



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 12:54 AM JST

PDB ID : 4U72
Title : Crystal structure of 4-phenylimidazole bound form of human indoleamine 2,3-dioxygenase (A260G mutant)
Authors : Sugimoto, H.; Horitani, M.; Kometani, E.; Shiro, Y.
Deposited on : 2014-07-30
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

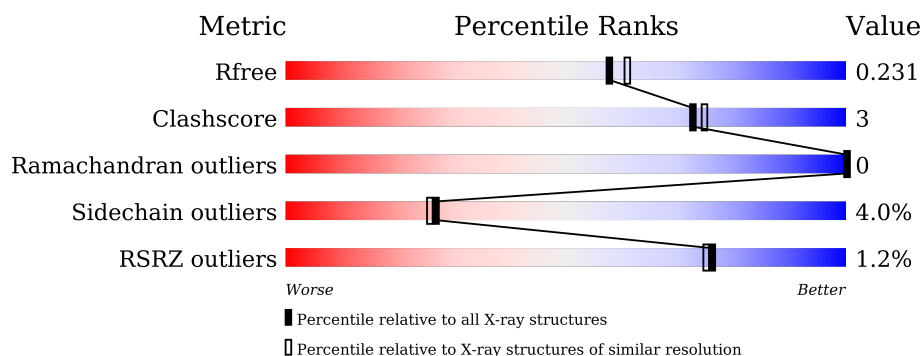
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	406	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	406	<div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6471 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.

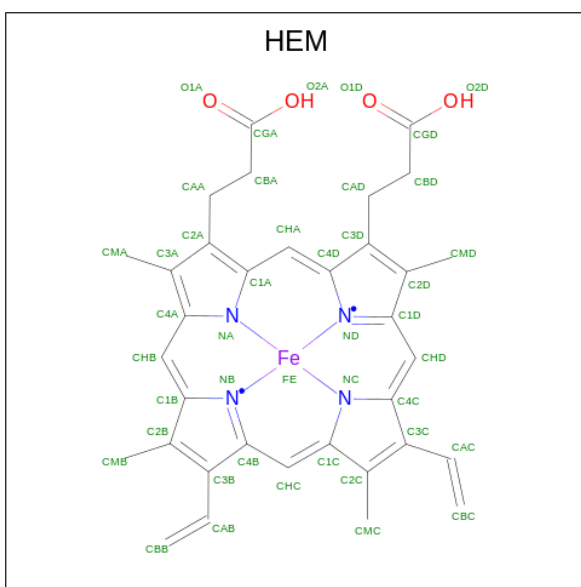
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2971	1908	507	539	17			
1	B	374	Total	C	N	O	S	0	4	0
			2979	1916	506	539	18			

There are 8 discrepancies between the modelled and reference sequences:

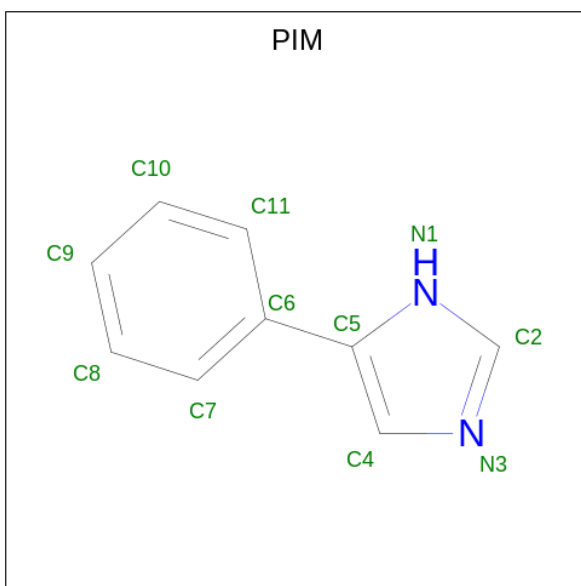
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14902
A	-1	SER	-	expression tag	UNP P14902
A	0	HIS	-	expression tag	UNP P14902
A	260	GLY	ALA	engineered mutation	UNP P14902
B	-2	GLY	-	expression tag	UNP P14902
B	-1	SER	-	expression tag	UNP P14902
B	0	HIS	-	expression tag	UNP P14902
B	260	GLY	ALA	engineered mutation	UNP P14902

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



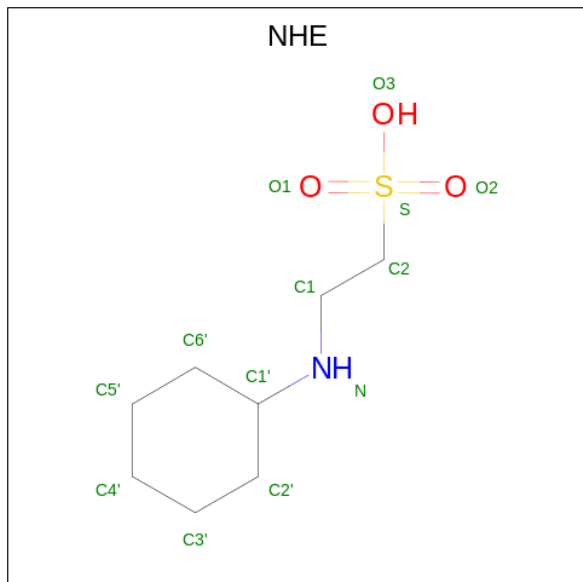
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (three-letter code: PIM) (formula: $C_9H_8N_2$).



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

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	1
			26	16	2	6	2		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	1
			26	16	2	6	2		

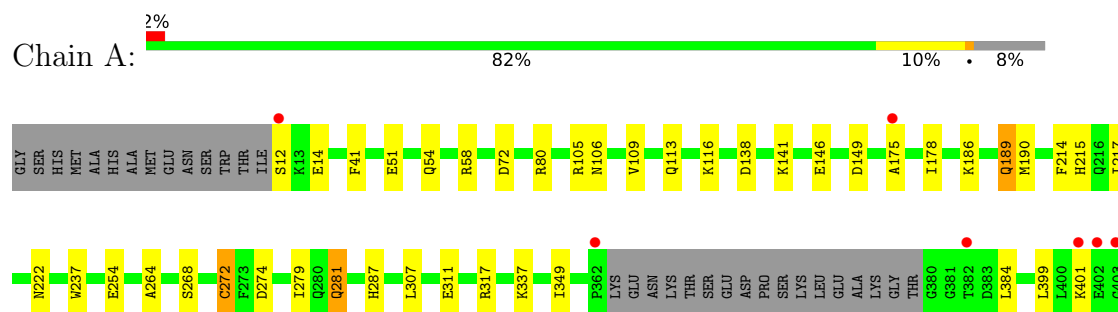
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	170	Total	O	0	0
			170	170		

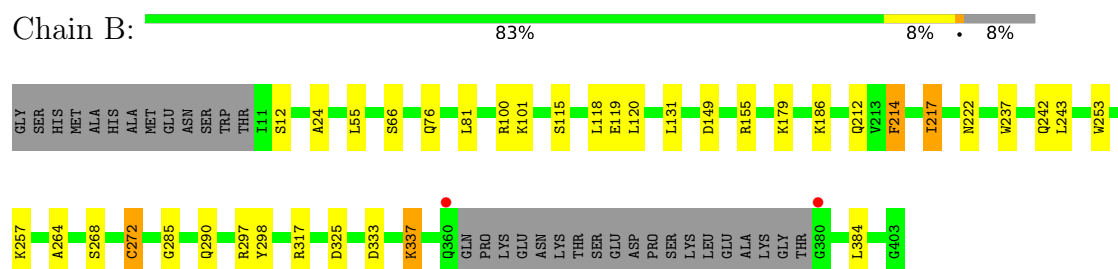
3 Residue-property plots [i](#)

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: Indoleamine 2,3-dioxygenase 1



• Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.97Å 98.89Å 131.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.00 19.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.76-2.00) 96.7 (19.76-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.231 0.186 , 0.231	Depositor DCC
R_{free} test set	3631 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: HEM, NHE, 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	1.02	1/3040 (0.0%)	0.99	8/4109 (0.2%)
1	B	1.05	2/3059 (0.1%)	1.00	9/4135 (0.2%)
All	All	1.03	3/6099 (0.0%)	1.00	17/8244 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	TYR	CG-CD1	6.01	1.47	1.39
1	B	119	GLU	CD-OE2	-5.32	1.19	1.25
1	A	146	GLU	CD-OE1	5.16	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ARG	NE-CZ-NH1	-10.06	115.27	120.30
1	B	317	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	B	100	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	149	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	B	325	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	317	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	155	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	80	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	317	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	72	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	149	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	155	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	100	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	B	217	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	A	116	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	B	81	LEU	CB-CG-CD2	-5.12	102.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ILE	C-N-CA	-5.05	109.06	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2971	0	2980	18	0
1	B	2979	0	3003	15	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	11	0	8	2	0
3	B	11	0	8	2	0
4	A	39	0	50	2	0
4	B	39	0	50	0	0
5	A	165	0	0	1	0
5	B	170	0	0	1	0
All	All	6471	0	6159	38	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 3.

All (38) 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:175:ALA:HA	1:A:178:ILE:HD12	1.68	0.76
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.70	0.73
1:A:384:LEU:HD11	2:A:501:HEM:HMA3	1.74	0.69
1:A:274:ASP:OD2	1:A:281:GLN:HG2	1.97	0.65
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.29	0.62
1:A:268:SER:O	1:A:272:CYS:HB3	2.00	0.61
1:A:138:ASP:OD2	1:A:141:LYS:HD2	2.00	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.83	0.61
1:B:101:LYS:HG2	1:B:243:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.82	0.60
1:B:285:GLY:O	1:B:290:GLN:NE2	2.34	0.57
1:A:287:HIS:HE1	4:A:504[A]:NHE:H4'2	1.72	0.55
1:B:101:LYS:HG2	1:B:243:LEU:HD22	1.89	0.55
1:A:54:GLN:O	1:A:58:ARG:HG2	2.08	0.54
1:A:106:ASN:HB2	5:A:760:HOH:O	2.09	0.53
1:A:307:LEU:O	1:A:311:GLU:HG2	2.10	0.52
1:A:41:PHE:CE2	1:A:58:ARG:NH2	2.79	0.50
1:B:214:PHE:HD1	1:B:214:PHE:O	1.93	0.50
1:B:333:ASP:O	1:B:337:LYS:HB2	2.12	0.49
1:A:384:LEU:CD1	2:A:501:HEM:HMA3	2.41	0.49
1:A:384:LEU:HD11	2:A:501:HEM:CMA	2.42	0.48
2:A:501:HEM:C1A	3:A:502:PIM:H2	2.49	0.48
1:B:24:ALA:HA	1:B:131:LEU:HB3	1.94	0.47
1:B:253:TRP:CE3	1:B:257:LYS:HG3	2.49	0.47
1:B:55:LEU:C	1:B:55:LEU:HD13	2.35	0.46
4:A:503:NHE:HC12	4:A:504[A]:NHE:HC21	1.98	0.44
1:B:115:SER:HB3	1:B:120:LEU:O	2.17	0.43
1:B:384:LEU:CD1	2:B:501:HEM:HMA2	2.48	0.43
1:B:268:SER:O	1:B:272[A]:CYS:HB3	2.19	0.43
1:B:297:ARG:HG3	5:B:729:HOH:O	2.18	0.42
1:A:399:LEU:HB3	1:A:401:LYS:O	2.19	0.42
1:B:264:ALA:H	3:B:502:PIM:HN1	1.66	0.42
1:B:242:GLN:O	1:B:243:LEU:HD23	2.20	0.41
1:A:109:VAL:O	1:A:113:GLN:HG3	2.21	0.41
1:A:189:GLN:HG3	1:A:190:MET:N	2.34	0.41
1:B:76:GLN:HB3	1:B:118:LEU:HD11	2.01	0.41
1:A:264:ALA:H	3:A:502:PIM:HN1	1.61	0.41
2:B:501:HEM:C1A	3:B:502:PIM:H2	2.55	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	371/406 (91%)	364 (98%)	7 (2%)	0	100	100
1	B	374/406 (92%)	365 (98%)	9 (2%)	0	100	100
All	All	745/812 (92%)	729 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	324/350 (93%)	310 (96%)	14 (4%)	25	23
1	B	327/350 (93%)	314 (96%)	13 (4%)	27	26
All	All	651/700 (93%)	624 (96%)	27 (4%)	27	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	14	GLU
1	A	51	GLU
1	A	105	ARG
1	A	186	LYS
1	A	189	GLN
1	A	214	PHE
1	A	215	HIS
1	A	222	ASN
1	A	237	TRP
1	A	254	GLU
1	A	272	CYS
1	A	281	GLN
1	A	337	LYS
1	B	12	SER
1	B	66	SER
1	B	149	ASP
1	B	179	LYS

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Mol	Chain	Res	Type
1	B	186	LYS
1	B	212	GLN
1	B	214	PHE
1	B	217	ILE
1	B	222	ASN
1	B	237	TRP
1	B	272[A]	CYS
1	B	272[B]	CYS
1	B	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	B	16	HIS
1	B	215	HIS
1	B	216	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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$
4	NHE	A	504[B]	-	13,13,13	1.73	1 (7%)	16,17,17	2.29	6 (37%)
4	NHE	B	504[A]	-	13,13,13	2.60	1 (7%)	16,17,17	1.66	5 (31%)
2	HEM	B	501	3,1	41,50,50	1.70	8 (19%)	45,82,82	2.09	14 (31%)
2	HEM	A	501	3,1	41,50,50	1.65	9 (21%)	45,82,82	2.41	14 (31%)
3	PIM	A	502	2	9,12,12	1.45	1 (11%)	7,15,15	1.47	1 (14%)
4	NHE	A	503	-	13,13,13	1.58	2 (15%)	16,17,17	2.63	6 (37%)
4	NHE	B	504[B]	-	13,13,13	2.28	2 (15%)	16,17,17	2.28	5 (31%)
4	NHE	B	503	-	13,13,13	1.19	1 (7%)	16,17,17	2.09	6 (37%)
3	PIM	B	502	2	9,12,12	1.47	1 (11%)	7,15,15	2.17	4 (57%)
4	NHE	A	504[A]	-	13,13,13	2.41	1 (7%)	16,17,17	1.59	3 (18%)

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
4	NHE	A	504[B]	-	-	2/7/15/15	0/1/1/1
4	NHE	B	504[A]	-	-	0/7/15/15	0/1/1/1
2	HEM	B	501	3,1	-	2/12/54/54	-
2	HEM	A	501	3,1	-	2/12/54/54	-
3	PIM	A	502	2	-	0/0/4/4	0/2/2/2
4	NHE	A	503	-	-	0/7/15/15	0/1/1/1
4	NHE	B	504[B]	-	-	5/7/15/15	0/1/1/1
4	NHE	B	503	-	-	0/7/15/15	0/1/1/1
3	PIM	B	502	2	-	0/0/4/4	0/2/2/2
4	NHE	A	504[A]	-	-	2/7/15/15	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504[A]	NHE	C2-S	-8.94	1.64	1.77
4	A	504[A]	NHE	C2-S	-8.22	1.65	1.77
4	B	504[B]	NHE	C2-S	-7.71	1.66	1.77
4	A	504[B]	NHE	C2-S	-5.87	1.69	1.77
2	A	501	HEM	C1B-NB	-5.02	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	NHE	C2-S	-4.60	1.71	1.77
2	B	501	HEM	C1B-NB	-4.01	1.33	1.40
2	B	501	HEM	CHB-C1B	3.28	1.43	1.35
2	B	501	HEM	CHA-C4D	3.24	1.43	1.35
2	B	501	HEM	C4B-NB	-3.24	1.32	1.38
2	B	501	HEM	C4D-ND	-3.21	1.34	1.40
2	A	501	HEM	C4B-NB	-3.09	1.32	1.38
2	B	501	HEM	C4D-C3D	2.93	1.50	1.45
2	A	501	HEM	C3C-C2C	-2.82	1.36	1.40
2	B	501	HEM	C3B-C4B	2.78	1.50	1.44
3	B	502	PIM	C8-C7	2.68	1.42	1.36
4	B	503	NHE	C2-S	-2.63	1.73	1.77
2	A	501	HEM	C1D-C2D	2.60	1.49	1.44
2	B	501	HEM	FE-NB	2.58	2.09	1.96
3	A	502	PIM	C9-C8	2.57	1.44	1.38
2	A	501	HEM	CHB-C1B	2.43	1.41	1.35
2	A	501	HEM	C4D-C3D	2.41	1.49	1.45
2	A	501	HEM	O2A-CGA	-2.38	1.22	1.30
4	B	504[B]	NHE	O2-S	2.30	1.51	1.45
2	A	501	HEM	FE-NB	2.28	2.08	1.96
4	A	503	NHE	C6'-C1'	2.09	1.56	1.52
2	A	501	HEM	C4D-ND	-2.05	1.36	1.40

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	7.81	113.14	105.07
2	B	501	HEM	C1B-NB-C4B	7.13	112.44	105.07
4	A	503	NHE	O3-S-C2	6.91	116.94	105.77
4	B	504[B]	NHE	O3-S-C2	6.50	116.28	105.77
4	A	504[B]	NHE	C1-N-C1'	6.32	126.56	114.14
2	A	501	HEM	CHC-C4B-NB	5.71	130.63	124.43
2	B	501	HEM	CHC-C4B-NB	5.00	129.86	124.43
2	A	501	HEM	C4B-C3B-C2B	-4.71	103.38	107.11
4	A	503	NHE	O1-S-C2	-4.43	101.58	106.92
2	B	501	HEM	CHA-C4D-ND	4.21	129.59	124.38
4	A	503	NHE	C4'-C3'-C2'	-4.15	102.96	111.42
4	B	503	NHE	O2-S-C2	-4.11	101.97	106.92
2	A	501	HEM	CHB-C1B-NB	4.00	129.32	124.38
4	B	503	NHE	O1-S-C2	3.96	111.69	106.92
4	A	504[A]	NHE	O3-S-C2	3.93	112.13	105.77
4	B	504[A]	NHE	C4'-C3'-C2'	-3.70	103.87	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	NHE	O3-S-C2	3.63	111.64	105.77
2	B	501	HEM	CHB-C1B-NB	3.62	128.86	124.38
2	A	501	HEM	C2C-C3C-C4C	3.61	109.42	106.90
4	B	504[B]	NHE	C1-N-C1'	3.34	120.70	114.14
2	A	501	HEM	CHD-C1D-C2D	-3.32	119.80	124.98
4	A	504[B]	NHE	C6'-C1'-C2'	-3.30	105.09	110.82
4	B	504[B]	NHE	C6'-C1'-C2'	-3.22	105.24	110.82
4	A	503	NHE	O3-S-O1	-3.17	103.54	111.27
3	B	502	PIM	C4-N3-C2	3.00	110.46	105.78
2	A	501	HEM	CMA-C3A-C4A	-3.00	123.86	128.46
2	A	501	HEM	C3B-C2B-C1B	2.98	108.70	106.49
2	B	501	HEM	CHA-C4D-C3D	-2.98	119.73	125.33
2	A	501	HEM	CHD-C1D-ND	2.97	127.66	124.43
2	B	501	HEM	CHD-C1D-C2D	-2.89	120.46	124.98
2	A	501	HEM	O2A-CGA-O1A	-2.85	116.20	123.30
4	A	504[B]	NHE	O1-S-C2	2.74	110.22	106.92
2	B	501	HEM	CHD-C1D-ND	2.73	127.39	124.43
4	B	504[A]	NHE	O1-S-C2	2.71	110.18	106.92
3	B	502	PIM	C7-C6-C11	2.67	121.02	118.65
3	B	502	PIM	C8-C7-C6	-2.57	116.43	120.44
2	B	501	HEM	CBA-CAA-C2A	-2.55	108.27	112.62
3	B	502	PIM	C9-C10-C11	-2.53	116.90	120.44
4	A	504[A]	NHE	C1-N-C1'	2.46	118.97	114.14
2	B	501	HEM	C2C-C3C-C4C	2.45	108.61	106.90
4	A	504[A]	NHE	C5'-C6'-C1'	2.44	115.70	111.11
2	B	501	HEM	C3C-C4C-NC	-2.42	106.37	110.94
4	B	503	NHE	C4'-C3'-C2'	-2.41	106.51	111.42
4	B	504[A]	NHE	C1-N-C1'	2.39	118.84	114.14
2	A	501	HEM	CMB-C2B-C1B	-2.38	121.42	125.04
4	B	504[A]	NHE	C4'-C5'-C6'	2.37	116.26	111.42
4	B	504[A]	NHE	C5'-C6'-C1'	2.37	115.56	111.11
2	A	501	HEM	C2B-C1B-NB	-2.33	107.08	109.84
4	B	503	NHE	C1-N-C1'	-2.32	109.58	114.14
4	B	504[B]	NHE	O3-S-O1	-2.32	105.61	111.27
4	A	504[B]	NHE	O3-S-O2	2.31	116.91	111.27
4	A	503	NHE	C4'-C5'-C6'	-2.29	106.74	111.42
3	A	502	PIM	C4-N3-C2	2.26	109.30	105.78
4	A	504[B]	NHE	O2-S-O1	-2.23	106.21	113.95
2	A	501	HEM	C3C-C4C-NC	-2.23	106.73	110.94
2	B	501	HEM	O2D-CGD-CBD	2.20	121.09	114.03
4	A	503	NHE	C1-N-C1'	-2.18	109.85	114.14
2	B	501	HEM	C4B-C3B-C2B	-2.16	105.40	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504[B]	NHE	O3-S-O2	-2.13	106.07	111.27
4	A	504[B]	NHE	O3-S-C2	2.11	109.18	105.77
4	B	503	NHE	C4'-C5'-C6'	-2.09	107.16	111.42
2	B	501	HEM	C1D-C2D-C3D	-2.08	104.77	106.96
2	A	501	HEM	CBB-CAB-C3B	-2.08	117.29	127.62
2	B	501	HEM	CMD-C2D-C1D	2.00	128.09	125.04

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504[A]	NHE	C6'-C1'-N-C1
4	A	504[A]	NHE	N-C1-C2-S
4	A	504[B]	NHE	N-C1-C2-S
4	B	504[B]	NHE	N-C1-C2-S
4	B	504[B]	NHE	C1-C2-S-O1
4	B	504[B]	NHE	C1-C2-S-O2
4	B	504[B]	NHE	C1-C2-S-O3
4	A	504[B]	NHE	C6'-C1'-N-C1
4	B	504[B]	NHE	C2-C1-N-C1'
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D

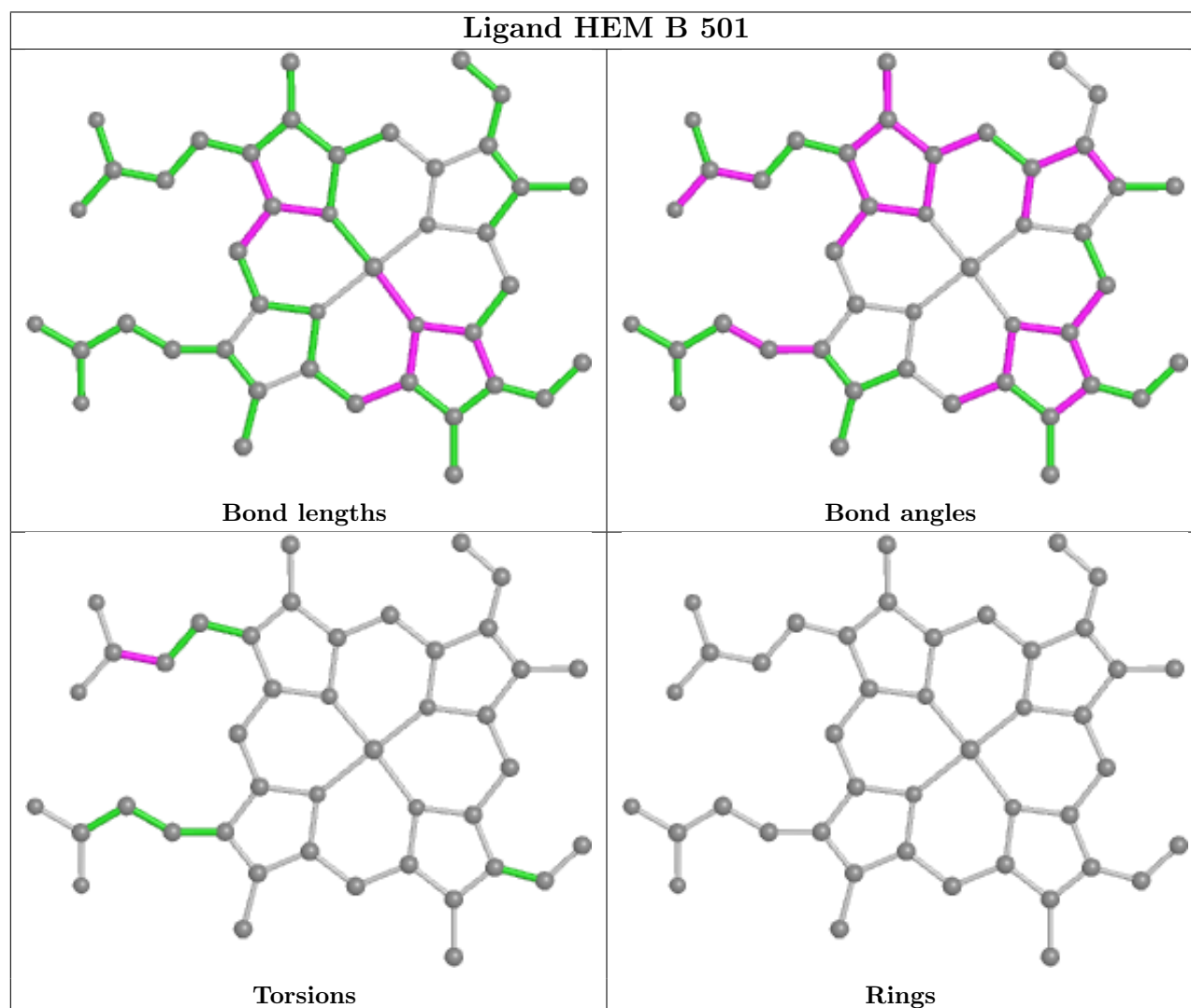
There are no ring outliers.

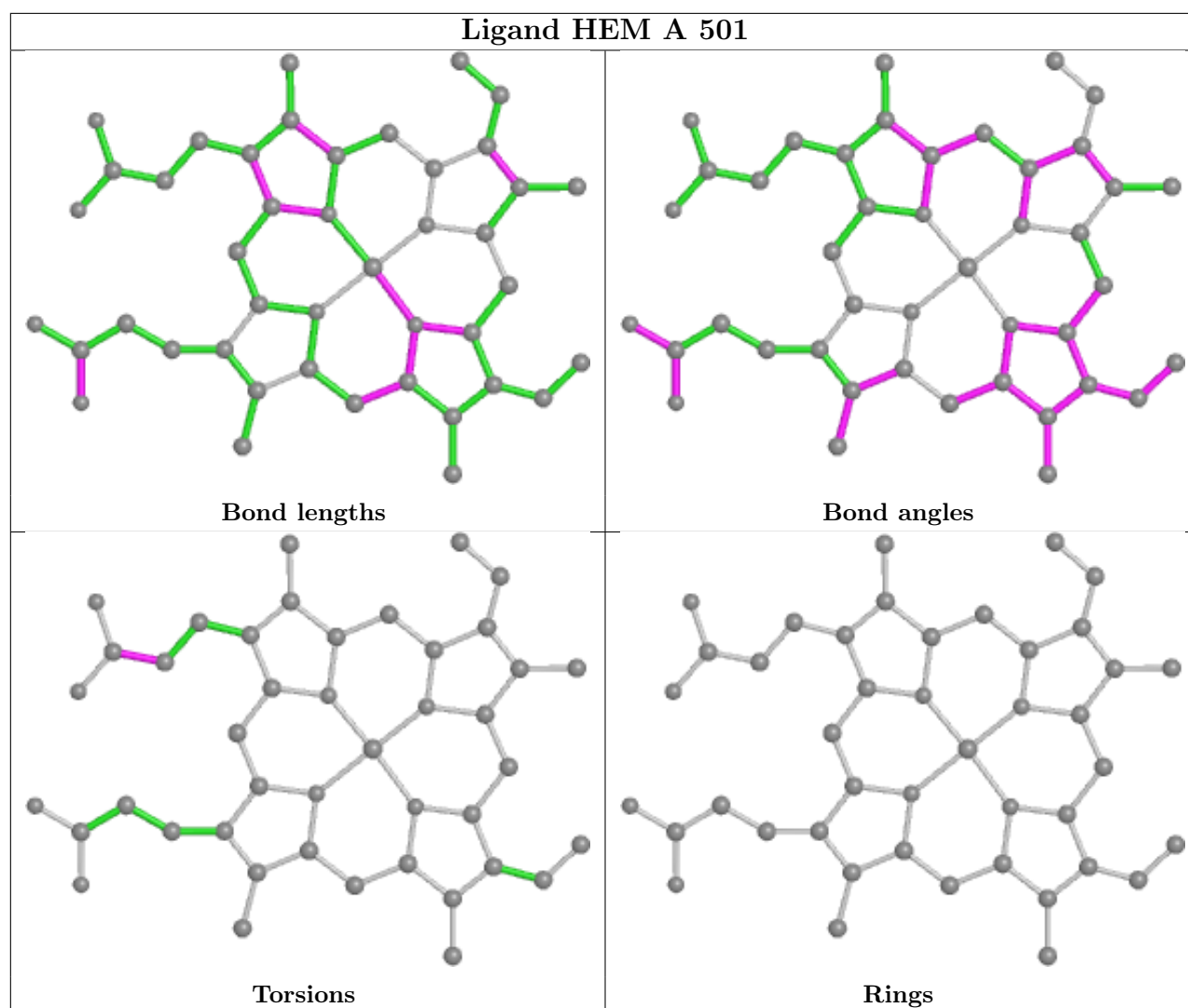
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	A	501	HEM	5	0
3	A	502	PIM	2	0
4	A	503	NHE	1	0
3	B	502	PIM	2	0
4	A	504[A]	NHE	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	375/406 (92%)	-0.48	7 (1%) 66 65	14, 25, 44, 111	0
1	B	374/406 (92%)	-0.48	2 (0%) 87 86	12, 25, 43, 58	4 (1%)
All	All	749/812 (92%)	-0.48	9 (1%) 76 75	12, 25, 43, 111	4 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	8.5
1	A	362	PRO	3.4
1	A	402	GLU	3.3
1	A	175	ALA	2.6
1	B	380	GLY	2.5
1	B	360	GLN	2.3
1	A	12	SER	2.2
1	A	382	THR	2.1
1	A	401	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

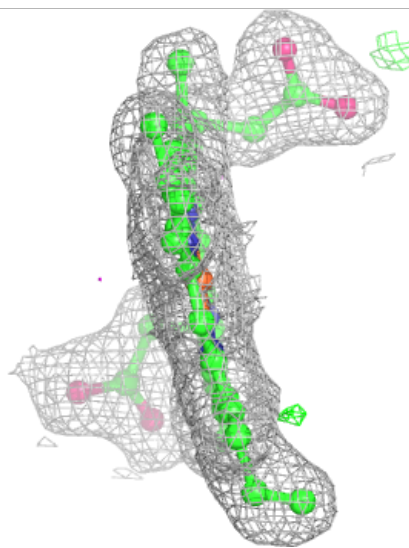
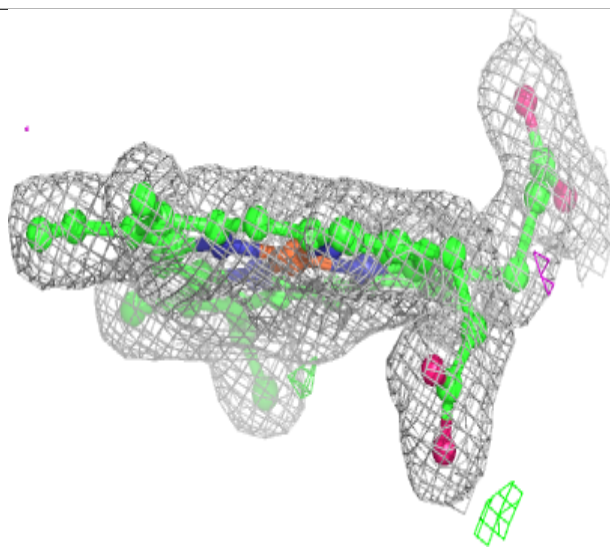
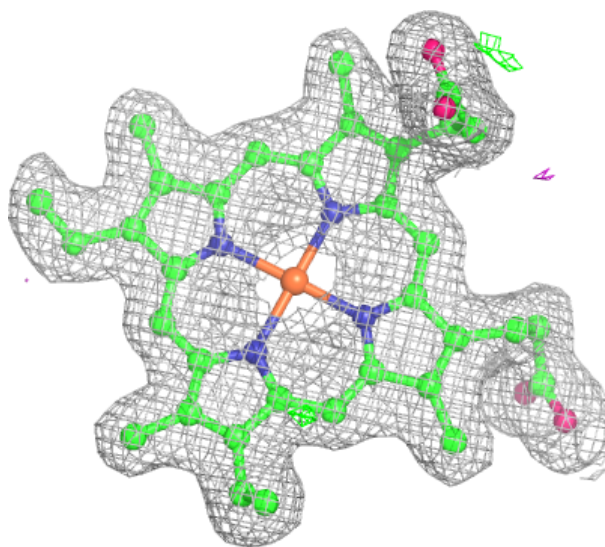
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NHE	B	504[A]	13/13	0.81	0.16	30,32,43,48	13
4	NHE	B	504[B]	13/13	0.81	0.16	37,39,40,41	13
4	NHE	A	504[A]	13/13	0.82	0.18	34,37,44,47	13
4	NHE	A	504[B]	13/13	0.82	0.18	24,26,28,29	13
4	NHE	A	503	13/13	0.94	0.09	24,28,32,33	0
4	NHE	B	503	13/13	0.95	0.07	21,28,39,40	0
3	PIM	A	502	11/11	0.98	0.04	12,13,14,15	0
3	PIM	B	502	11/11	0.98	0.04	13,14,14,15	0
2	HEM	A	501	43/43	0.99	0.04	14,16,18,19	0
2	HEM	B	501	43/43	0.99	0.04	15,18,22,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

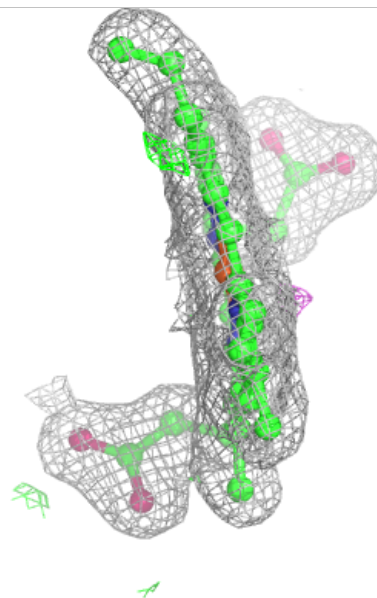
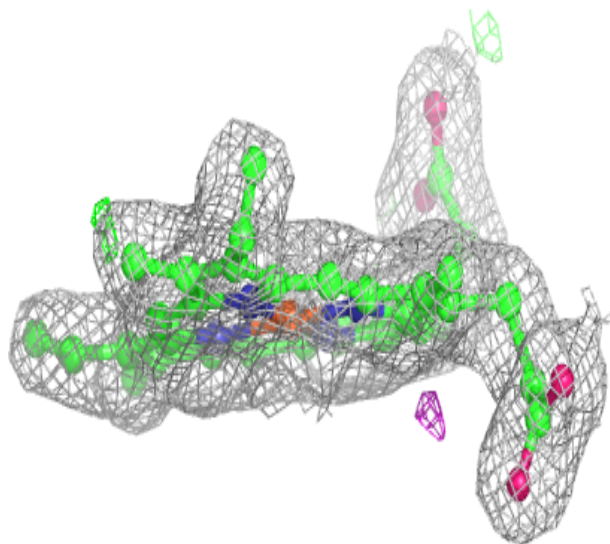
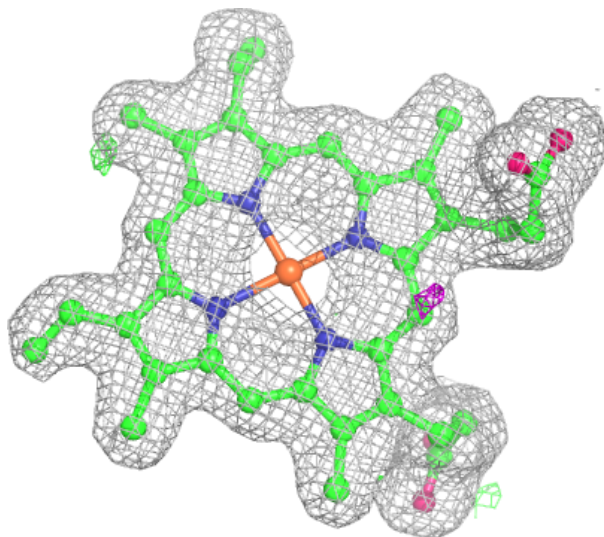
Electron density around HEM A 501:

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



Electron density around HEM B 501:

$2mF_o-DF_c$ (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.