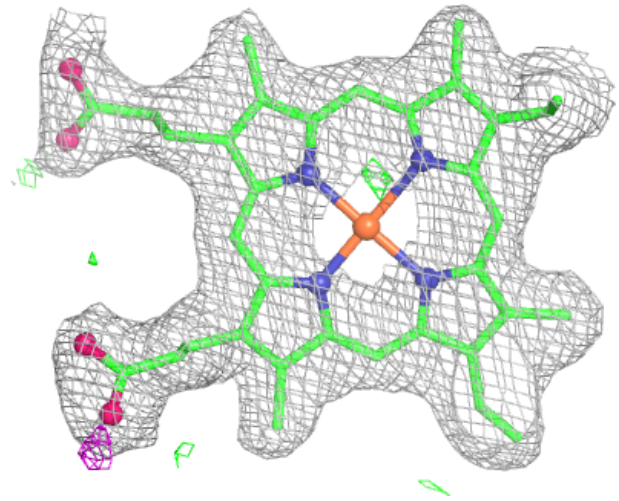


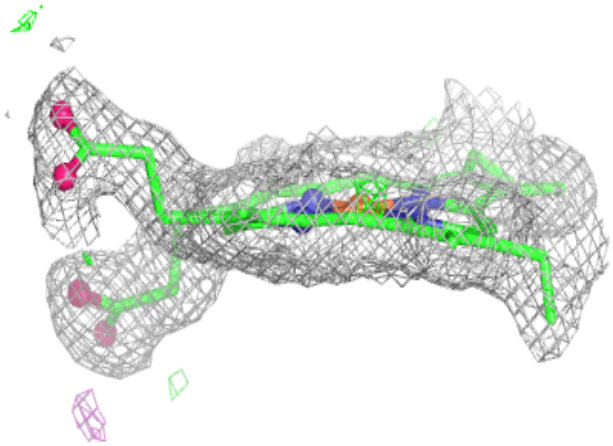


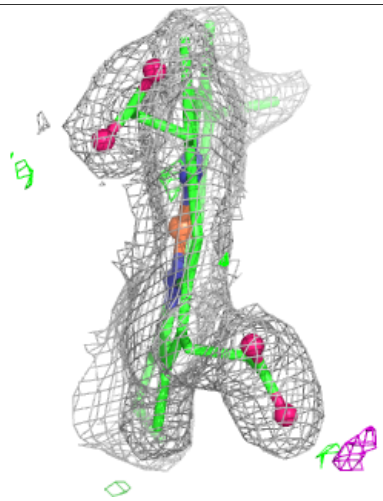


Electron density around HEC A 400:

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

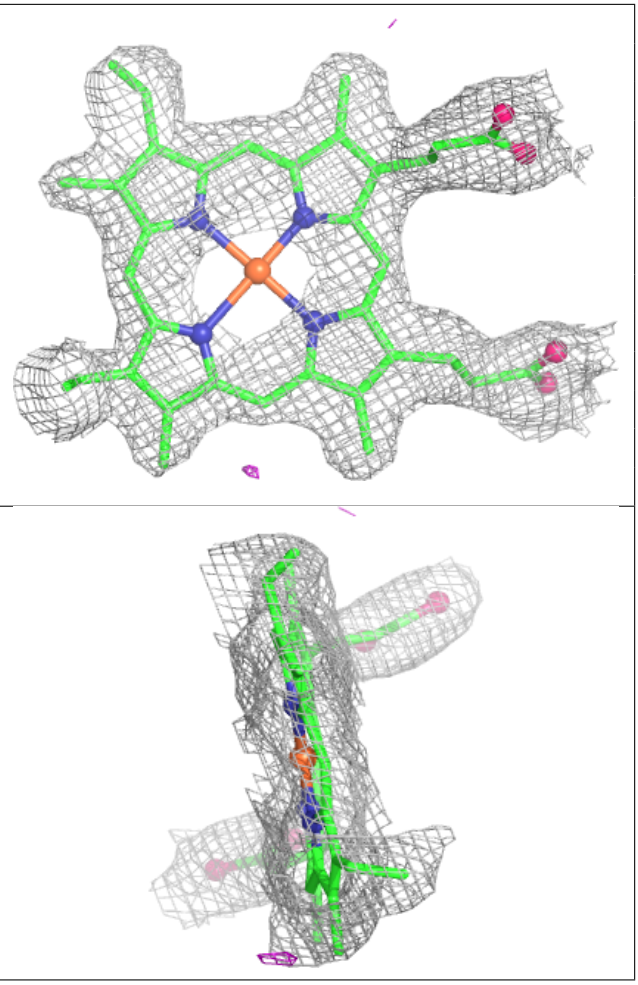






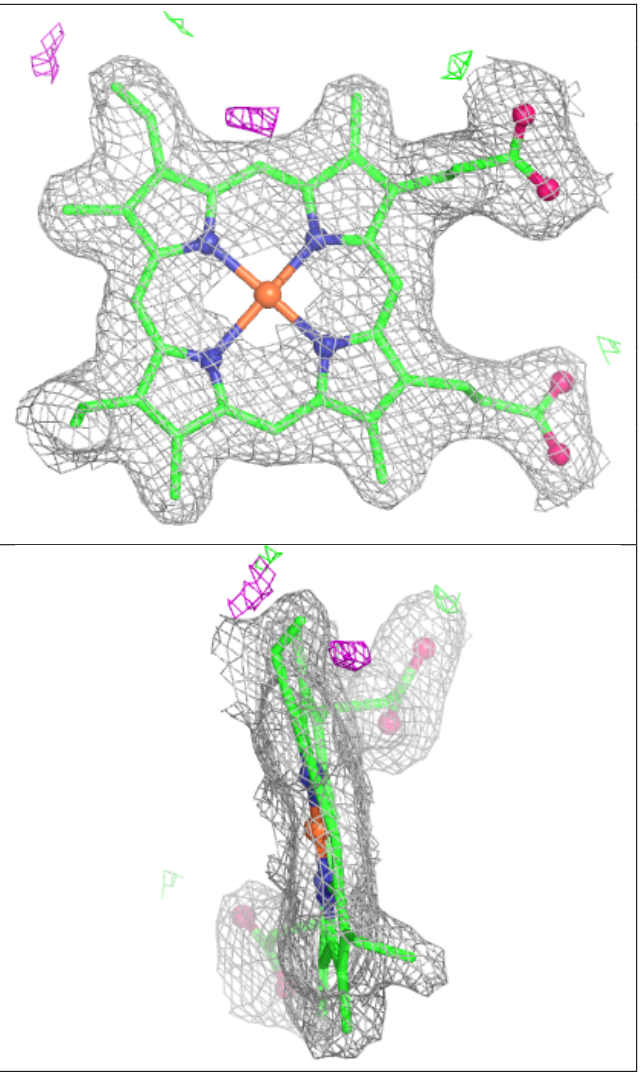
Electron density around HEC A 401:

$2mF_o$-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 400:

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.