



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 03:08 AM JST

PDB ID : 6KOF  
Title : Crystal structure of indoleamine 2,3-dioxygenase 1 (IDO1) in complex with compound 47  
Authors : Peng, Y.H.; Wu, S.Y.  
Deposited on : 2019-08-09  
Resolution : 2.26 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

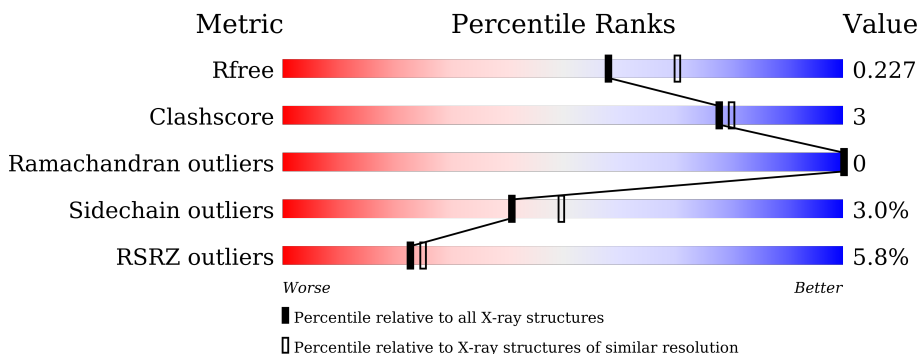
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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.

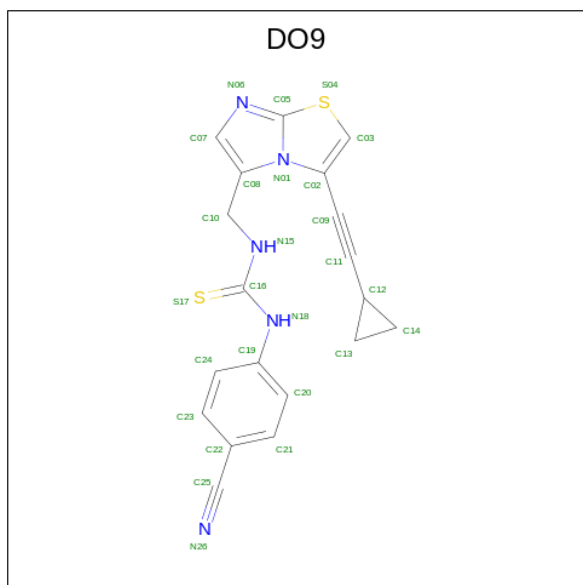


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	
1	B	403	





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			26	19	5	2		
3	B	1	Total	C	N	S	0	0
			26	19	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	93	Total	O	0	0
			93	93		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.42Å 92.57Å 130.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.26 29.68 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.68-2.26) 96.0 (29.68-2.26)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.26Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.195 , 0.227 0.195 , 0.227	Depositor DCC
$R_{free}$ test set	2370 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: DO9, 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	0.28	0/3005	0.43	0/4066
1	B	0.28	0/3031	0.44	0/4098
All	All	0.28	0/6036	0.43	0/8164

There are no bond length outliers.

There are no bond angle outliers.

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	2937	0	2946	18	0
1	B	2963	0	2979	14	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	26	0	0	3	0
3	B	26	0	0	2	0
4	A	46	0	0	0	0
4	B	93	0	0	0	0
All	All	6177	0	5985	35	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 (35) 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:269:VAL:HG23	1:A:270:PHE:HD1	1.59	0.67
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.80	0.62
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.80	0.62
1:A:231:ARG:HD2	3:A:502:DO9:C25	2.30	0.62
1:A:175:ALA:HA	1:A:178:ILE:HD12	1.82	0.62
1:B:279:ILE:HG22	1:B:281:GLN:HG2	1.84	0.60
1:A:308:CYS:SG	1:B:308:CYS:HB3	2.42	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HHD	1.87	0.56
1:B:282:THR:HB	1:B:293:GLN:HG2	1.90	0.53
1:A:267:SER:OG	1:A:269:VAL:HG22	2.09	0.52
1:A:99:VAL:HG11	1:A:243:LEU:HD11	1.91	0.52
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.91	0.51
1:A:264:ALA:HB3	2:A:501:HEM:C4D	2.47	0.50
1:B:281:GLN:HE22	1:B:391:VAL:HA	1.77	0.49
1:A:308:CYS:SG	1:B:308:CYS:CB	3.01	0.49
1:A:88:MET:HE1	1:A:123:ILE:HG13	1.96	0.48
1:A:36:TYR:OH	1:A:66:SER:O	2.20	0.47
1:A:269:VAL:HG23	1:A:270:PHE:CD1	2.45	0.46
1:A:72:ASP:OD1	1:A:72:ASP:N	2.40	0.45
1:A:39:TRP:CD2	1:A:83:LEU:HD21	2.51	0.45
1:B:136:LYS:HD3	1:B:139:PRO:HA	1.99	0.45
1:B:175:ALA:HA	1:B:178:ILE:HD12	1.99	0.44
1:B:279:ILE:O	1:B:281:GLN:N	2.49	0.44
1:B:264:ALA:HB3	2:B:501:HEM:C4D	2.53	0.43
1:A:58:ARG:HE	1:A:58:ARG:HB3	1.55	0.43
2:A:501:HEM:O2A	3:A:502:DO9:N15	2.51	0.43
1:B:72:ASP:OD1	1:B:75:SER:HB2	2.19	0.43
1:B:384:LEU:HD11	3:B:502:DO9:C21	2.49	0.43
1:A:42:ILE:HD12	1:A:62:LEU:HD11	2.01	0.43
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	2.00	0.43
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.95	0.41
1:B:221:VAL:HG12	1:B:353:TYR:CE2	2.55	0.41
1:A:61:LYS:HD3	1:A:61:LYS:HA	1.77	0.41
1:B:262:GLY:HA3	3:B:502:DO9:C13	2.51	0.41
1:A:264:ALA:HB2	3:A:502:DO9:C05	2.51	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	367/403 (91%)	360 (98%)	7 (2%)	0	100	100
1	B	370/403 (92%)	361 (98%)	9 (2%)	0	100	100
All	All	737/806 (91%)	721 (98%)	16 (2%)	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	320/348 (92%)	310 (97%)	10 (3%)	40	49
1	B	323/348 (93%)	314 (97%)	9 (3%)	43	52
All	All	643/696 (92%)	624 (97%)	19 (3%)	41	50

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	55	LEU
1	A	58	ARG
1	A	106	ASN
1	A	205	SER
1	A	231	ARG
1	A	237	TRP
1	A	272	CYS

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Mol	Chain	Res	Type
1	A	309	SER
1	A	393	SER
1	B	75	SER
1	B	80	ARG
1	B	116	LYS
1	B	214	PHE
1	B	231	ARG
1	B	263	SER
1	B	272	CYS
1	B	309	SER
1	B	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	B	189	GLN
1	B	281	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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
3	DO9	B	502	2	23,29,29	2.69	7 (30%)	26,40,40	1.91	5 (19%)
2	HEM	B	501	1,3	41,50,50	1.50	4 (9%)	45,82,82	1.49	8 (17%)
3	DO9	A	502	2	23,29,29	2.76	7 (30%)	26,40,40	1.83	3 (11%)
2	HEM	A	501	1,3	41,50,50	1.51	5 (12%)	45,82,82	1.54	9 (20%)

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	DO9	B	502	2	-	1/10/18/18	0/4/4/4
2	HEM	B	501	1,3	-	3/12/54/54	-
3	DO9	A	502	2	-	2/10/18/18	0/4/4/4
2	HEM	A	501	1,3	-	4/12/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	DO9	C16-N15	8.13	1.46	1.33
3	B	502	DO9	C16-N15	7.96	1.46	1.33
3	A	502	DO9	C16-N18	6.68	1.47	1.35
3	B	502	DO9	C16-N18	6.17	1.46	1.35
3	B	502	DO9	C02-C09	4.75	1.52	1.43
2	A	501	HEM	C3C-C2C	-4.69	1.33	1.40
2	B	501	HEM	C3C-C2C	-4.63	1.33	1.40
3	A	502	DO9	C02-C09	4.59	1.52	1.43
3	A	502	DO9	C22-C25	4.08	1.53	1.44
3	B	502	DO9	C22-C25	3.99	1.53	1.44
2	A	501	HEM	C3C-CAC	3.55	1.55	1.47
2	B	501	HEM	C3C-CAC	3.47	1.54	1.47
2	A	501	HEM	CAB-C3B	2.98	1.55	1.47
2	B	501	HEM	CAB-C3B	2.89	1.55	1.47
3	A	502	DO9	C19-N18	2.70	1.47	1.41
3	A	502	DO9	C16-S17	-2.66	1.61	1.68
3	B	502	DO9	C16-S17	-2.58	1.61	1.68
3	B	502	DO9	C19-N18	2.45	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAA-C2A	2.12	1.55	1.52
3	B	502	DO9	C12-C11	2.11	1.53	1.46
2	A	501	HEM	CAA-C2A	2.06	1.55	1.52
2	A	501	HEM	CMB-C2B	2.04	1.55	1.50
3	A	502	DO9	C12-C11	2.01	1.52	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	DO9	C02-C03-S04	-6.36	103.98	111.79
3	A	502	DO9	C02-C03-S04	-6.15	104.23	111.79
3	A	502	DO9	C08-C10-N15	-4.45	102.65	113.22
3	B	502	DO9	C08-C10-N15	-4.18	103.30	113.22
3	A	502	DO9	C10-C08-C07	-4.02	124.07	129.46
3	B	502	DO9	C10-C08-C07	-3.90	124.24	129.46
2	B	501	HEM	C4C-CHD-C1D	3.75	127.51	122.56
2	A	501	HEM	C4C-CHD-C1D	3.70	127.44	122.56
2	A	501	HEM	C4D-ND-C1D	3.37	108.56	105.07
2	B	501	HEM	C4D-ND-C1D	3.11	108.28	105.07
2	B	501	HEM	C1B-NB-C4B	2.85	108.02	105.07
2	A	501	HEM	C4B-CHC-C1C	2.65	126.05	122.56
3	B	502	DO9	C14-C12-C11	-2.58	112.05	119.06
2	A	501	HEM	C1B-NB-C4B	2.43	107.59	105.07
2	B	501	HEM	C4B-CHC-C1C	2.38	125.70	122.56
3	B	502	DO9	C10-N15-C16	-2.36	121.25	124.85
2	A	501	HEM	C3D-C4D-ND	-2.27	107.64	110.17
2	B	501	HEM	C3B-C2B-C1B	2.21	108.12	106.49
2	B	501	HEM	C4A-C3A-C2A	2.19	108.52	107.00
2	A	501	HEM	C2D-C1D-ND	-2.15	107.31	109.88
2	A	501	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
2	B	501	HEM	C3D-C4D-ND	-2.05	107.88	110.17
2	A	501	HEM	CHD-C1D-ND	2.03	126.64	124.43
2	A	501	HEM	CBA-CAA-C2A	-2.03	109.16	112.62
2	B	501	HEM	CMA-C3A-C4A	-2.01	125.37	128.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	DO9	C02-C09-C11-C12
3	A	502	DO9	C02-C09-C11-C12
2	A	501	HEM	C3D-CAD-CBD-CGD

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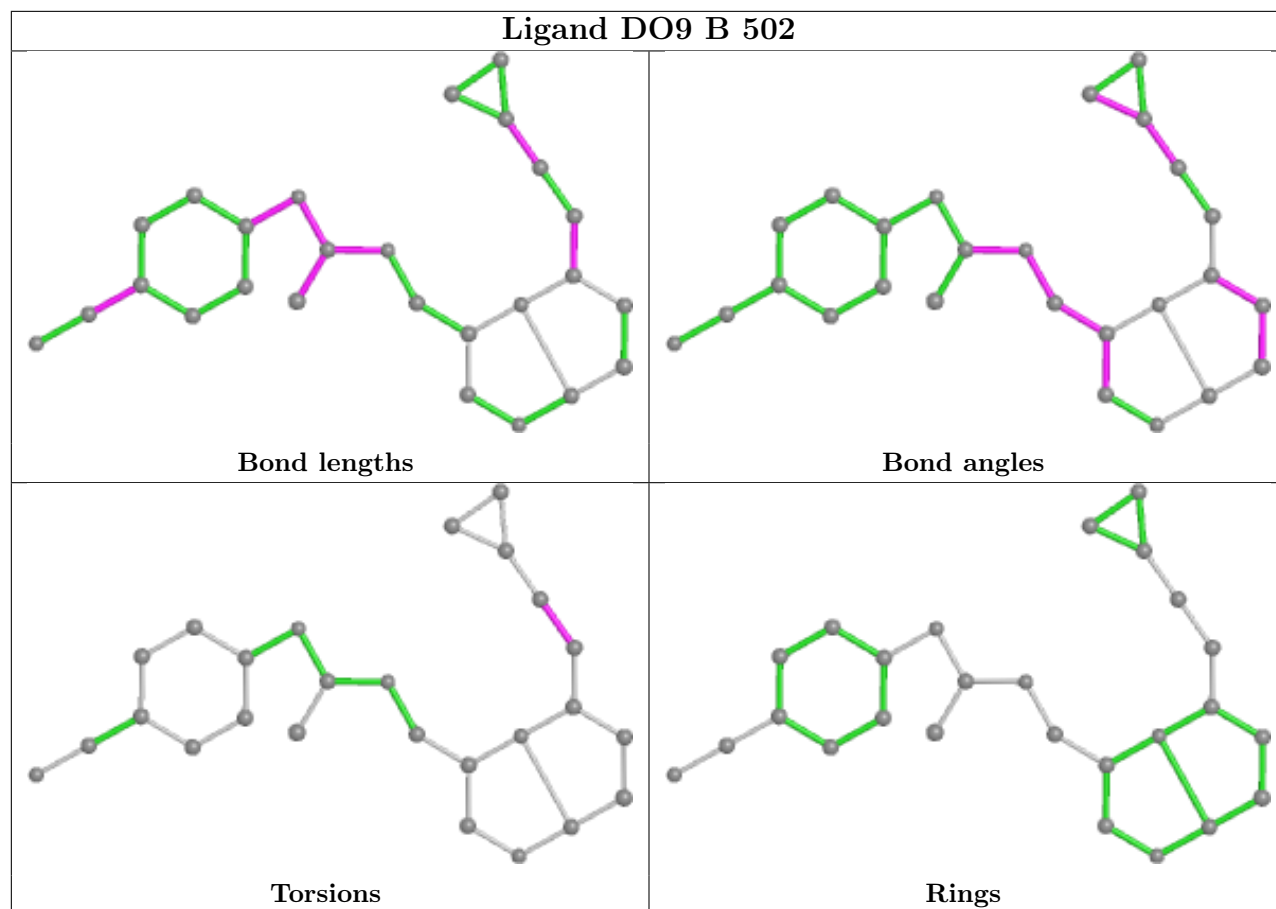
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
3	A	502	DO9	C21-C22-C25-N26

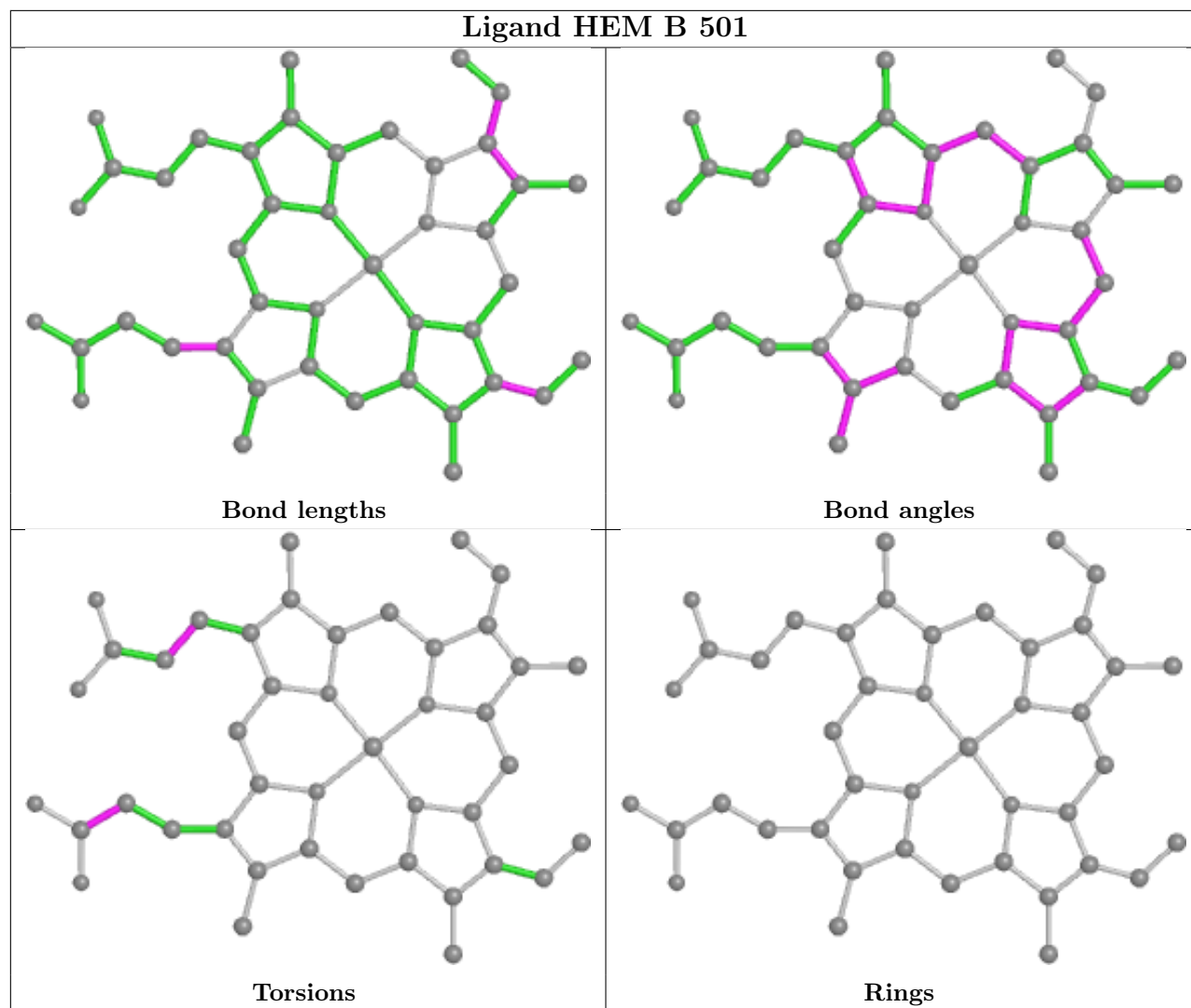
There are no ring outliers.

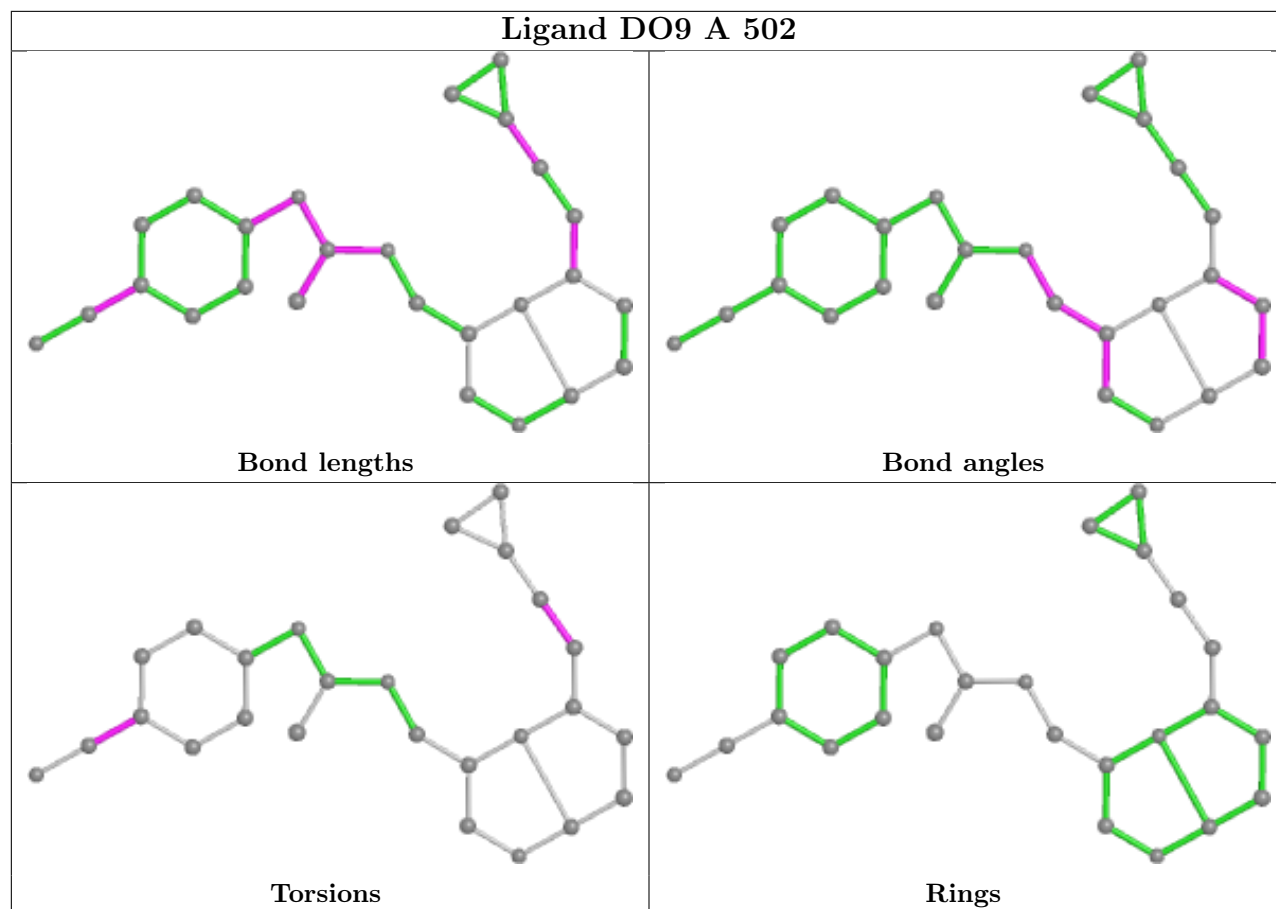
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	DO9	2	0
2	B	501	HEM	3	0
3	A	502	DO9	3	0
2	A	501	HEM	4	0

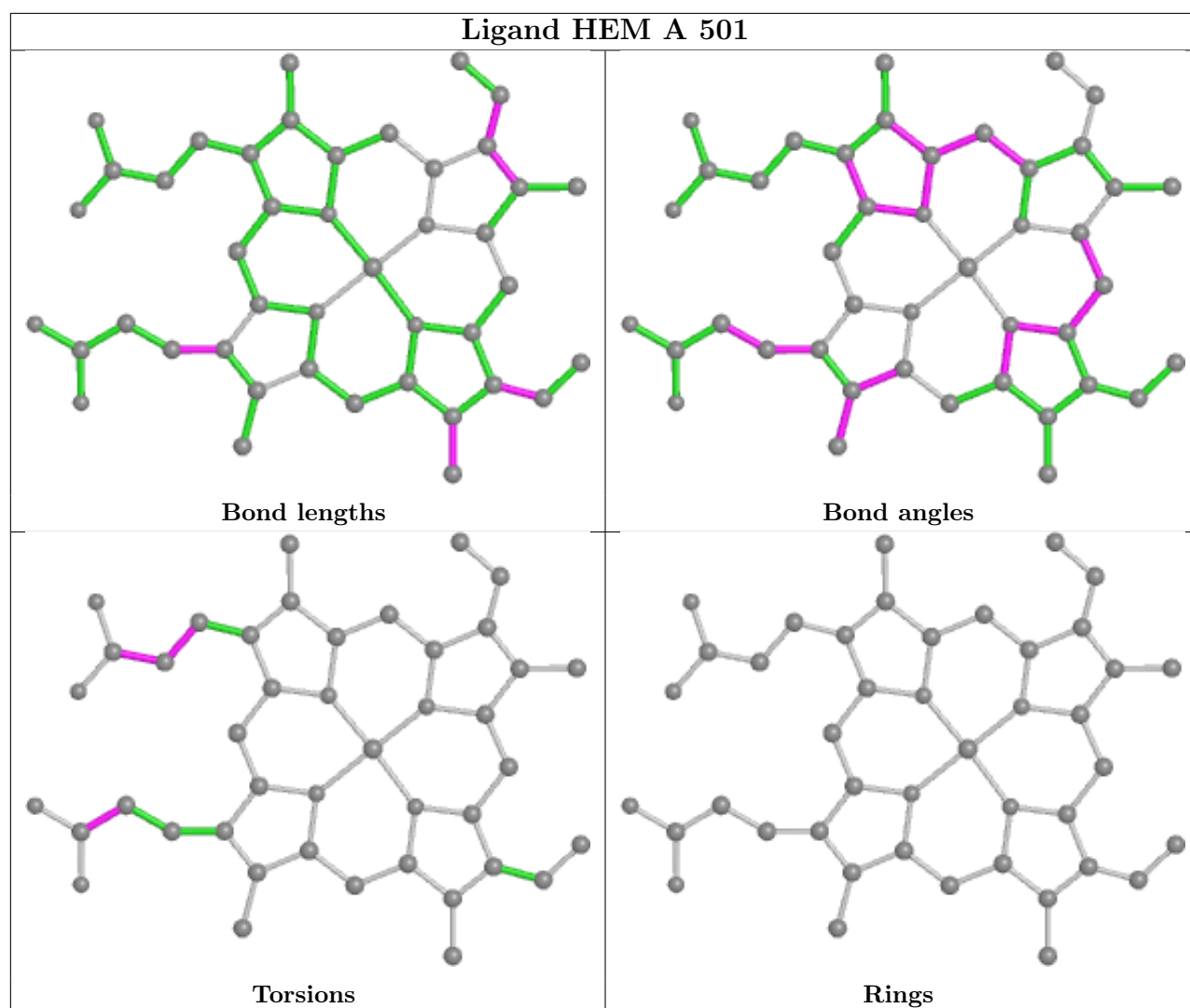
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

### 6.1 Protein, DNA and RNA chains

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	371/403 (92%)	0.29	29 (7%) 13 14	42, 56, 83, 94	0
1	B	374/403 (92%)	-0.06	14 (3%) 41 44	35, 47, 71, 88	0
All	All	745/806 (92%)	0.12	43 (5%) 23 25	35, 52, 80, 94	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	GLY	5.9
1	A	251	GLY	4.8
1	B	285	GLY	4.1
1	A	124	LEU	4.0
1	B	380	GLY	3.8
1	B	11	ILE	3.6
1	A	130	VAL	3.4
1	A	125	VAL	3.3
1	A	81	LEU	3.2
1	A	84	GLY	3.1
1	A	11	ILE	3.1
1	A	85	CYS	3.1
1	A	83	LEU	3.0
1	B	403	GLY	3.0
1	A	241	PRO	2.9
1	A	123	ILE	2.8
1	A	86	ILE	2.7
1	A	255	ASP	2.7
1	A	34	ASP	2.6
1	A	190	MET	2.6
1	B	84	GLY	2.5
1	B	86	ILE	2.5
1	A	254	GLU	2.5
1	A	252	PHE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	283	ALA	2.5
1	B	85	CYS	2.4
1	A	126	TYR	2.4
1	A	129	CYS	2.4
1	A	189	GLN	2.4
1	B	130	VAL	2.4
1	B	124	LEU	2.3
1	A	142	PRO	2.3
1	B	382	THR	2.2
1	A	68	ASP	2.2
1	A	128	ASP	2.2
1	A	396	GLU	2.1
1	B	126	TYR	2.1
1	A	71	THR	2.1
1	A	167	SER	2.1
1	A	88	MET	2.1
1	A	87	THR	2.0
1	A	61	LYS	2.0
1	B	359	SER	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](#)

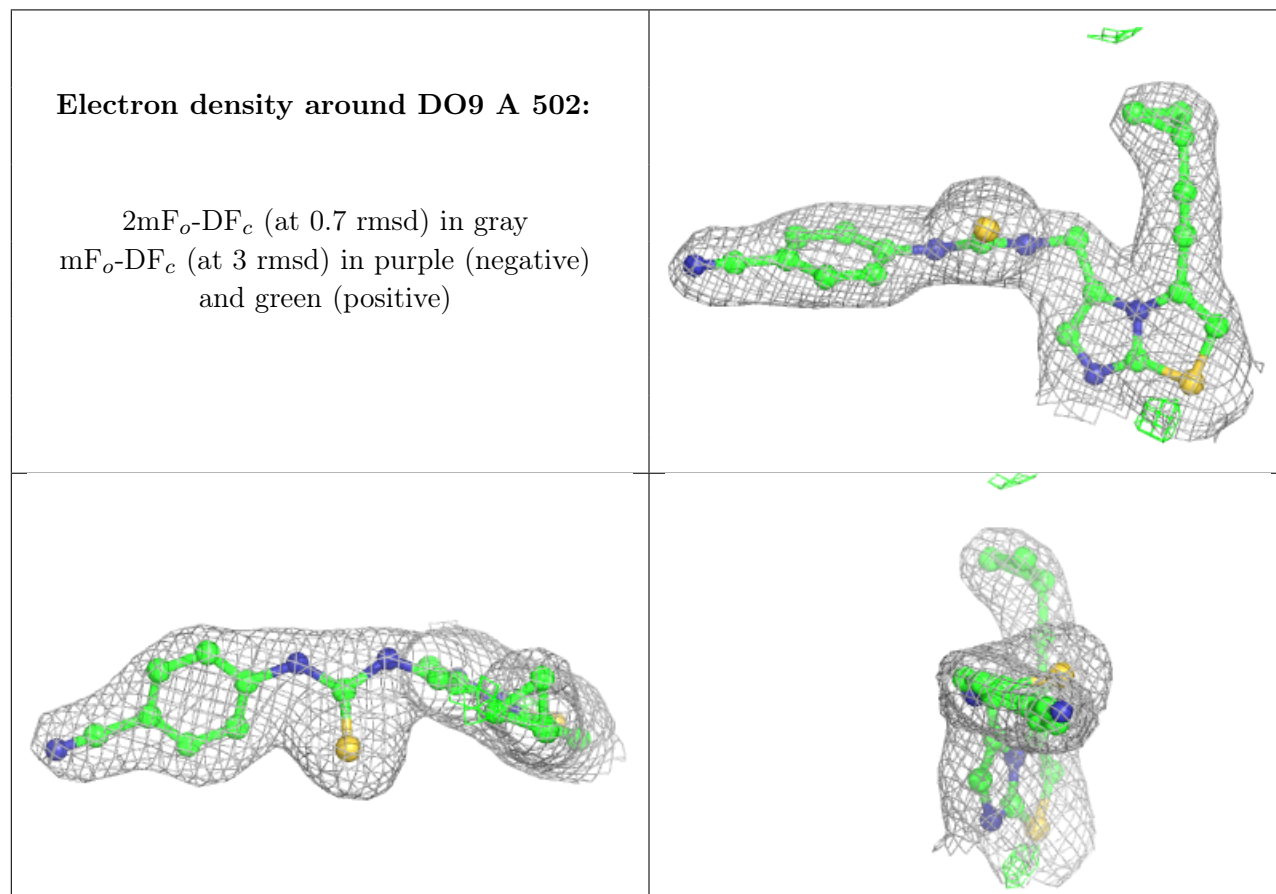
There are no monosaccharides in this entry.

## 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, 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.

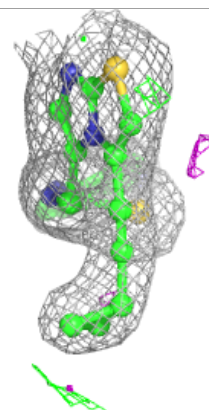
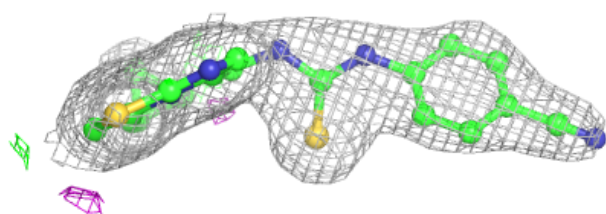
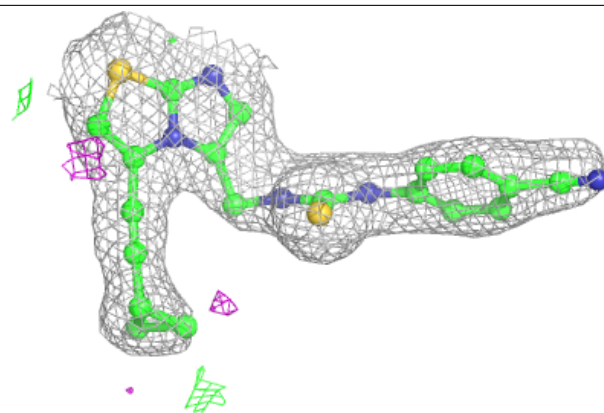
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DO9	A	502	26/26	0.94	0.20	37,44,48,52	0
3	DO9	B	502	26/26	0.96	0.18	30,41,46,67	0
2	HEM	A	501	43/43	0.97	0.12	36,43,50,62	0
2	HEM	B	501	43/43	0.98	0.14	32,40,48,58	0

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.



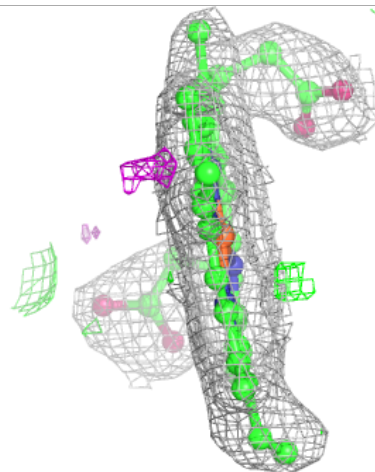
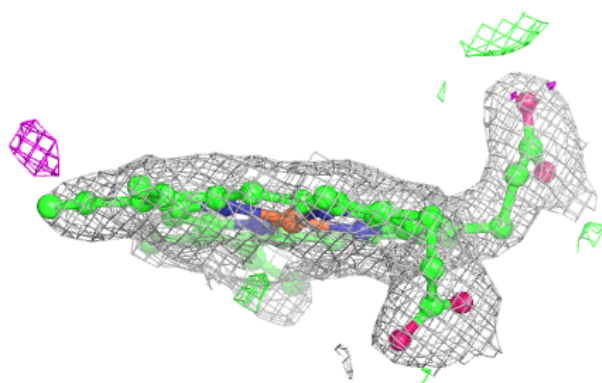
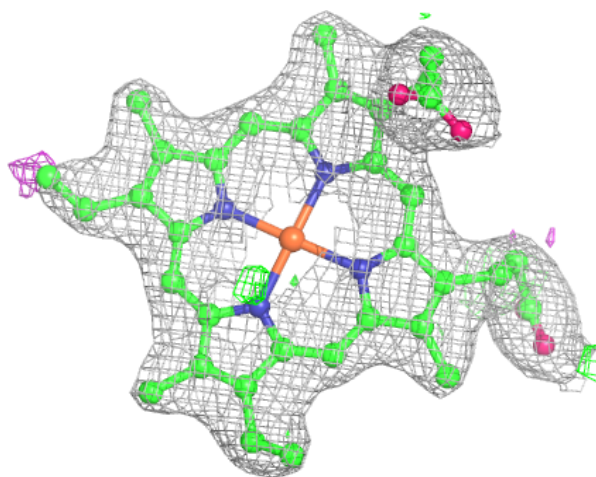
**Electron density around DO9 B 502:**

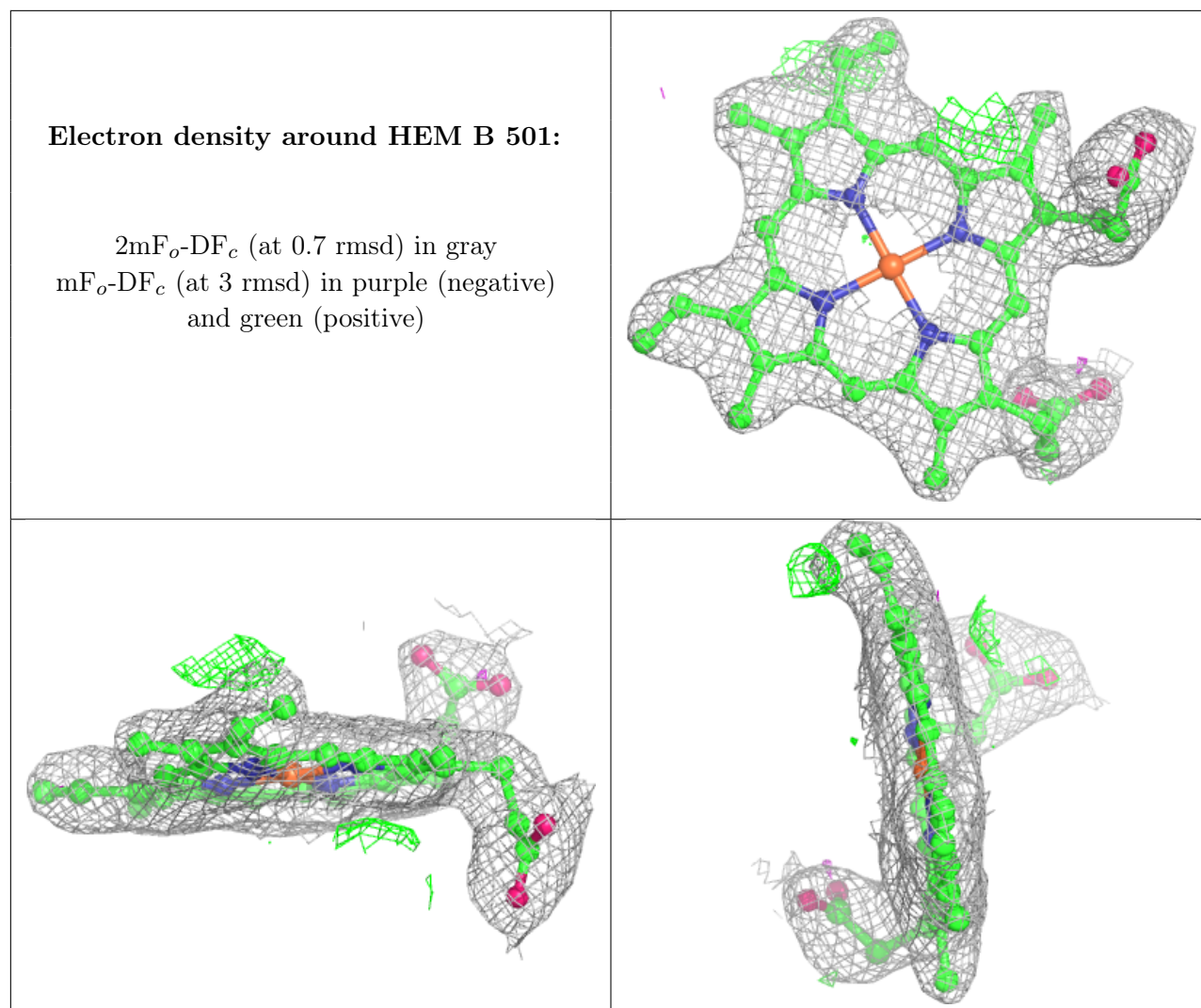
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.