



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:37 PM UTC

PDB ID : 1AEV / pdb\_00001aev  
Title : INTRODUCTION OF NOVEL SUBSTRATE OXIDATION INTO CYTOCHROME C PEROXIDASE BY CAVITY COMPLEMENTATION: OXIDATION OF 2-AMINOTHIAZOLE AND COVALENT MODIFICATION OF THE ENZYME (2-AMINOTHIAZOLE)  
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Deposited on : 1997-02-25  
Resolution : 2.10 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

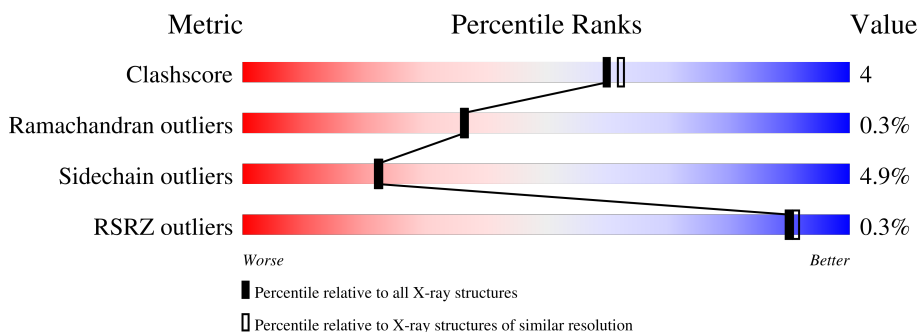
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	

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	AMT	A	296	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2941 atoms, of which 503 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.

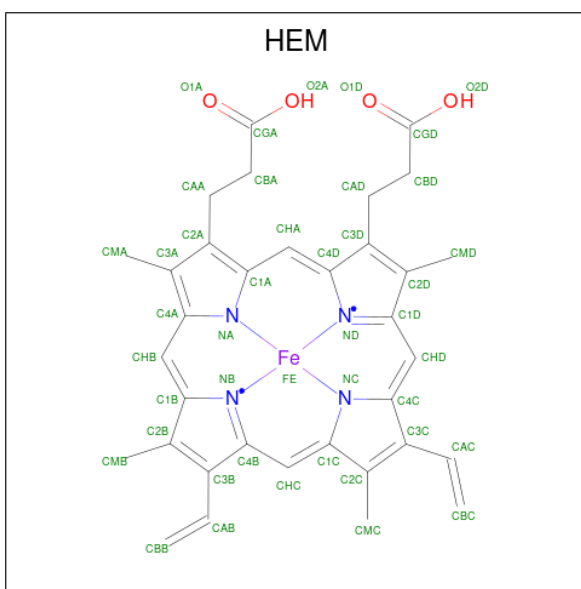
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	291	2841	1492	503	388	452	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

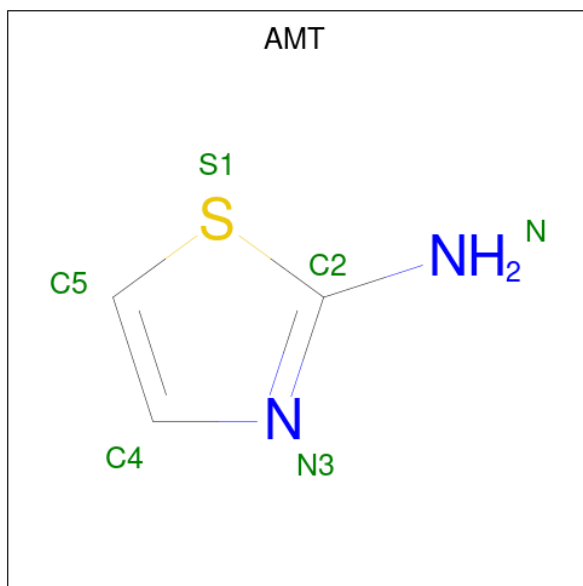
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	variant	UNP P00431
A	152	GLY	ASP	variant	UNP P00431
A	191	GLY	TRP	engineered mutation	UNP P00431
A	272	ASP	ASN	conflict	UNP P00431

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 3 is 2-AMINOTHIAZOLE (CCD ID: AMT) (formula: C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
3	A	1	6	3	2	1	0	0

- Molecule 4 is water.

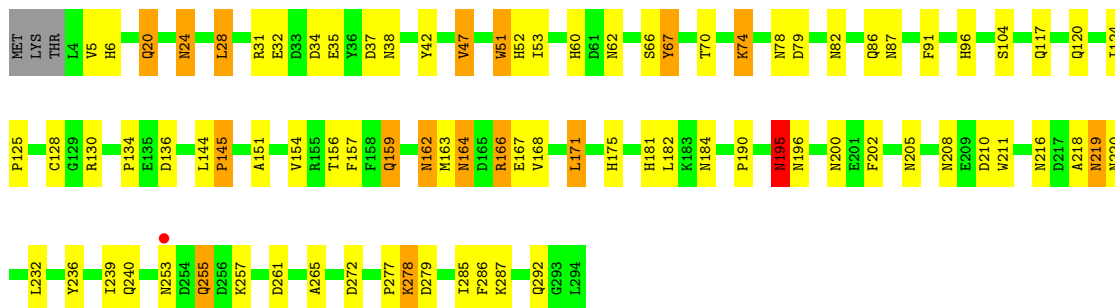
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	51	51	51	0	0

### 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.20Å 74.30Å 45.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10 7.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.0 (7.00-2.10) 85.0 (7.00-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 2.00Å)	Xtriage
Refinement program	XTALVIEW	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.62 , 91.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: AMT, HEM

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	1.08	8/2402 (0.3%)	1.96	76/3250 (2.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	47	VAL	CA-CB	6.65	1.63	1.54
1	A	60	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	6	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	175	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	52	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	6	HIS	CG-ND1	-5.24	1.32	1.38
1	A	53	ILE	CA-CB	5.00	1.60	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLN	OE1-CD-NE2	-10.31	112.29	122.60
1	A	124	ILE	O-C-N	-10.01	115.06	121.37
1	A	82	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	A	34	ASP	CA-CB-CG	9.24	121.84	112.60
1	A	62	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	A	208	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	A	278	LYS	CA-CB-CG	-8.46	97.19	114.10
1	A	195	ASN	N-CA-C	8.34	123.02	113.02
1	A	195	ASN	CA-CB-CG	8.30	120.90	112.60
1	A	240	GLN	OE1-CD-NE2	-8.17	114.43	122.60
1	A	52	HIS	N-CA-C	7.99	121.09	111.82
1	A	195	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	A	162	ASN	CA-CB-CG	7.92	120.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	A	164	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	5	VAL	O-C-N	-7.81	114.86	122.98
1	A	292	GLN	OE1-CD-NE2	-7.75	114.85	122.60
1	A	220	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	164	ASN	CA-CB-CG	7.39	120.00	112.60
1	A	162	ASN	N-CA-C	7.14	126.00	110.80
1	A	277	PRO	CA-C-O	-7.11	113.00	121.67
1	A	255	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	A	219	ASN	CB-CG-ND2	6.83	126.64	116.40
1	A	253	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	A	205	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	A	159	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	78	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	87	ASN	OD1-CG-ND2	-6.61	116.00	122.60
1	A	31	ARG	NE-CZ-NH2	-6.55	113.31	119.20
1	A	37	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	86	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	79	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	70	THR	N-CA-C	6.46	120.76	113.01
1	A	82	ASN	CB-CG-ND2	6.45	126.08	116.40
1	A	196	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	162	ASN	CA-C-O	6.27	129.47	120.51
1	A	265	ALA	N-CA-C	6.18	118.10	111.36
1	A	67	TYR	N-CA-C	6.16	118.50	111.11
1	A	91	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	181	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	A	66	SER	N-CA-C	6.01	120.22	113.01
1	A	128	CYS	O-C-N	-5.95	115.33	122.65
1	A	42	TYR	N-CA-C	5.95	120.40	113.20
1	A	38	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	184	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	145	PRO	N-CA-C	5.78	120.57	111.38
1	A	134	PRO	N-CA-C	5.77	120.28	111.34
1	A	210	ASP	CA-CB-CG	5.75	118.34	112.60
1	A	24	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	154	VAL	N-CA-C	5.69	115.89	110.42
1	A	279	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	232	LEU	CA-C-N	5.61	125.07	119.24
1	A	232	LEU	C-N-CA	5.61	125.07	119.24
1	A	211	TRP	N-CA-C	5.57	118.62	109.76
1	A	117	GLN	OE1-CD-NE2	-5.54	117.06	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	CA-CB-CG	5.49	125.08	114.10
1	A	51	TRP	CB-CG-CD1	-5.49	118.67	126.90
1	A	151	ALA	N-CA-C	5.48	118.01	111.71
1	A	104	SER	N-CA-C	5.43	116.89	110.97
1	A	163	MET	CG-SD-CE	-5.41	88.99	100.90
1	A	277	PRO	O-C-N	-5.40	116.42	123.06
1	A	32	GLU	N-CA-C	5.36	116.97	111.03
1	A	62	ASN	CB-CG-ND2	5.34	124.41	116.40
1	A	38	ASN	N-CA-C	5.26	118.65	111.39
1	A	136	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	60	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	286	PHE	N-CA-C	5.14	117.67	109.96
1	A	202	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	216	ASN	OD1-CG-ND2	-5.12	117.47	122.60
1	A	261	ASP	N-CA-C	5.12	116.94	111.36
1	A	51	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	272	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	182	LEU	N-CA-C	5.09	116.83	111.28
1	A	51	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	144	LEU	CA-C-N	5.06	124.97	119.85
1	A	144	LEU	C-N-CA	5.06	124.97	119.85

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2338	503	2209	18	0
2	A	43	0	30	2	0
3	A	6	0	4	1	0
4	A	51	0	0	1	0
All	All	2438	503	2243	20	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 4.

All (20) 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:74:LYS:HD2	1:A:74:LYS:H	1.64	0.63
1:A:20:GLN:HE22	1:A:287:LYS:N	2.02	0.58
1:A:20:GLN:HE22	1:A:287:LYS:H	1.55	0.53
2:A:295:HEM:C1A	3:A:296:AMT:H5	2.45	0.52
1:A:130:ARG:NE	4:A:326:HOH:O	2.44	0.50
1:A:167:GLU:O	1:A:171:LEU:HB2	2.12	0.50
1:A:24:ASN:O	1:A:28:LEU:HD22	2.12	0.49
1:A:145:PRO:HD3	1:A:157:PHE:CZ	2.48	0.48
1:A:164:ASN:O	1:A:168:VAL:HG23	2.14	0.48
1:A:195:ASN:HD22	1:A:195:ASN:H	1.64	0.46
1:A:166:ARG:HH21	1:A:257:LYS:NZ	2.14	0.45
1:A:218:ALA:O	1:A:219:ASN:HB2	2.17	0.44
1:A:166:ARG:HH21	1:A:257:LYS:HZ2	1.66	0.44
1:A:200:ASN:H	1:A:255:GLN:HE21	1.67	0.43
1:A:20:GLN:NE2	1:A:287:LYS:H	2.17	0.42
1:A:74:LYS:H	1:A:74:LYS:CD	2.32	0.41
1:A:125:PRO:HG3	1:A:285:ILE:CD1	2.50	0.41
1:A:236:TYR:CE1	1:A:239:ILE:HD11	2.55	0.41
1:A:67:TYR:HA	1:A:130:ARG:HG2	2.02	0.41
2:A:295:HEM:HBC2	2:A:295:HEM:HMC2	2.03	0.41

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	289/294 (98%)	282 (98%)	6 (2%)	1 (0%)	36 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

### 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	246/251 (98%)	234 (95%)	12 (5%)	22 22

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

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	47	VAL
1	A	51	TRP
1	A	74	LYS
1	A	156	THR
1	A	159	GLN
1	A	166	ARG
1	A	171	LEU
1	A	190	PRO
1	A	195	ASN
1	A	278	LYS

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	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	159	GLN
1	A	195	ASN
1	A	255	GLN
1	A	292	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	295	4,1	50,50,50	2.30	26 (52%)	67,82,82	1.07	3 (4%)
3	AMT	A	296	-	6,6,6	1.93	2 (33%)	7,7,7	3.00	4 (57%)

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	HEM	A	295	4,1	-	4/14/54/54	-
3	AMT	A	296	-	-	-	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	HEM	FE-NB	4.74	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	HEM	FE-ND	4.33	2.08	1.94
2	A	295	HEM	C3C-C4C	-4.06	1.38	1.46
2	A	295	HEM	C1B-NB	-3.66	1.33	1.40
3	A	296	AMT	C4-N3	-3.58	1.31	1.38
2	A	295	HEM	C1D-C2D	-3.55	1.37	1.44
2	A	295	HEM	C4D-C3D	-3.43	1.39	1.45
2	A	295	HEM	FE-NA	3.37	2.06	1.95
2	A	295	HEM	CBB-CAB	3.18	1.45	1.30
2	A	295	HEM	C4D-ND	-3.10	1.34	1.40
2	A	295	HEM	C4C-NC	-2.97	1.34	1.39
2	A	295	HEM	CBC-CAC	2.94	1.44	1.30
2	A	295	HEM	C1C-C2C	-2.79	1.39	1.45
2	A	295	HEM	CAB-C3B	-2.65	1.40	1.47
2	A	295	HEM	C1A-C2A	-2.64	1.39	1.44
2	A	295	HEM	C3B-C4B	-2.64	1.39	1.44
2	A	295	HEM	C1D-ND	-2.59	1.33	1.38
2	A	295	HEM	FE-NC	2.56	2.03	1.95
2	A	295	HEM	C4B-NB	-2.53	1.33	1.38
2	A	295	HEM	C1A-NA	-2.51	1.34	1.39
2	A	295	HEM	CAC-C3C	-2.45	1.40	1.47
2	A	295	HEM	C1B-C2B	-2.34	1.39	1.44
2	A	295	HEM	O2A-CGA	-2.33	1.23	1.30
2	A	295	HEM	C1C-NC	-2.32	1.35	1.39
3	A	296	AMT	C4-C5	2.26	1.39	1.34
2	A	295	HEM	C4A-C3A	-2.25	1.37	1.43
2	A	295	HEM	O2D-CGD	-2.22	1.23	1.30
2	A	295	HEM	CHD-C4C	2.03	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	AMT	C5-S1-C2	-4.69	84.69	90.05
3	A	296	AMT	S1-C2-N3	4.20	117.83	114.54
3	A	296	AMT	C4-C5-S1	3.43	114.64	110.27
3	A	296	AMT	C5-C4-N3	-2.95	111.86	116.12
2	A	295	HEM	C3C-C2C-C1C	-2.89	104.31	107.05
2	A	295	HEM	C3B-C2B-C1B	-2.27	104.70	106.41
2	A	295	HEM	C1C-CHC-C4B	2.01	130.30	126.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

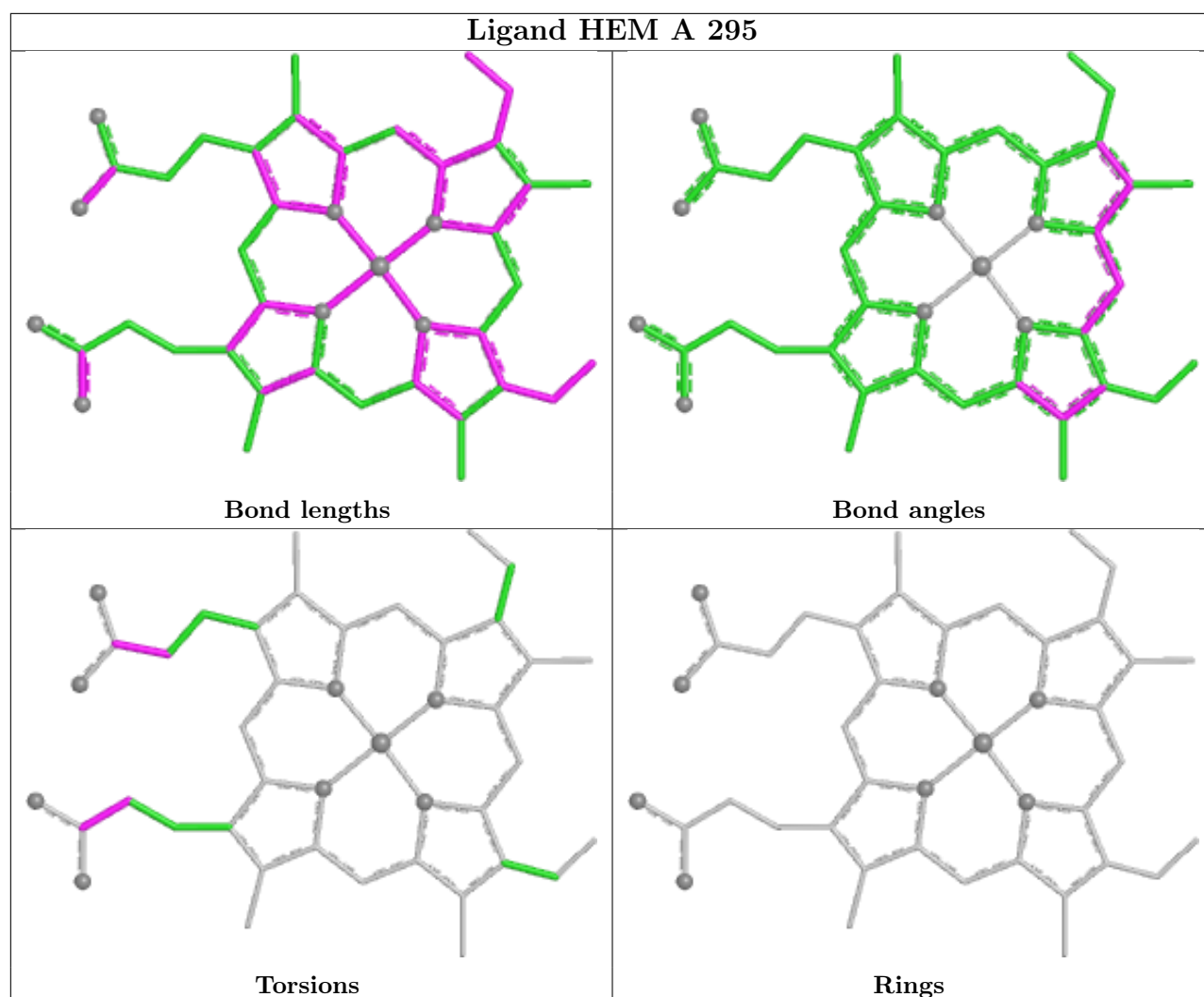
Mol	Chain	Res	Type	Atoms
2	A	295	HEM	CAA-CBA-CGA-O2A
2	A	295	HEM	CAA-CBA-CGA-O1A
2	A	295	HEM	CAD-CBD-CGD-O2D
2	A	295	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	HEM	2	0
3	A	296	AMT	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 than 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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	291/294 (98%)	-0.16	1 (0%) <b>90</b> <b>91</b>	8, 15, 26, 37	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	3.0

### 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](#)

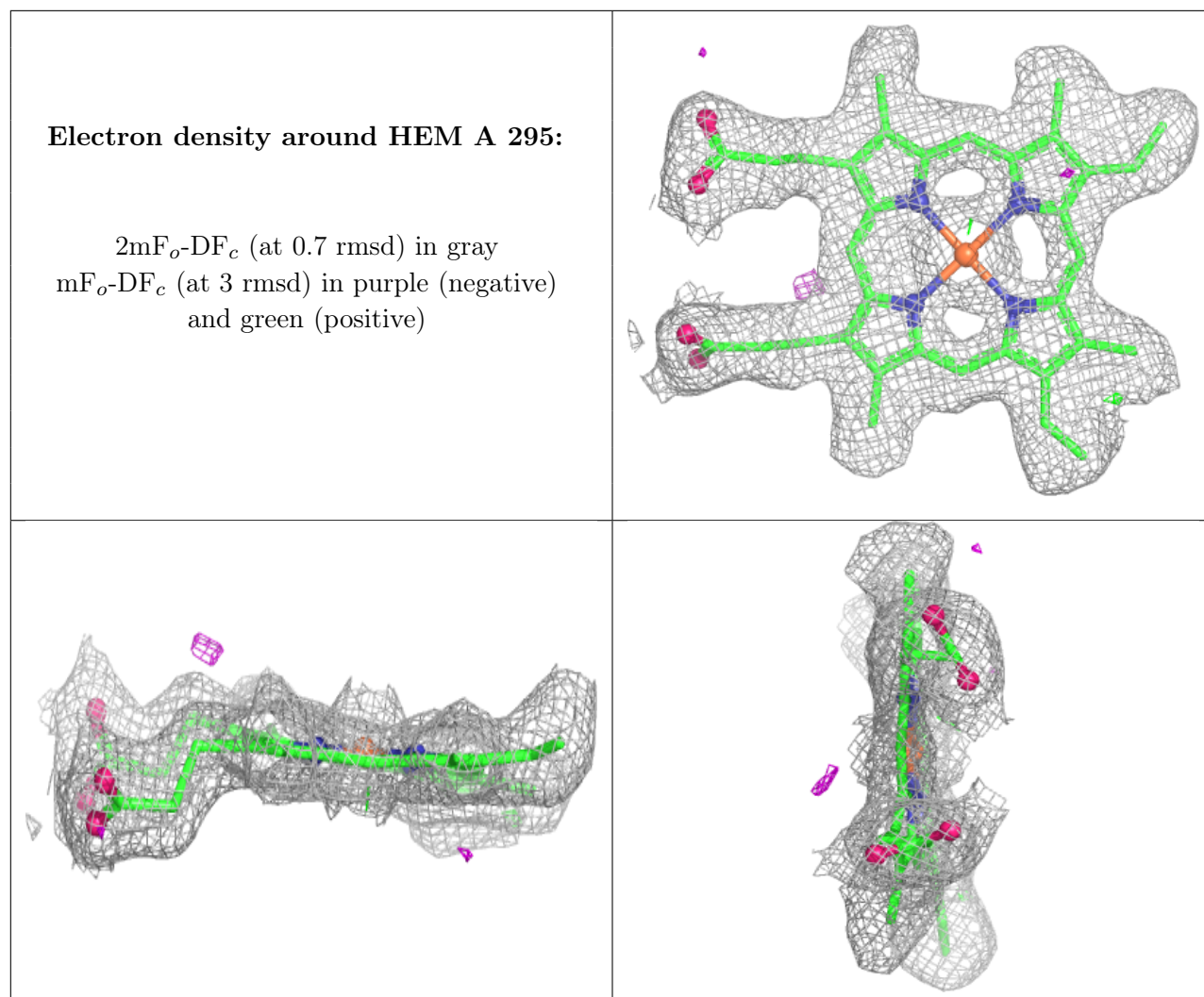
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	AMT	A	296	6/6	0.94	0.08	18,24,25,25	0
2	HEM	A	295	43/43	0.95	0.06	9,13,18,23	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.