



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:06 AM UTC

PDB ID : 3E5K / pdb_00003e5k
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (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

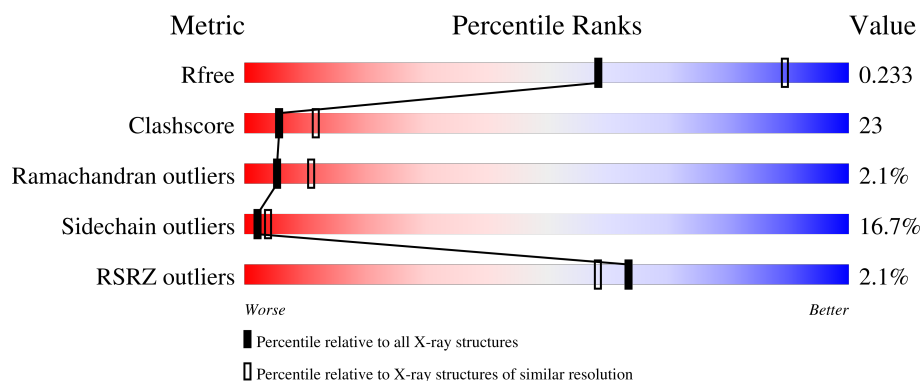
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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:

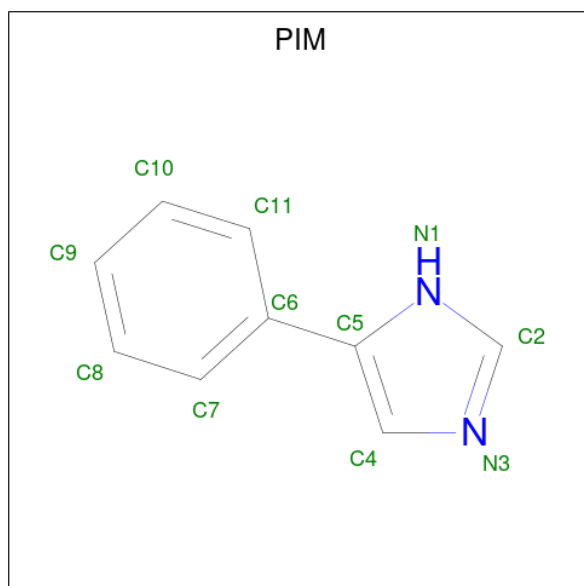
Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ILE	MET	engineered mutation	UNP Q93H81
A	400	HIS	-	expression tag	UNP Q93H81
A	401	HIS	-	expression tag	UNP Q93H81
A	402	HIS	-	expression tag	UNP Q93H81
A	403	HIS	-	expression tag	UNP Q93H81

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 (CCD ID: PIM) (formula: $C_9H_8N_2$).



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

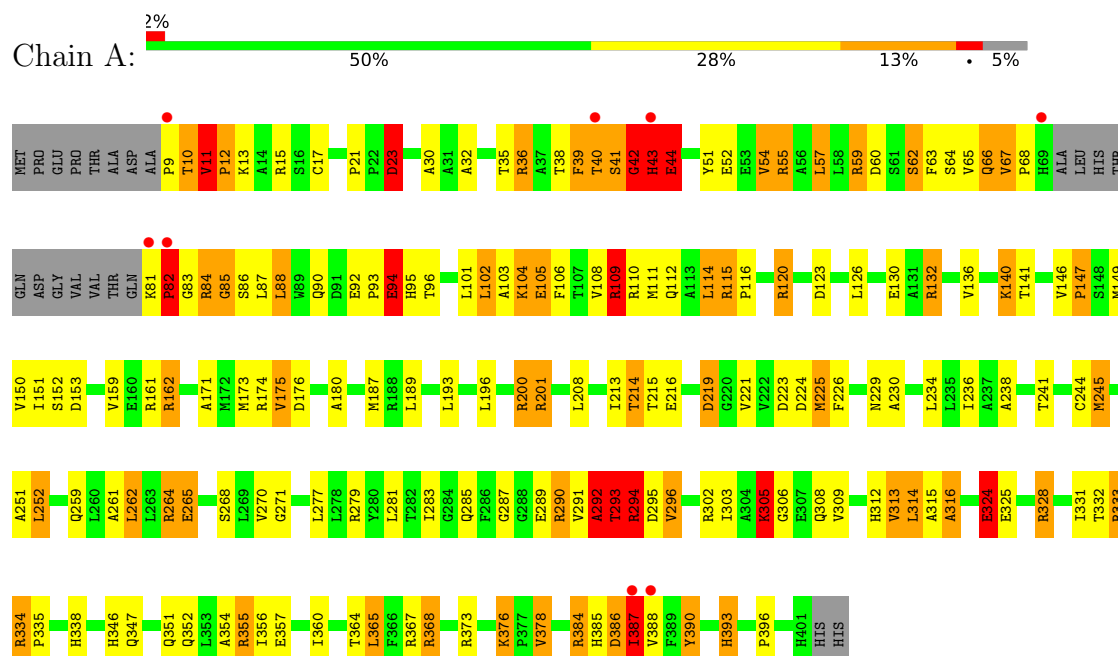
- Molecule 4 is water.

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, α , β , γ	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) 99.9 (34.52-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	49.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3148	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PIM, 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	0.89	0/3029	2.25	159/4115 (3.9%)

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

There are no bond length outliers.

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	N-CA-C	-10.70	99.33	111.00
1	A	365	LEU	CB-CA-C	-10.66	93.75	110.81
1	A	68	PRO	N-CA-C	10.49	129.38	113.75
1	A	41	SER	N-CA-C	-10.19	101.16	114.31
1	A	67	VAL	CB-CA-C	9.80	121.47	110.89
1	A	333	ARG	NE-CZ-NH2	-9.18	110.93	119.20
1	A	55	ARG	NE-CZ-NH1	-8.73	112.77	121.50
1	A	245	MET	CG-SD-CE	-8.58	82.02	100.90
1	A	355	ARG	N-CA-C	-8.52	101.21	111.69
1	A	316	ALA	N-CA-C	-8.31	102.18	111.82
1	A	386	ASP	N-CA-C	8.21	121.87	109.63
1	A	236	ILE	CB-CA-C	-8.13	101.16	112.14
1	A	378	VAL	CB-CA-C	-8.06	99.66	112.16
1	A	84	ARG	N-CA-C	7.92	121.88	110.24
1	A	108	VAL	N-CA-CB	7.82	120.25	110.47
1	A	109	ARG	N-CA-C	-7.80	102.85	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	N-CA-C	-7.80	101.88	111.40
1	A	11	VAL	CA-C-N	7.77	128.06	119.90
1	A	11	VAL	C-N-CA	7.77	128.06	119.90
1	A	140	LYS	N-CA-C	7.70	119.67	111.28
1	A	265	GLU	CG-CD-OE1	-7.56	101.01	118.40
1	A	279	ARG	N-CA-C	-7.51	103.17	111.36
1	A	234	LEU	N-CA-C	-7.50	103.10	111.28
1	A	338	HIS	CA-C-N	-7.43	111.49	122.86
1	A	338	HIS	C-N-CA	-7.43	111.49	122.86
1	A	252	LEU	N-CA-C	-7.43	102.56	111.69
1	A	287	GLY	O-C-N	7.42	129.38	122.99
1	A	376	LYS	CA-C-N	-7.36	112.41	119.85
1	A	376	LYS	C-N-CA	-7.36	112.41	119.85
1	A	293	THR	N-CA-C	7.32	126.39	110.80
1	A	214	THR	CB-CA-C	-7.24	96.98	110.01
1	A	95	HIS	N-CA-C	-7.22	103.49	111.36
1	A	12	PRO	N-CA-C	-7.14	100.01	110.80
1	A	175	VAL	CB-CA-C	7.06	119.96	111.20
1	A	13	LYS	N-CA-C	-7.06	105.60	114.56
1	A	101	LEU	N-CA-C	7.02	118.58	111.07
1	A	334	ARG	CB-CG-CD	-6.97	95.26	111.30
1	A	54	VAL	N-CA-C	-6.96	102.39	111.09
1	A	251	ALA	N-CA-C	-6.93	103.73	111.28
1	A	270	VAL	CG1-CB-CG2	-6.90	95.61	110.80
1	A	261	ALA	CA-C-O	-6.80	113.62	120.90
1	A	271	GLY	N-CA-C	-6.79	104.08	112.77
1	A	221	VAL	CA-C-N	-6.74	114.47	122.22
1	A	221	VAL	C-N-CA	-6.74	114.47	122.22
1	A	324	GLU	N-CA-C	6.74	120.26	110.28
1	A	85	GLY	N-CA-C	-6.74	105.93	115.43
1	A	360	ILE	N-CA-C	6.74	117.53	110.72
1	A	238	ALA	CA-C-O	6.74	127.89	120.82
1	A	238	ALA	N-CA-C	6.70	118.24	111.07
1	A	265	GLU	CA-CB-CG	-6.68	100.73	114.10
1	A	241	THR	CA-C-N	-6.61	110.91	120.29
1	A	241	THR	C-N-CA	-6.61	110.91	120.29
1	A	265	GLU	CB-CG-CD	-6.57	101.44	112.60
1	A	66	GLN	N-CA-C	-6.54	98.72	108.99
1	A	39	PHE	N-CA-C	6.54	124.73	110.80
1	A	252	LEU	CB-CG-CD2	6.51	130.24	110.70
1	A	270	VAL	N-CA-C	6.48	117.17	110.36
1	A	367	ARG	N-CA-C	-6.36	103.87	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LEU	CB-CA-C	-6.35	99.08	110.70
1	A	357	GLU	N-CA-CB	6.31	119.15	110.01
1	A	268	SER	N-CA-C	-6.29	105.47	113.01
1	A	290	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	A	67	VAL	N-CA-CB	6.24	115.89	110.08
1	A	120	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	A	387	ILE	CB-CA-C	-6.21	103.65	112.22
1	A	333	ARG	CB-CG-CD	6.20	125.56	111.30
1	A	230	ALA	N-CA-C	-6.19	104.08	111.69
1	A	333	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	264	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	A	141	THR	CA-C-O	-6.13	111.86	119.28
1	A	364	THR	N-CA-C	-6.09	103.97	111.40
1	A	332	THR	OG1-CB-CG2	-6.08	97.15	109.30
1	A	115	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	334	ARG	CD-NE-CZ	-6.05	115.92	124.40
1	A	393	HIS	CA-C-O	-6.05	114.46	120.70
1	A	303	ILE	CB-CA-C	-6.05	102.84	111.31
1	A	62	SER	N-CA-C	6.03	121.69	113.37
1	A	114	LEU	N-CA-C	6.03	120.24	113.01
1	A	292	ALA	CA-C-N	6.02	133.05	121.54
1	A	292	ALA	C-N-CA	6.02	133.05	121.54
1	A	15	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	A	105	GLU	N-CA-C	-5.93	106.68	114.04
1	A	17	CYS	CA-C-N	-5.90	113.60	119.56
1	A	17	CYS	C-N-CA	-5.90	113.60	119.56
1	A	162	ARG	N-CA-C	5.90	117.79	111.36
1	A	333	ARG	CG-CD-NE	-5.82	99.19	112.00
1	A	36	ARG	CA-C-N	-5.78	112.39	121.87
1	A	36	ARG	C-N-CA	-5.78	112.39	121.87
1	A	115	ARG	CB-CA-C	-5.77	99.86	112.38
1	A	214	THR	N-CA-CB	-5.76	101.63	110.44
1	A	32	ALA	CA-C-N	5.73	125.40	119.56
1	A	32	ALA	C-N-CA	5.73	125.40	119.56
1	A	82	PRO	CB-CA-C	5.72	121.00	111.56
1	A	373	ARG	CA-C-N	-5.71	111.91	121.39
1	A	373	ARG	C-N-CA	-5.71	111.91	121.39
1	A	264	ARG	CG-CD-NE	-5.70	99.47	112.00
1	A	305	LYS	CA-C-N	5.68	131.92	121.70
1	A	305	LYS	C-N-CA	5.68	131.92	121.70
1	A	114	LEU	N-CA-CB	-5.63	100.54	110.39
1	A	292	ALA	O-C-N	-5.63	116.66	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLU	N-CA-C	-5.60	98.86	110.80
1	A	175	VAL	CA-C-O	5.60	125.23	119.35
1	A	82	PRO	N-CA-C	5.58	123.98	112.47
1	A	201	ARG	N-CA-CB	5.58	118.43	110.06
1	A	214	THR	CA-CB-OG1	-5.58	101.23	109.60
1	A	10	THR	CB-CA-C	-5.55	100.37	109.53
1	A	390	TYR	N-CA-C	5.54	119.28	107.70
1	A	23	ASP	CA-C-N	-5.50	113.23	120.22
1	A	23	ASP	C-N-CA	-5.50	113.23	120.22
1	A	115	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	226	PHE	CA-C-N	-5.46	112.42	120.28
1	A	226	PHE	C-N-CA	-5.46	112.42	120.28
1	A	245	MET	N-CA-C	-5.46	105.35	112.23
1	A	265	GLU	OE1-CD-OE2	5.44	135.96	122.90
1	A	334	ARG	CB-CA-C	-5.44	99.46	110.17
1	A	244	CYS	CA-CB-SG	-5.39	102.01	114.40
1	A	55	ARG	NH1-CZ-NH2	5.33	126.24	119.30
1	A	109	ARG	CA-C-N	-5.32	113.15	120.28
1	A	109	ARG	C-N-CA	-5.32	113.15	120.28
1	A	130	GLU	CA-CB-CG	-5.30	103.49	114.10
1	A	262	LEU	CB-CG-CD1	5.28	126.55	110.70
1	A	332	THR	CA-CB-CG2	5.27	119.46	110.50
1	A	103	ALA	CA-C-O	5.27	125.90	119.05
1	A	171	ALA	CA-C-N	-5.25	111.34	121.58
1	A	171	ALA	C-N-CA	-5.25	111.34	121.58
1	A	175	VAL	N-CA-C	5.22	117.91	112.90
1	A	42	GLY	N-CA-C	5.22	125.54	113.18
1	A	214	THR	N-CA-C	5.20	119.61	113.16
1	A	17	CYS	CA-C-O	5.18	124.52	119.55
1	A	94	GLU	CB-CA-C	-5.18	99.64	109.95
1	A	305	LYS	CA-C-O	-5.17	114.86	120.81
1	A	43	HIS	CA-C-N	5.17	131.41	121.54
1	A	43	HIS	C-N-CA	5.17	131.41	121.54
1	A	15	ARG	CA-C-N	-5.16	112.10	121.14
1	A	15	ARG	C-N-CA	-5.16	112.10	121.14
1	A	140	LYS	CB-CA-C	-5.16	102.22	110.79
1	A	109	ARG	CA-CB-CG	5.16	124.42	114.10
1	A	264	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	356	ILE	N-CA-CB	-5.15	102.85	110.58
1	A	126	LEU	N-CA-CB	5.15	118.26	110.28
1	A	367	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	A	140	LYS	CA-C-N	-5.14	113.07	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LYS	C-N-CA	-5.14	113.07	122.38
1	A	354	ALA	N-CA-C	-5.14	105.76	111.36
1	A	96	THR	OG1-CB-CG2	5.13	119.57	109.30
1	A	44	GLU	N-CA-CB	5.13	119.16	110.49
1	A	351	GLN	CA-C-N	-5.12	111.98	120.68
1	A	351	GLN	C-N-CA	-5.12	111.98	120.68
1	A	30	ALA	N-CA-C	-5.12	105.40	111.69
1	A	88	LEU	CA-C-N	-5.08	114.59	122.67
1	A	88	LEU	C-N-CA	-5.08	114.59	122.67
1	A	356	ILE	CA-C-N	-5.08	113.84	120.44
1	A	356	ILE	C-N-CA	-5.08	113.84	120.44
1	A	67	VAL	N-CA-C	-5.07	103.98	108.95
1	A	287	GLY	CA-C-O	-5.05	116.24	120.89
1	A	259	GLN	CA-C-N	-5.03	113.15	120.29
1	A	259	GLN	C-N-CA	-5.03	113.15	120.29
1	A	84	ARG	CB-CG-CD	-5.02	99.75	111.30
1	A	151	ILE	O-C-N	-5.01	117.01	121.87

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2967	0	2956	132	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	140	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 23.

All (140) 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
1:A:42:GLY:HA3	1:A:43:HIS:O	1.82	0.78
1:A:289:GLU:CD	1:A:308:GLN:HE21	1.92	0.77
1:A:196:LEU:HG	1:A:200:ARG:NH1	2.03	0.74
1:A:57:LEU:C	1:A:57:LEU:HD23	2.14	0.73
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: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:293:THR:O	1:A:294:ARG:CB	2.42	0.67
1:A:289:GLU:CD	1:A:308:GLN:NE2	2.50	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:84:ARG:HH21	1:A:94:GLU:CB	2.17	0.56
1:A:245:MET:HE1	1:A:281:LEU:HD12	1.88	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:106:PHE:CE1	1:A:111:MET:HE2	2.43	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:9:PRO:N	1:A:38:THR:HG1	2.06	0.53
1:A:60:ASP:OD1	1:A:60:ASP:C	2.51	0.53
1:A:55:ARG:O	1:A:59:ARG:HB2	2.08	0.53
1:A:294:ARG:C	1:A:305:LYS:HB3	2.34	0.53
1:A:105:GLU:HA	1:A:105:GLU:OE1	2.09	0.52
1:A:57:LEU:C	1:A:57:LEU:CD2	2.83	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
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:109:ARG:O	1:A:110:ARG:C	2.52	0.49
1:A:305:LYS:O	1:A:305:LYS:HG3	2.11	0.49
1:A:390:TYR:C	1:A:390:TYR:CD2	2.85	0.48
1:A:196:LEU:HD21	1:A:200:ARG:HH11	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:223:ASP:O	1:A:224:ASP:C	2.57	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:313:VAL:O	1:A:314:LEU:C	2.57	0.46
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: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:283:ILE:HG12	1:A:314:LEU:HG	2.00	0.44
1:A:102:LEU:C	1:A:104:LYS:H	2.25	0.43
1:A:149:MET:HE2	1:A:149:MET:HB2	1.49	0.43
1:A:102:LEU:C	1:A:104:LYS:N	2.76	0.43
1:A:120:ARG:NH1	1:A:153:ASP:OD2	2.52	0.43
1:A:196:LEU:C	1:A:196:LEU:HD23	2.44	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: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:346:HIS:O	1:A:347:GLN:C	2.61	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:173:MET:HE3	1:A:173:MET:HB3	1.51	0.42
1:A:385:HIS:ND1	1:A:390:TYR:HE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:LEU:O	1:A:88:LEU:C	2.64	0.40
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%)	5 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	44	GLU
1	A	82	PRO

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Mol	Chain	Res	Type
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%)	259 (83%)	52 (17%)	2 4

All (52) 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	52	GLU
1	A	54	VAL
1	A	57	LEU
1	A	59	ARG
1	A	66	GLN
1	A	67	VAL
1	A	81	LYS
1	A	82	PRO
1	A	94	GLU
1	A	102	LEU
1	A	104	LYS
1	A	109	ARG
1	A	114	LEU

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Mol	Chain	Res	Type
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	187	MET
1	A	189	LEU
1	A	200	ARG
1	A	213	ILE
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	291	VAL
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	90	GLN
1	A	112	GLN
1	A	119	GLN
1	A	166	GLN
1	A	177	GLN
1	A	195	GLN
1	A	272	ASN

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Mol	Chain	Res	Type
1	A	308	GLN
1	A	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1408	1,3	50,50,50	1.92	11 (22%)	67,82,82	2.87	29 (43%)
3	PIM	A	501	2	11,12,12	2.04	3 (27%)	14,15,15	1.24	2 (14%)

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	1408	1,3	-	1/14/54/54	-
3	PIM	A	501	2	-	0/4/4/4	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1408	HEM	C3D-C2D	7.47	1.52	1.36
2	A	1408	HEM	FE-NB	4.70	2.09	1.94
3	A	501	PIM	C6-C5	-4.44	1.40	1.47
3	A	501	PIM	C5-N1	-4.17	1.33	1.38
2	A	1408	HEM	FE-NA	-3.56	1.83	1.95
2	A	1408	HEM	FE-NC	-3.51	1.83	1.95
2	A	1408	HEM	C1B-NB	-2.97	1.35	1.40
2	A	1408	HEM	CMB-C2B	2.88	1.56	1.50
2	A	1408	HEM	CMA-C3A	2.40	1.55	1.50
3	A	501	PIM	C4-N3	-2.38	1.33	1.37
2	A	1408	HEM	CAC-C3C	2.20	1.53	1.47
2	A	1408	HEM	C4D-ND	-2.19	1.36	1.40
2	A	1408	HEM	CAB-C3B	2.06	1.52	1.47
2	A	1408	HEM	FE-ND	2.04	2.01	1.94

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1408	HEM	C3B-C2B-C1B	-8.26	100.21	106.41
2	A	1408	HEM	C4B-C3B-C2B	6.98	113.69	107.28
2	A	1408	HEM	CHD-C4C-NC	6.48	131.51	124.45
2	A	1408	HEM	O2A-CGA-O1A	-5.37	109.53	123.33
2	A	1408	HEM	CBB-CAB-C3B	-5.33	100.91	127.53
2	A	1408	HEM	C3B-C4B-NB	-4.78	106.04	109.47
2	A	1408	HEM	C2A-C1A-NA	4.75	115.43	110.15
2	A	1408	HEM	C2B-C1B-NB	4.45	114.95	109.84
2	A	1408	HEM	CMB-C2B-C1B	4.24	131.65	125.03
2	A	1408	HEM	C3D-C4D-ND	4.20	114.78	110.17
2	A	1408	HEM	C4A-NA-C1A	-4.15	99.06	105.82
2	A	1408	HEM	O2A-CGA-CBA	3.93	126.43	114.00
2	A	1408	HEM	CHB-C4A-C3A	-3.86	116.22	127.43
2	A	1408	HEM	C4D-C3D-C2D	-3.80	101.36	106.89
2	A	1408	HEM	CBD-CAD-C3D	-3.71	102.28	112.53
2	A	1408	HEM	CMC-C2C-C1C	3.67	131.19	124.73
2	A	1408	HEM	CAB-C3B-C2B	-3.38	117.44	128.43
2	A	1408	HEM	C4C-C3C-C2C	3.32	109.70	106.81
2	A	1408	HEM	C3A-C4A-NA	3.25	115.35	110.14
2	A	1408	HEM	CMA-C3A-C2A	3.16	132.32	125.62
2	A	1408	HEM	CHD-C4C-C3C	-3.14	119.92	125.21
2	A	1408	HEM	CAA-CBA-CGA	-2.76	106.34	113.67
2	A	1408	HEM	CHA-C1A-C2A	-2.72	119.35	125.30
2	A	1408	HEM	CHB-C4A-NA	2.51	128.40	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1408	HEM	CHB-C1B-NB	-2.45	121.34	124.37
3	A	501	PIM	C6-C5-N1	2.21	126.28	123.72
3	A	501	PIM	C10-C11-C6	2.17	122.50	120.36
2	A	1408	HEM	CMA-C3A-C4A	-2.12	122.19	125.42
2	A	1408	HEM	CMC-C2C-C3C	-2.11	123.31	128.43
2	A	1408	HEM	CHC-C4B-C3B	2.11	129.28	125.07
2	A	1408	HEM	O1D-CGD-CBD	-2.05	116.58	123.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

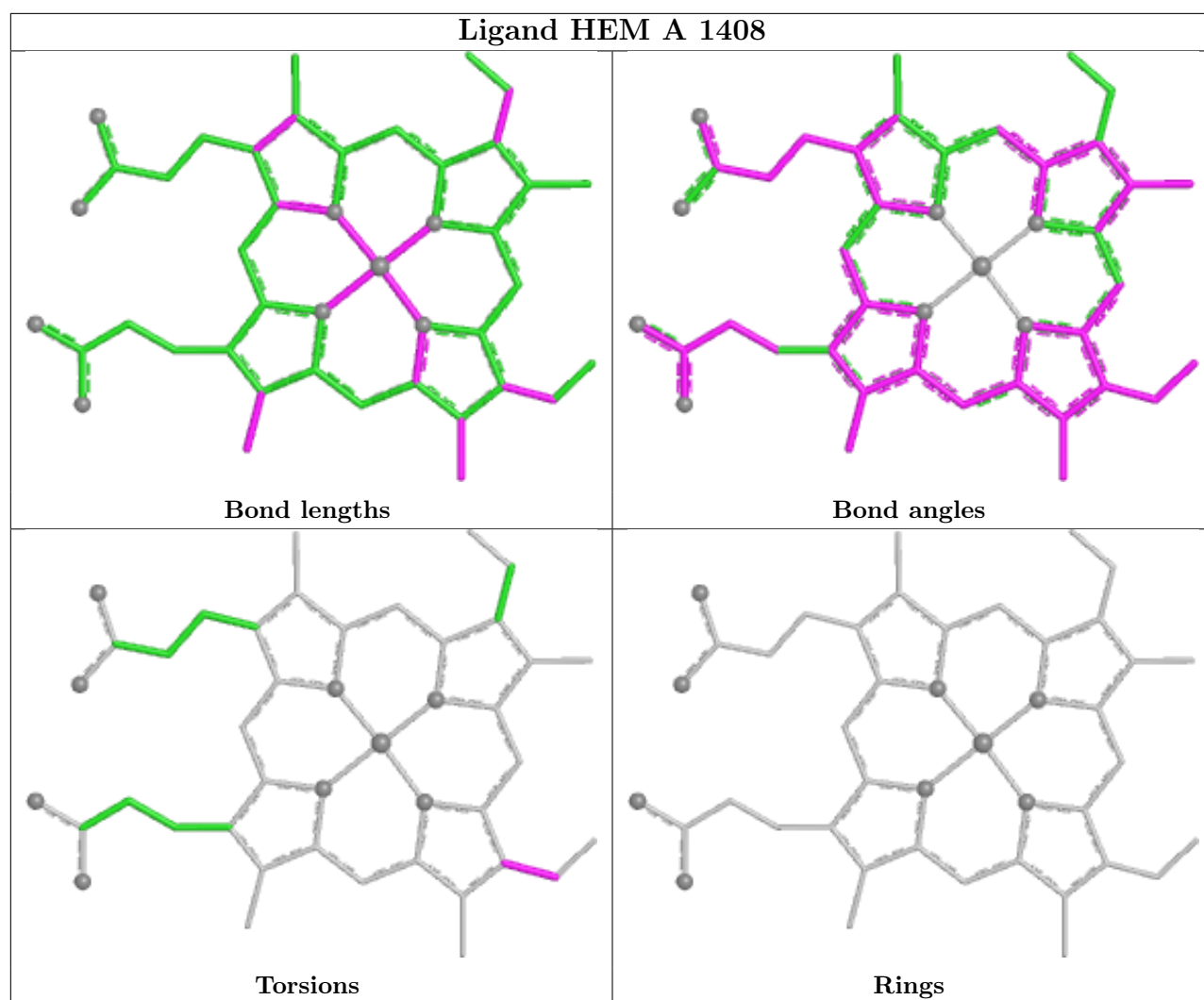
Mol	Chain	Res	Type	Atoms
2	A	1408	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1408	HEM	8	0
3	A	501	PIM	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/403 (94%)	-0.38	8 (2%) 63 58	21, 37, 61, 86	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	HIS	4.9
1	A	40	THR	3.4
1	A	9	PRO	3.1
1	A	81	LYS	3.0
1	A	388	VAL	3.0
1	A	82	PRO	2.9
1	A	43	HIS	2.2
1	A	387	ILE	2.2

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

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

6.3 Carbohydrates [i](#)

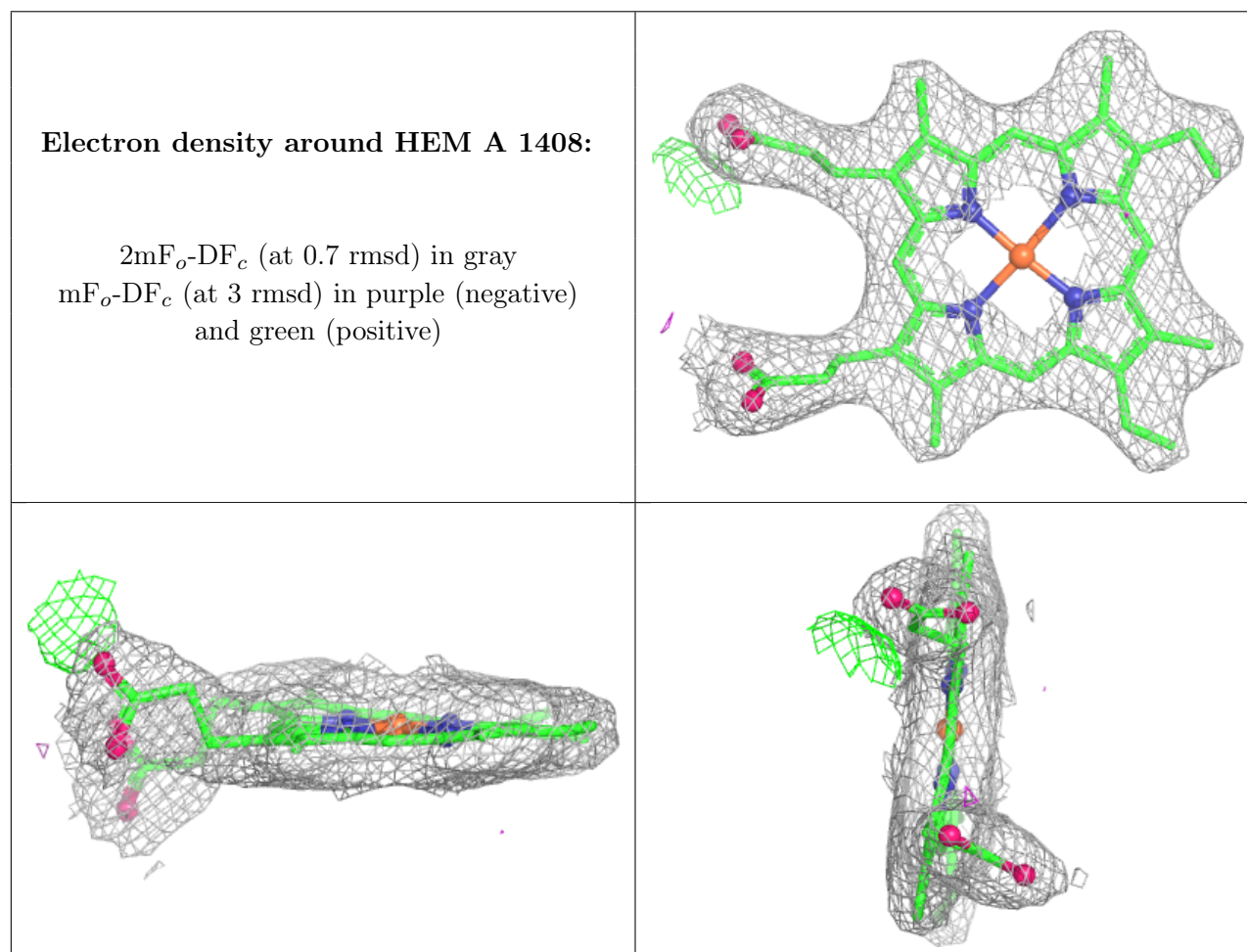
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PIM	A	501	11/11	0.97	0.09	38,44,47,49	0
2	HEM	A	1408	43/43	0.99	0.05	24,35,45,53	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.