

Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 10:11 AM EDT

PDB ID : 1AC8

Title : VARIATION IN THE STRENGTH OF A CH TO O HYDROGEN BOND IN

AN ARTIFICIAL PROTEIN CAVITY (3,4,5-TRIMETHYLTHIAZOLE)

Authors: Musah, R.A.; Jensen, G.M.; Bunte, S.W.; Rosenfeld, R.; Mcree, D.E.; Goodin,

D.B.

Deposited on : 1997-02-14

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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.23.2

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

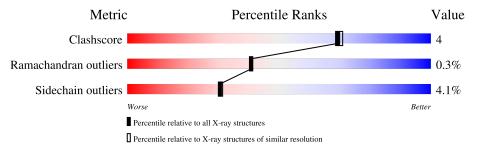
Validation Pipeline (wwPDB-VP) : 2.23.2

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	Similar resolution		
Metric	$(\# ext{Entries})$	$(\# \text{Entries, resolution range}(\text{\AA}))$		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (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 >=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%

Mol	Chain	Length	Quality of chain		
1	A	294	84%	14%	

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	TMZ	A	296	-	-	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2992 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.

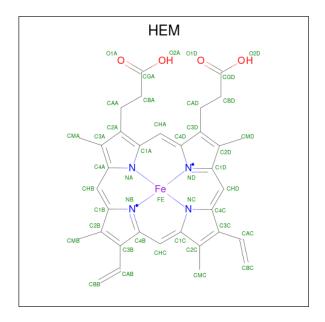
• Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	SEE REMARK 999	UNP P00431
A	152	GLY	ASP	SEE REMARK 999	UNP P00431
A	191	GLY	TRP	engineered mutation	UNP P00431
A	272	ASP	ASN	SEE REMARK 999	UNP P00431

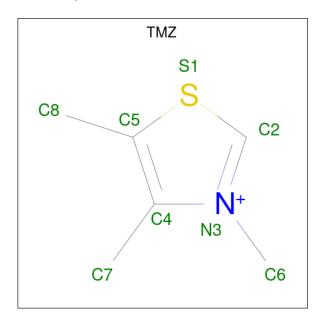
• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	Λ	1	Total	С	Fe	N	О	0	0
	2 A	1	43	34	1	4	4	0	U



 \bullet Molecule 3 is 3,4,5-TRIMETHYL-1,3-THIAZOLE (three-letter code: TMZ) (formula: $C_6H_{10}NS).$



Mol	Chain	Residues	Ato	ms		ZeroOcc	AltConf
3	A	1	Total (N 5 1	S 1	0	0

• Molecule 4 is water.

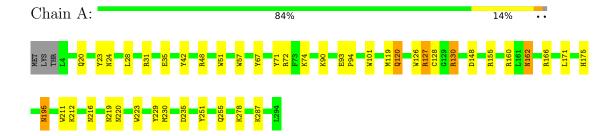
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0



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. 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. 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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	108.00Å 77.30Å 51.80Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 - 2.10	Depositor
Resolution (A)	21.10 - 1.95	EDS
% Data completeness	79.0 (7.00-2.10)	Depositor
(in resolution range)	66.3 (21.10-1.95)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	5.53 (at 1.95Å)	Xtriage
Refinement program	XTALVIEW	Depositor
D D.	(Not available) , (Not available)	Depositor
R, R_{free}	0.209 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 61.6	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2992	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: TMZ, 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	Boı	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.83	$1/2402 \ (0.0\%)$	1.58	46/3250 (1.4%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
1	A	42	TYR	CD2-CE2	-6.72	1.29	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	166	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	48	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	31	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	127	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	101	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	126	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	127	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	51	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	A	57	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	126	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	223	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	71	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	A	127	ARG	CB-CG-CD	-7.38	92.40	111.60
1	A	223	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	51	TRP	CB-CG-CD1	-7.33	117.47	127.00
1	A	51	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	229	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	A	130	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	162	ASN	CA-C-N	-7.09	101.60	117.20
1	A	101	TRP	CE2-CD2-CG	-6.90	101.78	107.30

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	211	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	211	TRP	CD1-CG-CD2	6.58	111.56	106.30
1	A	160	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	57	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	A	51	TRP	CG-CD2-CE3	6.42	139.68	133.90
1	A	162	ASN	N-CA-C	6.29	128.00	111.00
1	A	160	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	31	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	42	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	130	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	130	ARG	CG-CD-NE	-6.01	99.18	111.80
1	A	251	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	126	TRP	CG-CD2-CE3	5.66	138.99	133.90
1	A	148	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	101	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	57	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	255	GLN	CG-CD-NE2	5.24	129.27	116.70
1	A	48	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	155	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	90	LYS	CA-CB-CG	-5.21	101.94	113.40
1	A	230	MET	CA-CB-CG	5.16	122.06	113.30
1	A	126	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	166	ARG	CG-CD-NE	-5.08	101.13	111.80
1	A	255	GLN	OE1-CD-NE2	-5.08	110.22	121.90
1	A	162	ASN	CA-C-O	5.07	130.74	120.10
1	A	223	TRP	CG-CD2-CE3	5.02	138.42	133.90

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2338	503	2209	15	0
2	A	43	0	30	2	0
3	A	8	0	10	4	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	100	0	0	4	0
All	All	2489	503	2249	17	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 (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)	
1:A:128:CYS:HA	4:A:326:HOH:O	1.62	0.99	
1:A:235:ASP:OD2	3:A:296:TMZ:H2	1.94	0.67	
1:A:175:HIS:O	3:A:296:TMZ:H72	1.96	0.66	
1:A:130:ARG:NE	4:A:442:HOH:O	2.37	0.57	
1:A:20:GLN:HE22	1:A:287:LYS:H	1.52	0.57	
1:A:195:ASN:HD22	1:A:195:ASN:H	1.54	0.55	
1:A:67:TYR:HA	1:A:130:ARG:HG2	1.89	0.53	
1:A:130:ARG:CZ	4:A:442:HOH:O	2.57	0.52	
1:A:119:MET:O	1:A:120:GLN:HG2	2.11	0.50	
1:A:130:ARG:NH2	4:A:442:HOH:O	2.45	0.49	
1:A:93:GLU:HB3	1:A:94:PRO:HD2	1.97	0.46	
1:A:195:ASN:H	1:A:195:ASN:ND2	2.14	0.44	
2:A:295:HEM:HAD2	3:A:296:TMZ:H83	2.01	0.43	
1:A:23:TYR:HD1	1:A:24:ASN:HD22	1.66	0.42	
1:A:216:ASN:HD21	1:A:220:ASN:HB2	1.84	0.42	
2:A:295:HEM:HAD2	3:A:296:TMZ:C8	2.50	0.41	
1:A:127:ARG:HH11	1:A:127:ARG:HD3	1.78	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%)	283 (98%)	5 (2%)	1 (0%)	41 41	

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	Analysed Rotameric Out		Percentiles
1	A	246/251 (98%)	236 (96%)	10 (4%)	30 31

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	72	ARG
1	A	74	LYS
1	A	120	GLN
1	A	171	LEU
1	A	195	ASN
1	A	212	LYS
1	A	219	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	78	ASN
1	A	195	ASN
1	A	220	ASN

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	240	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 monosaccharides 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	Trme	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Clasies	Chain	Chain	Dec	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2												
2	HEM	A	295	1,4	27,50,50	1.45	4 (14%)	17,82,82	1.67	3 (17%)												
3	TMZ	A	296	-	4,8,8	2.93	2 (50%)	4,11,11	2.98	2 (50%)												

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	1,4	-	0/6/54/54	-
3	TMZ	A	296	-	-	-	0/1/1/1



All (6) bond length outlier	s are listed below:
-----------------------------	---------------------

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	A	296	TMZ	C6-N3	-5.33	1.35	1.47
2	A	295	HEM	C3B-CAB	-3.88	1.40	1.47
2	A	295	HEM	C3C-CAC	-2.97	1.41	1.47
2	A	295	HEM	CBC-CAC	2.56	1.46	1.29
2	A	295	HEM	CBB-CAB	2.54	1.46	1.29
3	A	296	TMZ	C4-N3	2.35	1.42	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	296	TMZ	C7-C4-N3	-4.75	116.53	122.53
2	A	295	HEM	CMB-C2B-C3B	4.21	132.55	124.68
3	A	296	TMZ	C5-C4-N3	3.58	114.96	107.38
2	A	295	HEM	CMC-C2C-C3C	3.33	130.91	124.68
2	A	295	HEM	C1D-C2D-C3D	-2.41	105.32	107.00

There are no chirality outliers.

There are no torsion outliers.

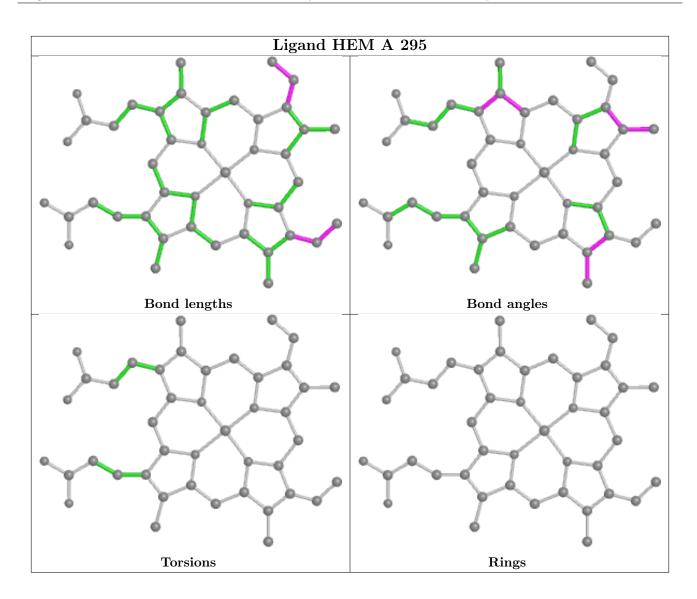
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	HEM	2	0
3	A	296	TMZ	4	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.





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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

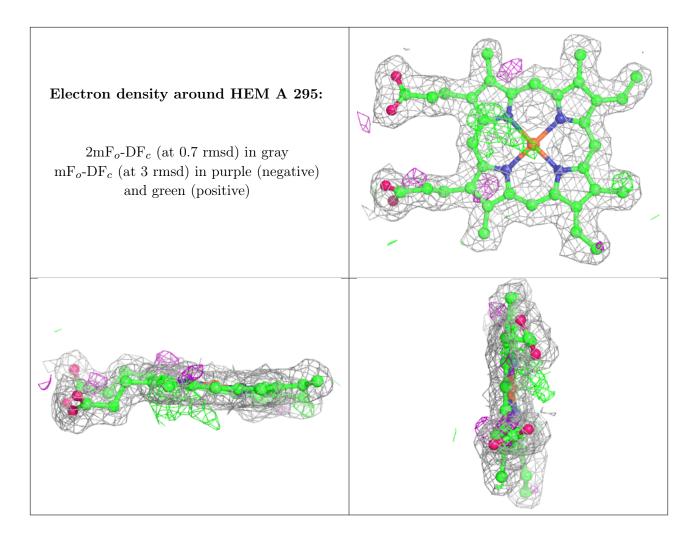
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

