



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 04:48 AM EDT

PDB ID : 3E5K  
Title : Crystal structure of CYP105P1 wild-type 4-phenylimidazole complex  
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Deposited on : 2008-08-14  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.23.2  
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

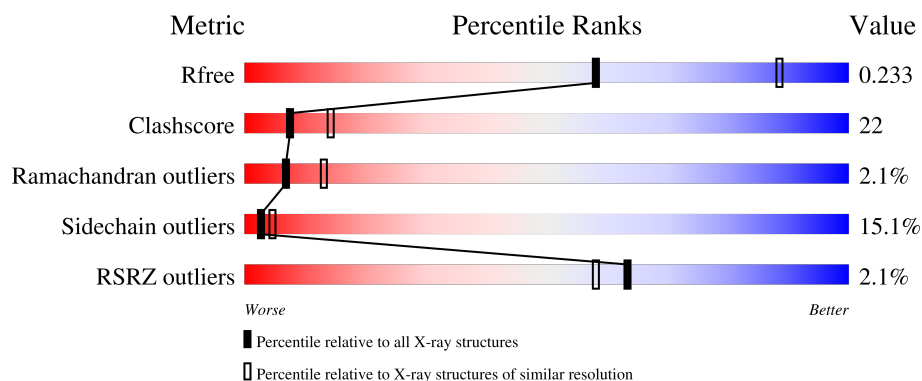
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	403	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3148 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.

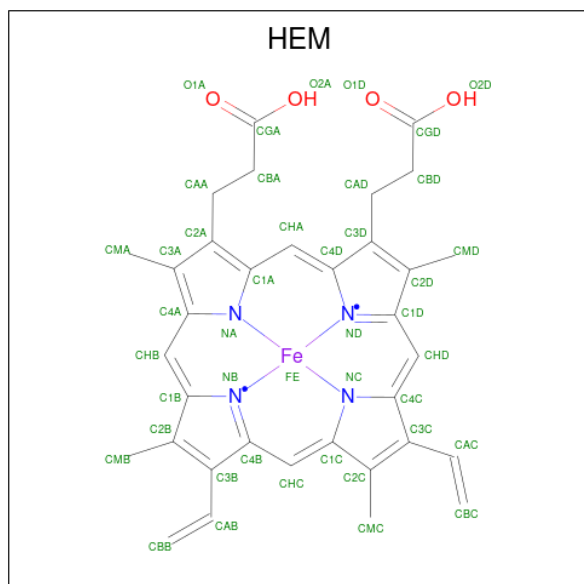
- Molecule 1 is a protein called Cytochrome P450 (Cytochrome P450 hydroxylase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2967	1876	532	548	11	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

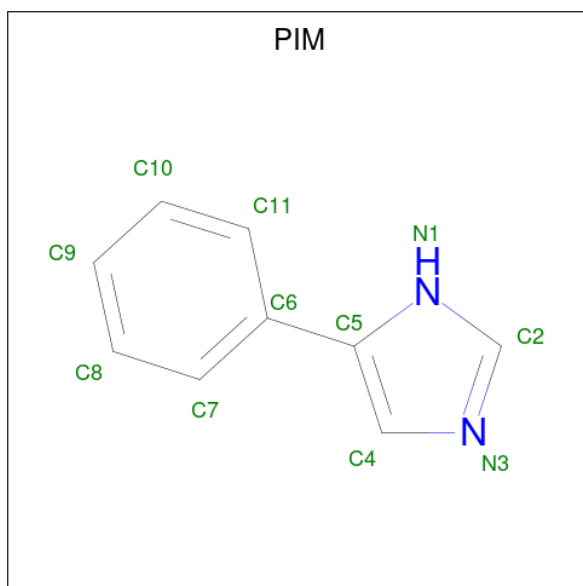
Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ILE	MET	engineered mutation	UNP Q93H81
A	400	HIS	-	expression tag	UNP Q93H81
A	401	HIS	-	expression tag	UNP Q93H81
A	402	HIS	-	expression tag	UNP Q93H81
A	403	HIS	-	expression tag	UNP Q93H81

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



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

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (three-letter code: PIM) (formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N		
			11	9	2		
						0	0

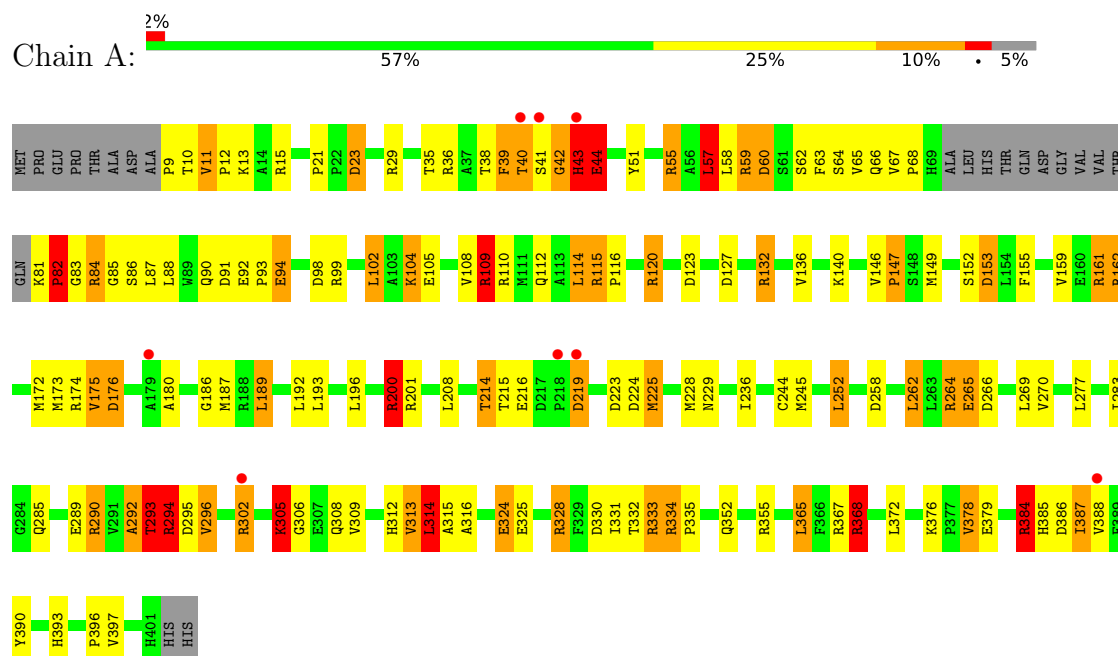
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O		
			127	127		
					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 P450 (Cytochrome P450 hydroxylase)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.72Å 143.72Å 70.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.52 – 2.60 34.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.52-2.60) 100.0 (34.52-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.236 0.172 , 0.233	Depositor DCC
$R_{free}$ test set	1331 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: HEM, PIM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	1/3029 (0.0%)	1.90	84/4115 (2.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	CYS	CB-SG	5.61	1.91	1.82

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ARG	NE-CZ-NH2	-18.73	110.93	120.30
1	A	55	ARG	NE-CZ-NH1	-15.05	112.77	120.30
1	A	333	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	A	264	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	A	15	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	A	245	MET	CG-SD-CE	-11.36	82.02	100.20
1	A	252	LEU	CB-CG-CD2	11.32	130.24	111.00
1	A	99	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	A	265	GLU	OE1-CD-OE2	10.55	135.96	123.30
1	A	270	VAL	CG1-CB-CG2	-9.55	95.61	110.90
1	A	94	GLU	OE1-CD-OE2	9.22	134.37	123.30
1	A	330	ASP	CB-CG-OD2	-9.21	110.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	CB-CG-CD1	9.15	126.55	111.00
1	A	290	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	A	120	ARG	NE-CZ-NH2	8.99	124.79	120.30
1	A	115	ARG	NE-CZ-NH2	8.74	124.67	120.30
1	A	365	LEU	CB-CA-C	-8.66	93.75	110.20
1	A	265	GLU	CG-CD-OE1	-8.65	101.01	118.30
1	A	115	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	A	127	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	A	84	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	200	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	368	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	60	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	384	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	98	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	330	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	29	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	367	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	A	161	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	A	15	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	314	LEU	CB-CG-CD2	6.81	122.58	111.00
1	A	244	CYS	CA-CB-SG	-6.66	102.01	114.00
1	A	68	PRO	N-CA-C	6.65	129.38	112.10
1	A	120	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	109	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	334	ARG	CB-CG-CD	-6.29	95.26	111.60
1	A	55	ARG	NH1-CZ-NH2	6.21	126.24	119.40
1	A	102	LEU	CB-CG-CD2	6.19	121.52	111.00
1	A	378	VAL	CB-CA-C	-6.18	99.66	111.40
1	A	379	GLU	OE1-CD-OE2	-6.17	115.90	123.30
1	A	368	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	333	ARG	CG-CD-NE	-6.00	99.19	111.80
1	A	58	LEU	CA-CB-CG	-5.92	101.69	115.30
1	A	264	ARG	CG-CD-NE	-5.87	99.47	111.80
1	A	252	LEU	CB-CA-C	-5.86	99.08	110.20
1	A	57	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	A	258	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	397	VAL	CA-CB-CG1	-5.78	102.24	110.90
1	A	265	GLU	CA-CB-CG	-5.76	100.73	113.40
1	A	189	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	A	264	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	293	THR	N-CA-C	5.70	126.39	111.00
1	A	378	VAL	CG1-CB-CG2	5.63	119.92	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	THR	OG1-CB-CG2	-5.59	97.15	110.00
1	A	200	ARG	NH1-CZ-NH2	-5.57	113.28	119.40
1	A	94	GLU	CG-CD-OE2	-5.53	107.25	118.30
1	A	334	ARG	CD-NE-CZ	-5.48	115.92	123.60
1	A	153	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	334	ARG	CB-CA-C	-5.47	99.46	110.40
1	A	98	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	305	LYS	CA-C-N	5.45	127.10	116.20
1	A	214	THR	CB-CA-C	-5.41	96.98	111.60
1	A	94	GLU	CB-CA-C	-5.38	99.64	110.40
1	A	333	ARG	CB-CG-CD	5.37	125.56	111.60
1	A	108	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	A	192	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	175	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	A	67	VAL	CB-CA-C	5.30	121.47	111.40
1	A	115	ARG	CB-CA-C	-5.27	99.86	110.40
1	A	155	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	A	228	MET	CG-SD-CE	5.23	108.57	100.20
1	A	13	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	236	ILE	CB-CA-C	-5.22	101.16	111.60
1	A	266	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	114	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	91	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	269	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	302	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	39	PHE	N-CA-C	5.08	124.73	111.00
1	A	162	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	332	THR	CA-CB-CG2	5.05	119.46	112.40
1	A	372	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	A	109	ARG	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ALA	Peptide
1	A	43	HIS	Peptide

## 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	2967	0	2956	125	0
2	A	43	0	30	8	0
3	A	11	0	8	2	0
4	A	127	0	0	7	0
All	All	3148	0	2994	133	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 22.

All (133) 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:42:GLY:HA2	1:A:43:HIS:HB2	1.25	1.15
2:A:1408:HEM:HBB2	2:A:1408:HEM:HHC	1.12	1.11
1:A:84:ARG:HH21	1:A:94:GLU:HG2	1.12	1.10
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.22	1.03
1:A:294:ARG:H	1:A:305:LYS:HB2	1.27	0.98
1:A:87:LEU:H	1:A:90:GLN:HE21	1.10	0.97
1:A:82:PRO:CB	1:A:83:GLY:HA2	1.94	0.97
1:A:214:THR:O	1:A:214:THR:HG22	1.66	0.93
1:A:84:ARG:NH2	1:A:94:GLU:HG2	1.82	0.93
2:A:1408:HEM:HBB2	2:A:1408:HEM:CHC	1.74	0.93
1:A:42:GLY:HA2	1:A:43:HIS:CB	1.98	0.91
1:A:84:ARG:HH21	1:A:94:GLU:CG	1.84	0.91
1:A:294:ARG:HG3	1:A:295:ASP:N	1.86	0.89
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.37	0.89
1:A:62:SER:O	1:A:293:THR:HB	1.74	0.87
1:A:293:THR:O	1:A:294:ARG:HB3	1.74	0.87
1:A:328:ARG:HG2	1:A:328:ARG:NH1	1.89	0.86
1:A:289:GLU:OE1	1:A:308:GLN:NE2	2.08	0.86
1:A:214:THR:O	1:A:214:THR:CG2	2.26	0.83
1:A:384:ARG:HG3	1:A:384:ARG:NH1	1.89	0.83
1:A:104:LYS:HE2	4:A:1485:HOH:O	1.80	0.82
1:A:82:PRO:HB2	1:A:83:GLY:HA2	1.61	0.80
1:A:42:GLY:CA	1:A:43:HIS:O	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:HA3	1:A:43:HIS:O	1.82	0.78
1:A:196:LEU:HG	1:A:200:ARG:NH1	2.03	0.74
1:A:292:ALA:O	1:A:306:GLY:HA2	1.88	0.73
1:A:294:ARG:N	1:A:305:LYS:HB2	2.03	0.73
1:A:289:GLU:CD	1:A:308:GLN:HE21	1.92	0.72
1:A:324:GLU:O	1:A:333:ARG:NH2	2.23	0.70
1:A:115:ARG:HB2	1:A:116:PRO:HD3	1.73	0.69
1:A:57:LEU:C	1:A:57:LEU:HD23	2.14	0.68
1:A:293:THR:O	1:A:294:ARG:CB	2.42	0.67
1:A:312:HIS:HD2	1:A:315:ALA:H	1.43	0.66
1:A:196:LEU:HG	1:A:200:ARG:HH12	1.59	0.65
1:A:196:LEU:CG	1:A:200:ARG:HH12	2.10	0.65
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.06	0.64
1:A:159:VAL:HG22	1:A:162:ARG:HH21	1.64	0.63
1:A:23:ASP:OD1	1:A:23:ASP:N	2.27	0.63
1:A:325:GLU:HB3	1:A:328:ARG:HD3	1.81	0.62
1:A:196:LEU:CG	1:A:200:ARG:NH1	2.62	0.62
1:A:82:PRO:HB3	1:A:83:GLY:HA2	1.80	0.62
1:A:293:THR:O	1:A:293:THR:HG22	1.99	0.62
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.06	0.62
1:A:289:GLU:CD	1:A:308:GLN:NE2	2.50	0.61
1:A:42:GLY:HA2	1:A:43:HIS:O	1.99	0.61
1:A:115:ARG:HH11	1:A:115:ARG:HG3	1.67	0.60
1:A:293:THR:O	1:A:293:THR:CG2	2.50	0.59
2:A:1408:HEM:CMC	2:A:1408:HEM:HBC2	2.32	0.58
1:A:87:LEU:H	1:A:90:GLN:NE2	1.93	0.57
1:A:172:MET:HE3	1:A:186:GLY:HA2	1.87	0.56
1:A:9:PRO:N	1:A:38:THR:HG1	2.02	0.56
1:A:84:ARG:HH21	1:A:94:GLU:CB	2.17	0.56
1:A:87:LEU:N	1:A:90:GLN:HE21	1.91	0.55
1:A:386:ASP:HB2	1:A:387:ILE:HG13	1.89	0.55
1:A:51:TYR:HA	1:A:316:ALA:HB1	1.88	0.54
1:A:176:ASP:OD1	1:A:176:ASP:N	2.41	0.54
1:A:294:ARG:N	1:A:305:LYS:HD2	2.23	0.53
1:A:55:ARG:O	1:A:59:ARG:HB2	2.08	0.53
1:A:105:GLU:HA	1:A:105:GLU:OE1	2.09	0.52
1:A:82:PRO:CB	1:A:83:GLY:CA	2.79	0.52
2:A:1408:HEM:HBC2	2:A:1408:HEM:HMC1	1.92	0.52
1:A:85:GLY:H	1:A:90:GLN:HE22	1.58	0.52
1:A:219:ASP:N	1:A:219:ASP:OD1	2.43	0.52
1:A:115:ARG:HG3	1:A:115:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:O	1:A:11:VAL:CG2	2.59	0.51
1:A:112:GLN:HE21	1:A:115:ARG:HH12	1.59	0.50
1:A:86:SER:O	1:A:87:LEU:HB2	2.11	0.49
1:A:159:VAL:HA	1:A:162:ARG:HE	1.76	0.49
1:A:285:GLN:HB2	4:A:1469:HOH:O	2.12	0.49
1:A:387:ILE:HD12	1:A:388:VAL:HG23	1.94	0.49
1:A:60:ASP:OD1	1:A:60:ASP:C	2.51	0.49
1:A:305:LYS:O	1:A:305:LYS:HG3	2.11	0.49
1:A:196:LEU:HD21	1:A:200:ARG:HH11	1.78	0.48
1:A:294:ARG:C	1:A:305:LYS:HB3	2.34	0.48
1:A:196:LEU:HD21	1:A:200:ARG:NH1	2.27	0.48
1:A:295:ASP:O	1:A:296:VAL:HG13	2.14	0.48
1:A:63:PHE:HB3	1:A:290:ARG:HB3	1.95	0.48
1:A:201:ARG:HG2	4:A:1503:HOH:O	2.12	0.48
1:A:149:MET:O	1:A:149:MET:HG3	2.14	0.47
1:A:57:LEU:C	1:A:57:LEU:CD2	2.83	0.47
1:A:196:LEU:CD2	1:A:200:ARG:NH1	2.77	0.47
1:A:115:ARG:NH1	1:A:115:ARG:CG	2.77	0.47
1:A:43:HIS:HA	1:A:44:GLU:HB2	1.95	0.47
1:A:292:ALA:HB1	1:A:294:ARG:O	2.16	0.46
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.59	0.46
1:A:84:ARG:HH21	1:A:94:GLU:HB3	1.80	0.46
1:A:57:LEU:HD11	1:A:309:VAL:HG12	1.98	0.45
1:A:208:LEU:O	1:A:208:LEU:HG	2.16	0.45
1:A:39:PHE:HB3	1:A:40:THR:H	1.43	0.45
1:A:109:ARG:O	1:A:110:ARG:C	2.52	0.45
1:A:387:ILE:HG13	1:A:387:ILE:H	1.21	0.45
2:A:1408:HEM:NB	3:A:501:PIM:H2	2.31	0.45
1:A:393:HIS:HB3	4:A:1512:HOH:O	2.16	0.44
1:A:334:ARG:HH11	1:A:334:ARG:HD2	1.50	0.44
2:A:1408:HEM:HMC1	2:A:1408:HEM:CBC	2.47	0.44
1:A:86:SER:HB3	1:A:229:ASN:HB3	2.00	0.44
1:A:149:MET:SD	1:A:162:ARG:HD3	2.57	0.44
1:A:335:PRO:HA	4:A:1489:HOH:O	2.17	0.44
1:A:390:TYR:C	1:A:390:TYR:CD2	2.85	0.44
1:A:173:MET:HE2	1:A:173:MET:HB3	1.67	0.44
1:A:283:ILE:HG12	1:A:314:LEU:HG	2.00	0.44
1:A:120:ARG:NH1	1:A:153:ASP:OD2	2.52	0.43
1:A:385:HIS:ND1	1:A:390:TYR:CE2	2.84	0.43
1:A:115:ARG:HH11	1:A:115:ARG:CG	2.28	0.43
1:A:223:ASP:O	1:A:224:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:HIS:HD1	1:A:390:TYR:HE2	1.64	0.42
1:A:136:VAL:O	1:A:396:PRO:HA	2.19	0.42
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.64	0.42
1:A:223:ASP:O	1:A:225:MET:N	2.52	0.42
1:A:331:ILE:HD13	1:A:331:ILE:HG21	1.86	0.42
1:A:86:SER:O	1:A:88:LEU:N	2.46	0.42
2:A:1408:HEM:CMC	2:A:1408:HEM:CBC	2.97	0.42
1:A:355:ARG:HH11	1:A:355:ARG:HD2	1.66	0.42
2:A:1408:HEM:C4B	3:A:501:PIM:H2	2.55	0.42
1:A:313:VAL:O	1:A:314:LEU:C	2.57	0.42
1:A:385:HIS:ND1	1:A:390:TYR:HE2	2.17	0.42
1:A:146:VAL:HB	1:A:147:PRO:HD3	2.00	0.42
1:A:123:ASP:HA	1:A:368:ARG:HH21	1.84	0.41
1:A:57:LEU:HD11	1:A:309:VAL:CG1	2.50	0.41
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.87	0.41
1:A:376:LYS:HD2	1:A:376:LYS:HA	1.66	0.41
1:A:65:VAL:HG12	1:A:290:ARG:HD2	2.02	0.41
1:A:384:ARG:CD	1:A:386:ASP:OD2	2.68	0.41
1:A:59:ARG:HD2	1:A:59:ARG:HA	1.02	0.41
1:A:115:ARG:HB2	1:A:116:PRO:CD	2.47	0.41
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.86	0.41
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.36	0.40
1:A:21:PRO:HD3	4:A:1467:HOH:O	2.20	0.40
1:A:92:GLU:HB2	1:A:93:PRO:HA	2.03	0.40
1:A:264:ARG:CD	4:A:1470:HOH:O	2.69	0.40
1:A:64:SER:O	1:A:290:ARG:HA	2.22	0.40
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.92	0.40
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.82	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	378/403 (94%)	352 (93%)	18 (5%)	8 (2%)	7	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	44	GLU
1	A	82	PRO
1	A	294	ARG
1	A	43	HIS
1	A	293	THR
1	A	180	ALA
1	A	132	ARG

### 5.3.2 Protein sidechains ⓘ

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	311/328 (95%)	264 (85%)	47 (15%)	3	4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	11	VAL
1	A	23	ASP
1	A	35	THR
1	A	36	ARG
1	A	40	THR
1	A	41	SER
1	A	44	GLU
1	A	57	LEU
1	A	59	ARG
1	A	66	GLN
1	A	81	LYS
1	A	82	PRO

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	104	LYS
1	A	109	ARG
1	A	114	LEU
1	A	132	ARG
1	A	140	LYS
1	A	147	PRO
1	A	152	SER
1	A	174	ARG
1	A	175	VAL
1	A	176	ASP
1	A	187	MET
1	A	189	LEU
1	A	200	ARG
1	A	215	THR
1	A	216	GLU
1	A	219	ASP
1	A	225	MET
1	A	252	LEU
1	A	265	GLU
1	A	294	ARG
1	A	296	VAL
1	A	302	ARG
1	A	305	LYS
1	A	313	VAL
1	A	314	LEU
1	A	324	GLU
1	A	328	ARG
1	A	352	GLN
1	A	365	LEU
1	A	368	ARG
1	A	378	VAL
1	A	384	ARG
1	A	387	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	90	GLN
1	A	112	GLN
1	A	119	GLN

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	195	GLN
1	A	272	ASN
1	A	308	GLN
1	A	312	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 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PIM	A	501	2	10,12,12	1.97	2 (20%)	11,15,15	0.84	0
2	HEM	A	1408	3,1	27,50,50	2.06	6 (22%)	17,82,82	2.76	9 (52%)

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	PIM	A	501	2	-	0/4/4/4	0/2/2/2
2	HEM	A	1408	3,1	-	0/6/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PIM	C6-C5	-5.53	1.40	1.48
2	A	1408	HEM	C3D-C2D	5.14	1.52	1.37
2	A	1408	HEM	C3B-C2B	-4.75	1.33	1.40
2	A	1408	HEM	C3C-C2C	-4.38	1.34	1.40
2	A	1408	HEM	C3C-CAC	2.65	1.53	1.47
2	A	1408	HEM	C3B-CAB	2.43	1.52	1.47
2	A	1408	HEM	CMB-C2B	2.14	1.56	1.51
3	A	501	PIM	C4-C5	-2.04	1.34	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1408	HEM	CBD-CAD-C3D	-5.53	102.28	112.48
2	A	1408	HEM	CMA-C3A-C4A	-4.08	122.19	128.46
2	A	1408	HEM	C4C-C3C-C2C	4.01	109.70	106.90
2	A	1408	HEM	CMA-C3A-C2A	3.91	132.32	124.94
2	A	1408	HEM	CAA-CBA-CGA	-3.77	106.34	112.67
2	A	1408	HEM	C4A-C3A-C2A	-2.69	105.12	107.00
2	A	1408	HEM	C3B-C4B-NB	-2.46	106.04	109.21
2	A	1408	HEM	CAD-CBD-CGD	-2.44	108.58	112.67
2	A	1408	HEM	C1D-C2D-C3D	-2.09	105.54	107.00

There are no chirality outliers.

There are no torsion outliers.

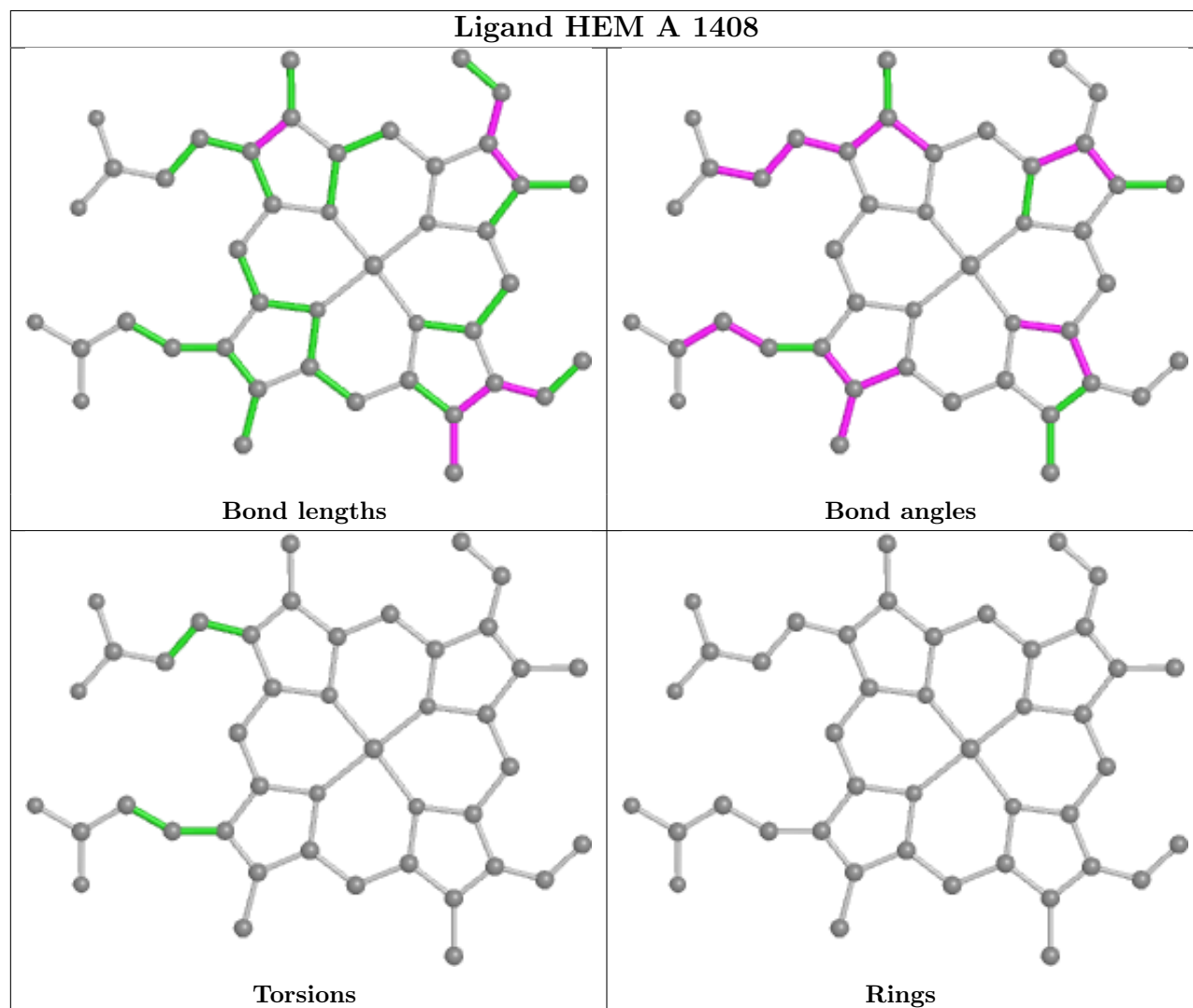
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PIM	2	0
2	A	1408	HEM	8	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	382/403 (94%)	-0.49	8 (2%) 63 58	21, 37, 61, 86	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	THR	3.2
1	A	43	HIS	3.1
1	A	218	PRO	2.9
1	A	219	ASP	2.9
1	A	302	ARG	2.9
1	A	41	SER	2.5
1	A	179	ALA	2.3
1	A	388	VAL	2.1

### 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](#)

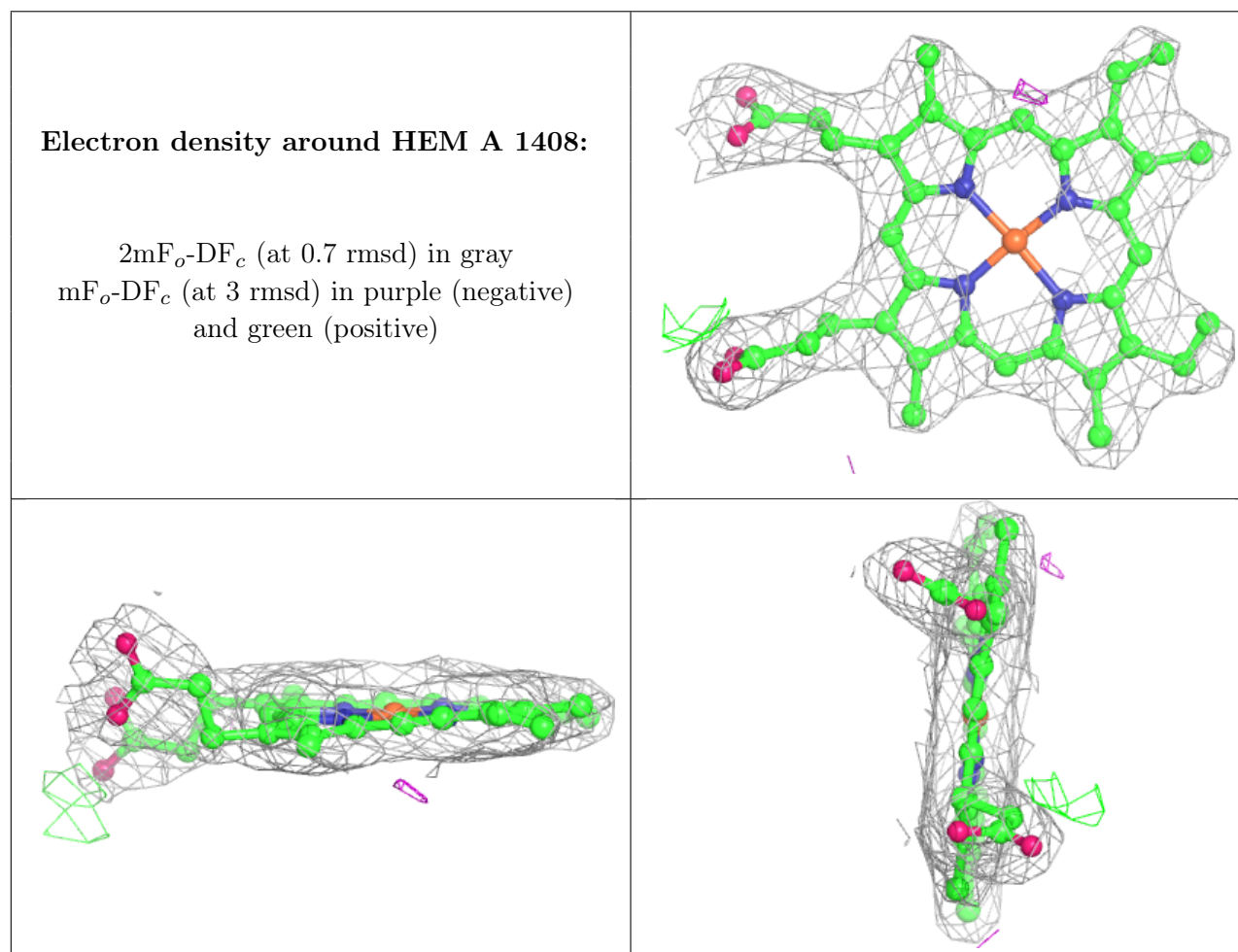
There are no monosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	1408	43/43	0.99	0.15	24,35,45,53	0
3	PIM	A	501	11/11	0.99	0.15	38,44,47,49	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.