



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:29 am BST

PDB ID : 1I3E  
Title : HUMAN AZIDO-MET HEMOGLOBIN BART'S (GAMMA4)  
Authors : Kidd, R.D.; Baker, H.M.; Mathews, A.J.; Brittain, T.; Baker, E.N.  
Deposited on : 2001-02-15  
Resolution : 1.86 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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

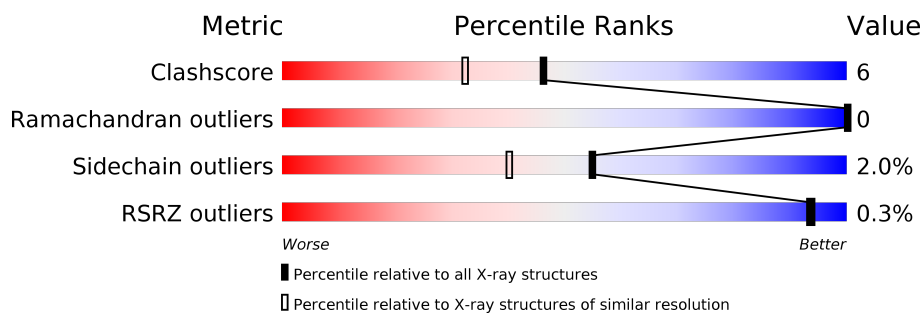
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	146	 72% 21% 7%
1	B	146	 64% 30% 5% •

## 2 Entry composition [i](#)

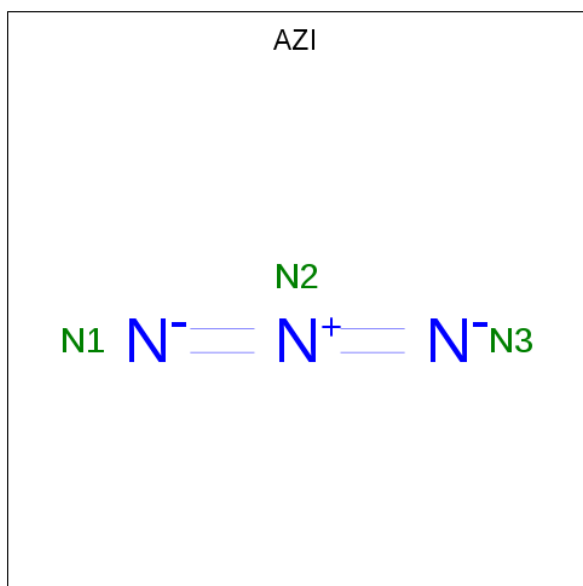
There are 4 unique types of molecules in this entry. The entry contains 2596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMOGLOBIN GAMMA CHAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	3	0	0
			1131	724	193	211	3			
1	B	146	Total	C	N	O	S	12	0	0
			1131	724	193	211	3			

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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		

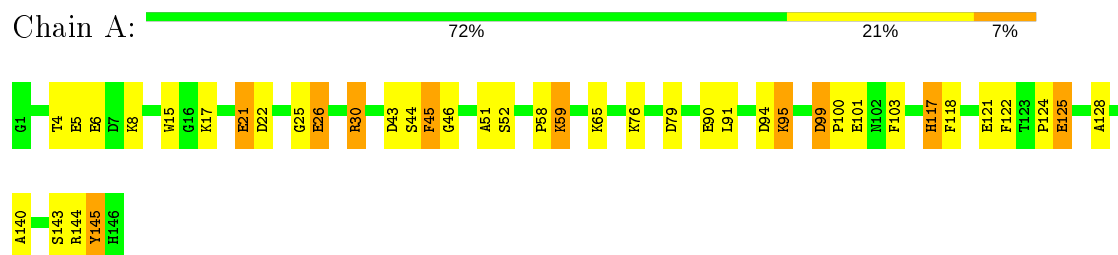
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	108	Total	O	0	0
			108	108		

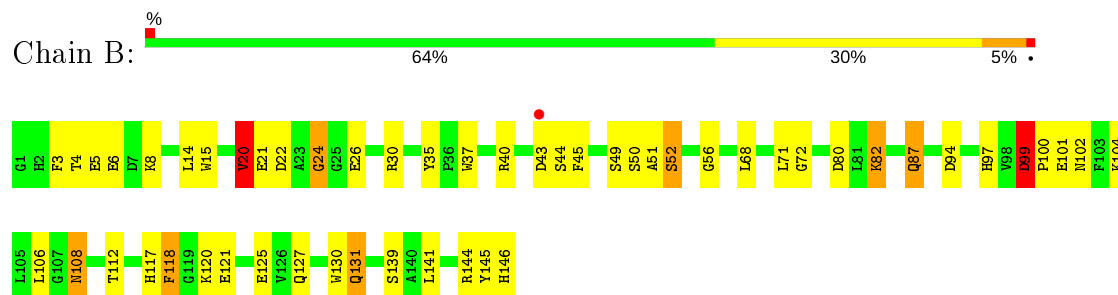
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: HEMOGLOBIN GAMMA CHAINS



#### • Molecule 1: HEMOGLOBIN GAMMA CHAINS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.54Å 81.62Å 53.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.86 18.38 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.86) 98.3 (18.38-1.86)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 1.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.184 , 0.220 0.171 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2596	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 8.72% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, 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	2.48	52/1157 (4.5%)	1.56	17/1565 (1.1%)
1	B	2.56	61/1157 (5.3%)	1.74	30/1565 (1.9%)
All	All	2.52	113/2314 (4.9%)	1.65	47/3130 (1.5%)

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	B	0	1

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	GLU	CD-OE2	17.73	1.45	1.25
1	A	26	GLU	CD-OE2	-16.27	1.07	1.25
1	B	101	GLU	CD-OE2	15.77	1.43	1.25
1	A	26	GLU	CG-CD	13.50	1.72	1.51
1	A	21	GLU	CG-CD	-13.42	1.31	1.51
1	B	52	SER	CA-CB	13.15	1.72	1.52
1	A	6	GLU	CD-OE1	-12.34	1.12	1.25
1	B	125	GLU	CD-OE2	-11.96	1.12	1.25
1	B	43	ASP	CB-CG	-11.12	1.28	1.51
1	A	30	ARG	NE-CZ	10.96	1.47	1.33
1	B	20	VAL	C-N	-10.65	1.09	1.34
1	B	21	GLU	C-O	10.55	1.43	1.23
1	A	90	GLU	CD-OE2	10.34	1.37	1.25
1	A	117	HIS	CE1-NE2	10.25	1.56	1.32
1	B	82	LYS	CD-CE	10.24	1.76	1.51
1	A	52	SER	CA-CB	9.97	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	CD2-CE2	9.58	1.52	1.41
1	B	87	GLN	CD-NE2	-9.58	1.08	1.32
1	B	144	ARG	CZ-NH1	9.52	1.45	1.33
1	B	26	GLU	CD-OE2	-9.42	1.15	1.25
1	A	144	ARG	CZ-NH2	9.28	1.45	1.33
1	B	6	GLU	CD-OE2	8.81	1.35	1.25
1	B	44	SER	CA-CB	-8.80	1.39	1.52
1	B	20	VAL	C-O	8.73	1.40	1.23
1	A	143	SER	CA-CB	8.60	1.65	1.52
1	B	21	GLU	CG-CD	8.26	1.64	1.51
1	A	21	GLU	CD-OE1	8.26	1.34	1.25
1	B	15	TRP	CD2-CE3	-7.97	1.28	1.40
1	A	145	TYR	CE1-CZ	7.78	1.48	1.38
1	A	6	GLU	CG-CD	7.66	1.63	1.51
1	A	118	PHE	CE1-CZ	7.62	1.51	1.37
1	B	125	GLU	CG-CD	7.39	1.63	1.51
1	B	94	ASP	N-CA	7.33	1.61	1.46
1	A	51	ALA	CA-CB	7.32	1.67	1.52
1	B	6	GLU	CD-OE1	7.31	1.33	1.25
1	A	94	ASP	N-CA	7.06	1.60	1.46
1	B	20	VAL	CB-CG1	-6.94	1.38	1.52
1	B	101	GLU	CG-CD	-6.87	1.41	1.51
1	A	43	ASP	CG-OD2	6.84	1.41	1.25
1	B	44	SER	CB-OG	6.75	1.51	1.42
1	B	5	GLU	CG-CD	6.70	1.61	1.51
1	B	49	SER	CA-CB	6.67	1.62	1.52
1	A	17	LYS	C-N	-6.65	1.18	1.34
1	B	56	GLY	CA-C	6.62	1.62	1.51
1	B	5	GLU	CB-CG	-6.54	1.39	1.52
1	B	131	GLN	CD-NE2	-6.48	1.16	1.32
1	A	121	GLU	CD-OE2	6.47	1.32	1.25
1	A	45	PHE	CG-CD1	-6.47	1.29	1.38
1	A	118	PHE	CG-CD1	6.43	1.48	1.38
1	A	76	LYS	CG-CD	6.42	1.74	1.52
1	B	22	ASP	CB-CG	6.40	1.65	1.51
1	B	35	TYR	CE1-CZ	-6.38	1.30	1.38
1	B	5	GLU	CA-CB	6.35	1.68	1.53
1	A	101	GLU	CD-OE1	6.32	1.32	1.25
1	A	143	SER	C-N	-6.27	1.19	1.34
1	B	52	SER	CB-OG	6.26	1.50	1.42
1	A	122	PHE	CE1-CZ	6.23	1.49	1.37
1	B	20	VAL	N-CA	6.22	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	NE-CZ	-6.20	1.25	1.33
1	B	121	GLU	CD-OE2	6.20	1.32	1.25
1	B	108	ASN	CG-ND2	6.19	1.48	1.32
1	B	102	ASN	CB-CG	6.10	1.65	1.51
1	A	145	TYR	CG-CD1	-6.06	1.31	1.39
1	B	43	ASP	CG-OD2	6.04	1.39	1.25
1	B	26	GLU	CG-CD	6.03	1.60	1.51
1	A	30	ARG	CZ-NH1	-6.02	1.25	1.33
1	B	139	SER	CB-OG	6.00	1.50	1.42
1	B	43	ASP	N-CA	5.96	1.58	1.46
1	A	26	GLU	CD-OE1	5.94	1.32	1.25
1	B	35	TYR	CE2-CZ	5.94	1.46	1.38
1	B	94	ASP	C-N	5.93	1.47	1.34
1	B	145	TYR	CD2-CE2	-5.88	1.30	1.39
1	B	97	HIS	CG-CD2	-5.84	1.25	1.35
1	A	5	GLU	CG-CD	5.81	1.60	1.51
1	A	128	ALA	CA-CB	5.81	1.64	1.52
1	B	37	TRP	CE3-CZ3	5.78	1.48	1.38
1	B	80	ASP	CG-OD1	5.77	1.38	1.25
1	A	4	THR	C-N	5.75	1.47	1.34
1	A	144	ARG	CZ-NH1	5.67	1.40	1.33
1	B	15	TRP	CE2-CZ2	-5.66	1.30	1.39
1	B	21	GLU	CA-CB	-5.63	1.41	1.53
1	B	50	SER	CA-CB	5.60	1.61	1.52
1	B	99	ASP	CB-CG	-5.59	1.40	1.51
1	B	22	ASP	C-O	5.58	1.33	1.23
1	A	15	TRP	CE3-CZ3	5.57	1.48	1.38
1	A	145	TYR	CG-CD2	5.49	1.46	1.39
1	B	72	GLY	N-CA	-5.47	1.37	1.46
1	A	140	ALA	C-O	5.46	1.33	1.23
1	B	80	ASP	CA-CB	-5.45	1.42	1.53
1	A	8	LYS	CG-CD	5.45	1.71	1.52
1	A	44	SER	CA-CB	5.45	1.61	1.52
1	A	59	LYS	CE-NZ	5.44	1.62	1.49
1	B	15	TRP	CD2-CE2	5.43	1.47	1.41
1	A	43	ASP	N-CA	5.43	1.57	1.46
1	B	45	PHE	C-N	-5.41	1.23	1.33
1	A	121	GLU	CB-CG	5.36	1.62	1.52
1	A	124	PRO	N-CD	5.32	1.55	1.47
1	A	46	GLY	N-CA	5.31	1.54	1.46
1	A	103	PHE	CG-CD1	5.29	1.46	1.38
1	A	25	GLY	CA-C	-5.28	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	LYS	CD-CE	5.26	1.64	1.51
1	A	125	GLU	CD-OE1	5.20	1.31	1.25
1	A	95	LYS	CG-CD	5.20	1.70	1.52
1	B	3	PHE	CG-CD1	-5.14	1.31	1.38
1	A	15	TRP	CG-CD1	5.13	1.44	1.36
1	A	117	HIS	CD2-NE2	5.11	1.52	1.42
1	B	4	THR	CA-C	-5.08	1.39	1.52
1	B	37	TRP	CD2-CE2	-5.08	1.35	1.41
1	B	8	LYS	CA-C	-5.06	1.39	1.52
1	B	130	TRP	CD2-CE2	-5.04	1.35	1.41
1	B	30	ARG	CZ-NH2	5.03	1.39	1.33
1	B	24	GLY	N-CA	5.02	1.53	1.46
1	A	45	PHE	CD1-CE1	5.00	1.49	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ASP	CB-CG-OD1	18.15	134.63	118.30
1	B	40	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	43	ASP	CB-CG-OD1	11.92	129.03	118.30
1	A	144	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	A	21	GLU	OE1-CD-OE2	-9.51	111.89	123.30
1	A	45	PHE	CB-CG-CD2	-8.92	114.55	120.80
1	B	40	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	146	HIS	CA-C-O	-7.75	103.82	120.10
1	B	43	ASP	OD1-CG-OD2	-7.71	108.65	123.30
1	B	101	GLU	OE1-CD-OE2	-7.42	114.39	123.30
1	B	80	ASP	CB-CG-OD2	7.12	124.70	118.30
1	B	21	GLU	CB-CA-C	-7.05	96.29	110.40
1	B	45	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	A	30	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	99	ASP	CB-CG-OD2	6.79	124.42	118.30
1	B	99	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	15	TRP	CD1-CG-CD2	6.53	111.53	106.30
1	B	71	LEU	CB-CG-CD1	-6.49	99.97	111.00
1	A	79	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	30	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	118	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	B	6	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	B	94	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	15	TRP	CE2-CD2-CG	-6.12	102.41	107.30
1	B	112	THR	CA-CB-CG2	-5.89	104.15	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ARG	NH1-CZ-NH2	5.88	125.86	119.40
1	B	20	VAL	CA-C-N	5.78	129.91	117.20
1	B	125	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	B	145	TYR	CZ-CE2-CD2	5.73	124.96	119.80
1	A	122	PHE	CD1-CE1-CZ	-5.66	113.31	120.10
1	A	117	HIS	CG-CD2-NE2	-5.64	98.48	109.20
1	B	37	TRP	CG-CD2-CE3	-5.48	128.96	133.90
1	B	101	GLU	CG-CD-OE1	5.47	129.24	118.30
1	B	82	LYS	CD-CE-NZ	-5.44	99.20	111.70
1	A	26	GLU	OE1-CD-OE2	5.41	129.80	123.30
1	A	15	TRP	CD1-CG-CD2	5.40	110.62	106.30
1	A	145	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	B	30	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	20	VAL	CA-C-O	-5.31	108.95	120.10
1	A	43	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	B	35	TYR	CZ-CE2-CD2	-5.15	115.17	119.80
1	B	21	GLU	N-CA-CB	5.14	119.86	110.60
1	A	15	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	B	87	GLN	CG-CD-OE1	-5.08	111.44	121.60
1	A	101	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	B	35	TYR	CG-CD2-CE2	5.07	125.36	121.30
1	B	37	TRP	CE2-CD2-CG	5.04	111.33	107.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	VAL	Mainchain

## 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	1131	0	1126	10	0
1	B	1131	0	1127	21	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	134	0	0	2	1
4	B	108	0	0	6	0
All	All	2596	0	2313	29	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 6.

All (29) 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:82:LYS:CD	1:B:82:LYS:CE	1.76	1.57
1:B:82:LYS:NZ	1:B:82:LYS:CD	2.43	0.79
1:B:131:GLN:HG3	4:B:277:HOH:O	1.91	0.71
1:B:20:VAL:HG13	1:B:68:LEU:HB3	1.77	0.65
1:B:106:LEU:HD23	1:B:106:LEU:O	2.01	0.61
1:B:106:LEU:HD23	1:B:106:LEU:C	2.23	0.59
1:A:30:ARG:HD3	1:B:127:GLN:OE1	2.03	0.57
1:A:22:ASP:O	1:A:26:GLU:HG3	2.06	0.56
1:B:82:LYS:CG	1:B:82:LYS:CE	2.77	0.55
1:A:100:PRO:HG3	1:A:145:TYR:CD2	2.42	0.54
1:B:131:GLN:NE2	4:B:277:HOH:O	2.35	0.52
1:A:45:PHE:HA	1:A:59:LYS:HD3	1.91	0.51
1:A:26:GLU:OE1	1:A:117:HIS:NE2	2.44	0.51
1:B:99:ASP:OD2	1:B:99:ASP:N	2.45	0.48
1:B:117:HIS:HB2	4:B:433:HOH:O	2.14	0.47
1:B:131:GLN:CG	4:B:277:HOH:O	2.54	0.45
1:A:91:LEU:HD12	1:A:95:LYS:HD3	1.98	0.45
1:A:125:GLU:HG3	1:B:51:ALA:CB	2.47	0.44
1:B:108:ASN:ND2	4:B:439:HOH:O	2.50	0.44
1:A:21:GLU:OE2	1:A:65:LYS:HE3	2.17	0.43
1:B:24:GLY:N	1:B:68:LEU:HD22	2.34	0.42
1:B:24:GLY:CA	1:B:68:LEU:HD22	2.49	0.42
1:B:99:ASP:HA	1:B:100:PRO:HD3	1.89	0.42
1:A:26:GLU:HG2	4:A:394:HOH:O	2.20	0.41
1:A:58:PRO:HD2	4:A:404:HOH:O	2.21	0.41
1:B:141:LEU:HD11	3:B:147:HEM:CAB	2.51	0.41
1:B:14:LEU:HD11	1:B:118:PHE:CG	2.56	0.41
1:B:104:LYS:HG3	4:B:371:HOH:O	2.20	0.41
1:B:141:LEU:CD1	3:B:147:HEM:HAB	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:A:244:HOH:O	4:A:244:HOH:O[2_545]	0.30	1.90

## 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	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
All	All	288/292 (99%)	285 (99%)	3 (1%)	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	122/122 (100%)	121 (99%)	1 (1%)	81	76
1	B	122/122 (100%)	118 (97%)	4 (3%)	38	21
All	All	244/244 (100%)	239 (98%)	5 (2%)	55	40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	B	52	SER
1	B	87	GLN
1	B	99	ASP
1	B	120	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	B	39	GLN
1	B	77	HIS
1	B	87	GLN
1	B	97	HIS
1	B	108	ASN
1	B	117	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AZI	B	148	3	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	A	148	3	0,2,2	0.00	-	0,1,1	0.00	-
3	HEM	A	147	1,2	27,50,50	2.78	10 (37%)	17,82,82	1.84	5 (29%)
3	HEM	B	147	1,2	27,50,50	3.01	14 (51%)	17,82,82	1.94	6 (35%)

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	HEM	A	147	1,2	-	0/6/54/54	-
3	HEM	B	147	1,2	-	0/6/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	147	HEM	C3B-C2B	-7.08	1.30	1.40
3	B	147	HEM	CMA-C3A	6.81	1.65	1.51
3	B	147	HEM	C1D-ND	6.67	1.49	1.36
3	A	147	HEM	C4D-C3D	5.62	1.55	1.42
3	A	147	HEM	CMA-C3A	5.05	1.62	1.51
3	B	147	HEM	C1D-CHD	-4.91	1.27	1.41
3	B	147	HEM	C3B-C2B	-4.47	1.34	1.40
3	A	147	HEM	C3B-CAB	4.13	1.56	1.47
3	A	147	HEM	C1C-C2C	4.04	1.51	1.42
3	A	147	HEM	CMB-C2B	3.97	1.61	1.51
3	B	147	HEM	C4D-C3D	3.95	1.51	1.42
3	B	147	HEM	C3C-C2C	-3.81	1.35	1.40
3	A	147	HEM	CBB-CAB	3.74	1.54	1.29
3	B	147	HEM	C3C-CAC	3.72	1.55	1.47
3	B	147	HEM	C1C-C2C	3.60	1.50	1.42
3	B	147	HEM	CBB-CAB	3.01	1.49	1.29
3	A	147	HEM	C3C-C2C	-2.85	1.36	1.40
3	B	147	HEM	CBC-CAC	2.84	1.48	1.29
3	B	147	HEM	CAA-C2A	2.82	1.56	1.52
3	A	147	HEM	CBC-CAC	2.70	1.47	1.29
3	B	147	HEM	C3B-CAB	2.66	1.53	1.47
3	B	147	HEM	C4A-NA	2.53	1.41	1.36
3	B	147	HEM	CMB-C2B	2.27	1.57	1.51
3	A	147	HEM	C1A-NA	2.26	1.40	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	147	HEM	C4A-C3A-C2A	3.94	109.73	107.00
3	B	147	HEM	CBD-CAD-C3D	-3.93	105.23	112.48
3	A	147	HEM	C1D-C2D-C3D	-3.90	104.29	107.00
3	B	147	HEM	C4C-C3C-C2C	3.54	109.37	106.90
3	B	147	HEM	CMC-C2C-C3C	3.02	130.33	124.68
3	A	147	HEM	CBD-CAD-C3D	-2.66	107.58	112.48
3	B	147	HEM	C3B-C4B-NB	2.51	112.46	109.21
3	A	147	HEM	CAA-CBA-CGA	-2.47	108.53	112.67
3	A	147	HEM	CMC-C2C-C3C	2.20	128.80	124.68
3	B	147	HEM	CAA-CBA-CGA	-2.12	109.11	112.67
3	B	147	HEM	CMB-C2B-C3B	2.12	128.64	124.68

There are no chirality outliers.

There are no torsion outliers.

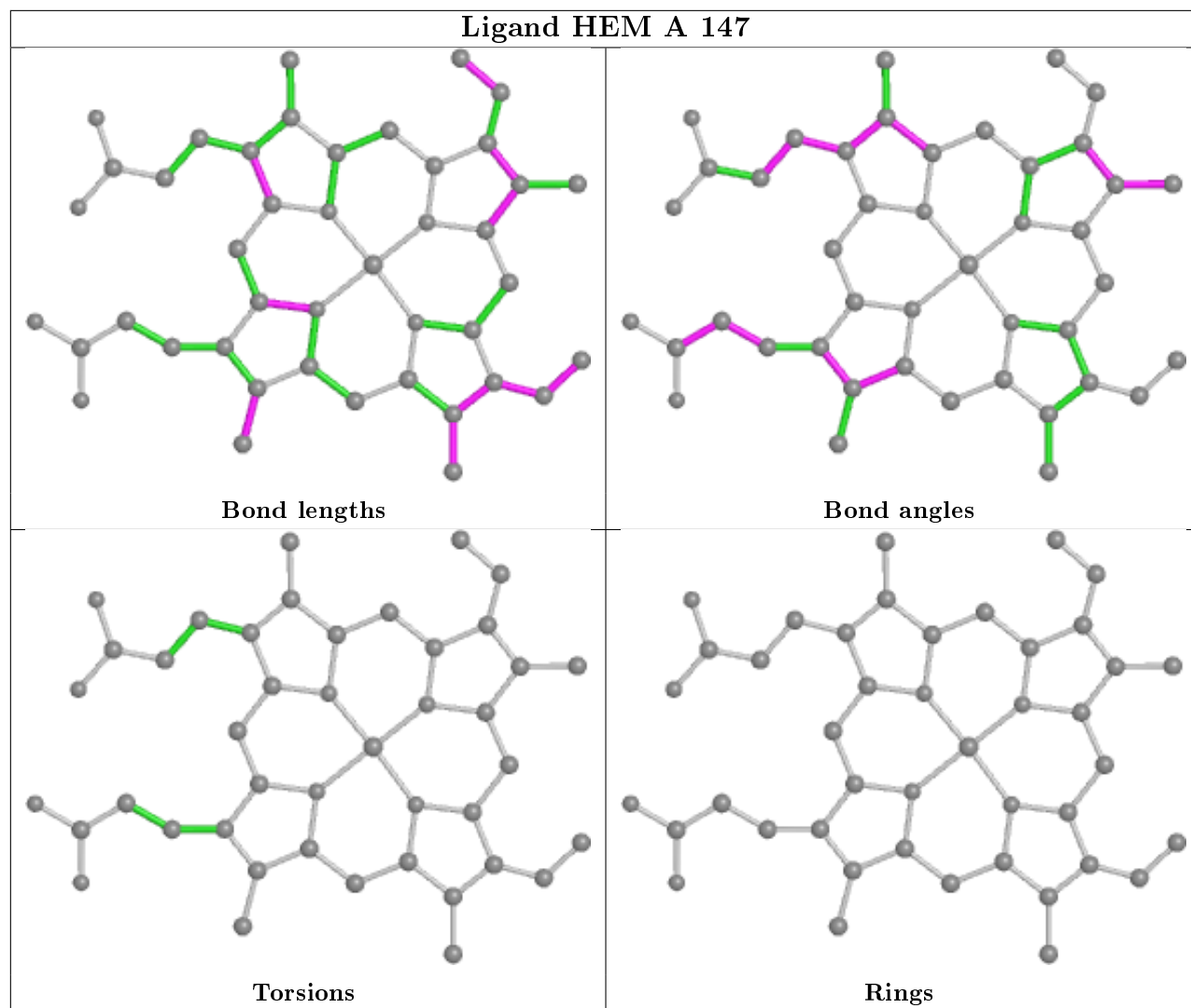
There are no ring outliers.

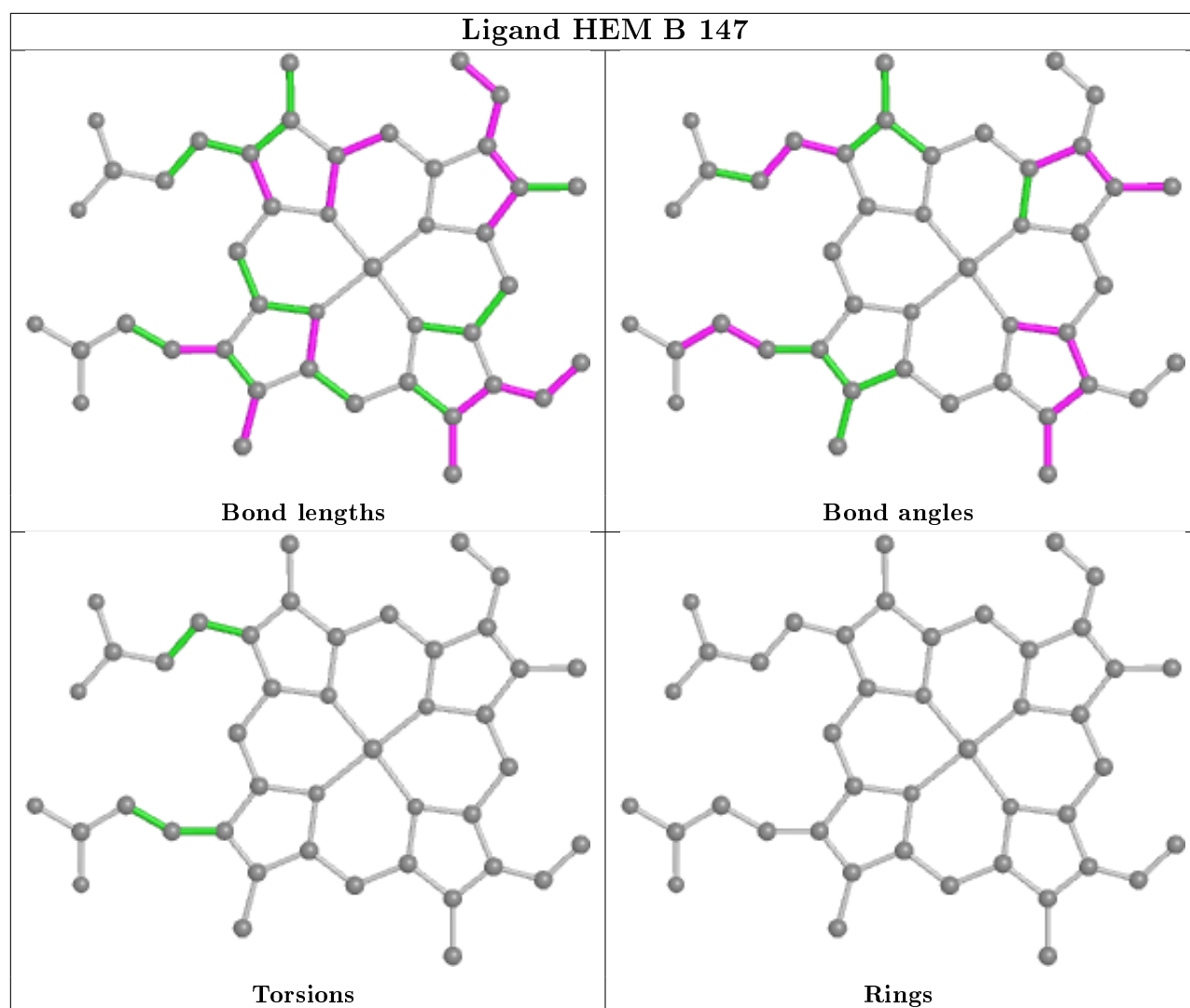
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	143:SER	C	144:ARG	N	1.19
1	A	17:LYS	C	18:VAL	N	1.18
1	B	20:VAL	C	21:GLU	N	1.09

## 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	146/146 (100%)	-0.24	0 100 100	9, 14, 20, 25	12 (8%)
1	B	146/146 (100%)	-0.14	1 (0%) 87 88	10, 16, 23, 29	16 (10%)
All	All	292/292 (100%)	-0.19	1 (0%) 94 93	9, 15, 22, 29	28 (9%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ASP	2.6

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

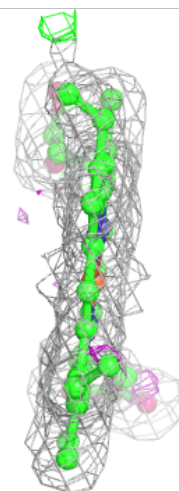
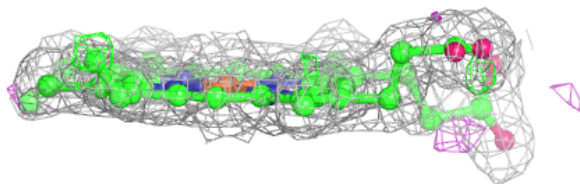
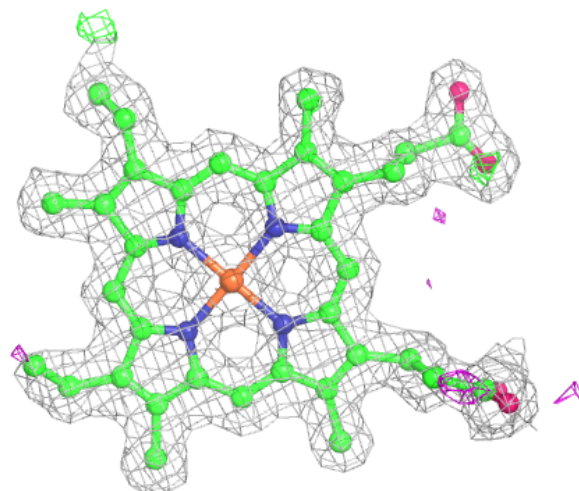
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

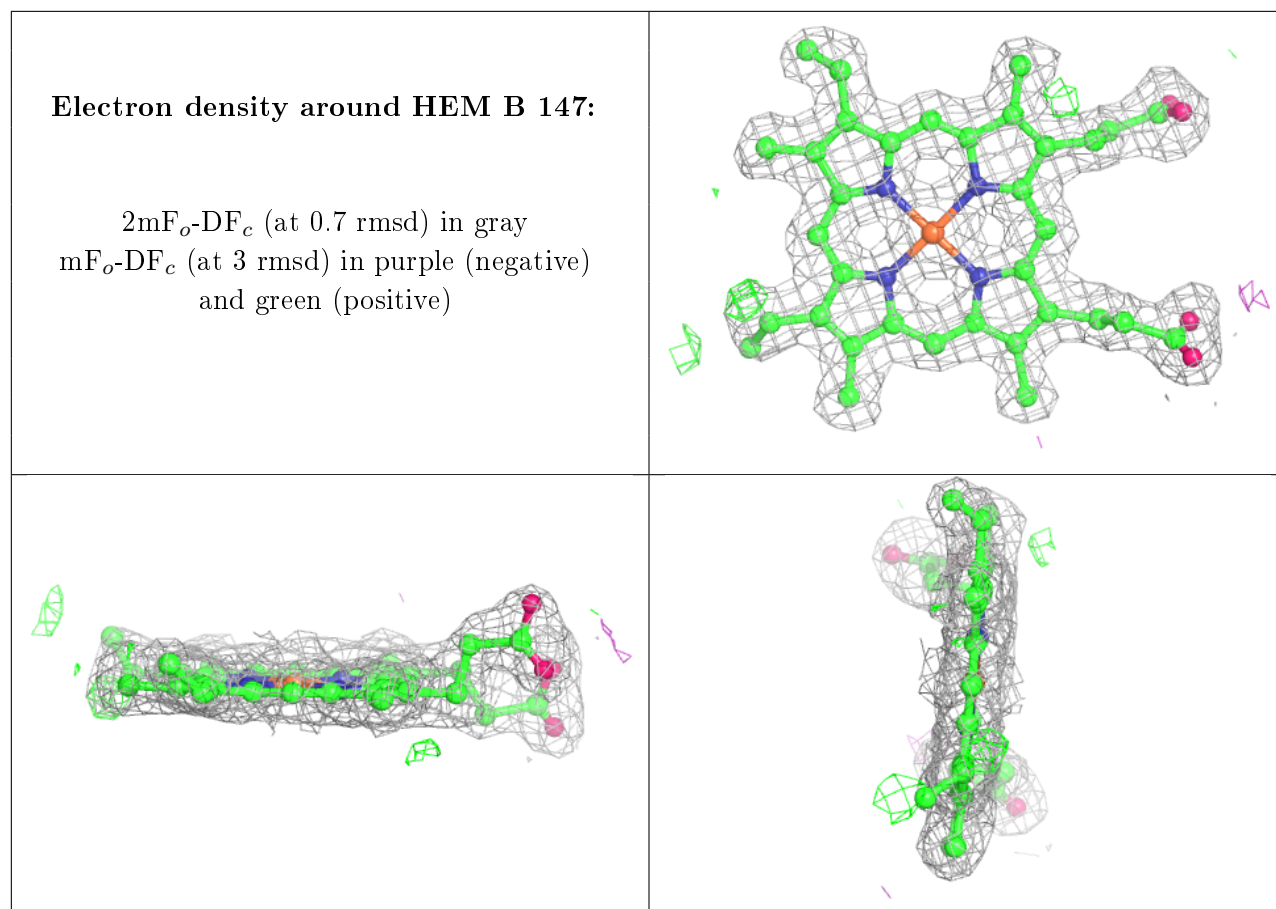
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HEM	A	147	43/43	0.96	0.12	8,12,18,21	2
3	HEM	B	147	43/43	0.96	0.11	10,14,24,31	1
2	AZI	B	148	3/3	0.98	0.09	14,14,14,15	0
2	AZI	A	148	3/3	0.98	0.09	13,13,15,17	0

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 HEM A 147:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.