



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 26, 2025 – 12:09 pm GMT

PDB ID : 9ESF  
Title : Holo IDO with a bound inhibitor  
Authors : Wicki, M.; Mac Sweeney, A.  
Deposited on : 2024-03-26  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, 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)	:	2.41

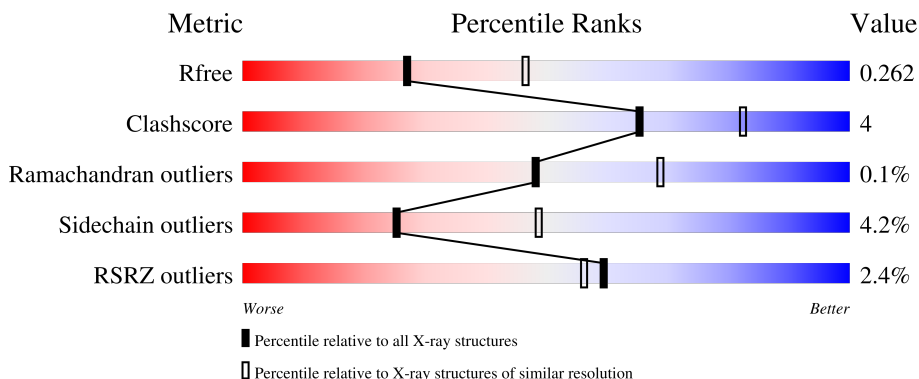
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	365	
1	B	365	
1	C	365	
1	D	365	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11162 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2706	1732	465	497	12			
1	B	328	Total	C	N	O	S	0	1	0
			2734	1749	472	501	12			
1	C	330	Total	C	N	O	S	0	0	0
			2735	1751	469	503	12			
1	D	331	Total	C	N	O	S	0	0	0
			2741	1753	472	504	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P20351
A	380	LEU	-	expression tag	UNP P20351
A	381	GLU	-	expression tag	UNP P20351
A	382	HIS	-	expression tag	UNP P20351
A	383	HIS	-	expression tag	UNP P20351
A	384	HIS	-	expression tag	UNP P20351
A	385	HIS	-	expression tag	UNP P20351
A	386	HIS	-	expression tag	UNP P20351
A	387	HIS	-	expression tag	UNP P20351
B	23	MET	-	initiating methionine	UNP P20351
B	380	LEU	-	expression tag	UNP P20351
B	381	GLU	-	expression tag	UNP P20351
B	382	HIS	-	expression tag	UNP P20351
B	383	HIS	-	expression tag	UNP P20351
B	384	HIS	-	expression tag	UNP P20351
B	385	HIS	-	expression tag	UNP P20351
B	386	HIS	-	expression tag	UNP P20351
B	387	HIS	-	expression tag	UNP P20351
C	23	MET	-	initiating methionine	UNP P20351
C	380	LEU	-	expression tag	UNP P20351
C	381	GLU	-	expression tag	UNP P20351

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Chain	Residue	Modelled	Actual	Comment	Reference
C	382	HIS	-	expression tag	UNP P20351
C	383	HIS	-	expression tag	UNP P20351
C	384	HIS	-	expression tag	UNP P20351
C	385	HIS	-	expression tag	UNP P20351
C	386	HIS	-	expression tag	UNP P20351
C	387	HIS	-	expression tag	UNP P20351
D	23	MET	-	initiating methionine	UNP P20351
D	380	LEU	-	expression tag	UNP P20351
D	381	GLU	-	expression tag	UNP P20351
D	382	HIS	-	expression tag	UNP P20351
D	383	HIS	-	expression tag	UNP P20351
D	384	HIS	-	expression tag	UNP P20351
D	385	HIS	-	expression tag	UNP P20351
D	386	HIS	-	expression tag	UNP P20351
D	387	HIS	-	expression tag	UNP P20351

- # HEM

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
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

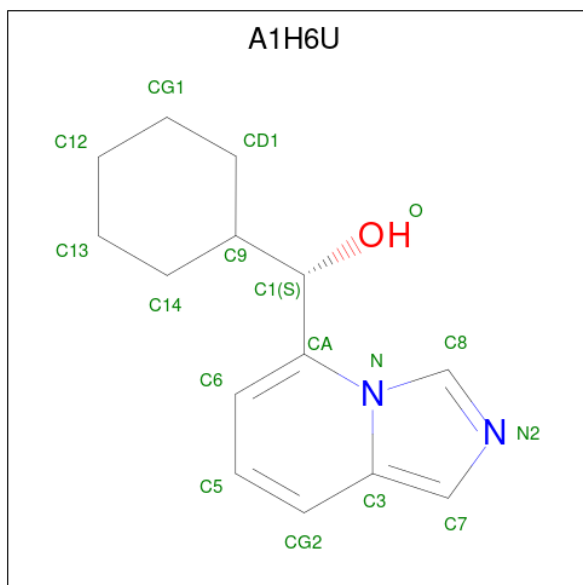


WORLD WIDE  
PDB  
PROTEIN DATA BANK

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

- Molecule 3 is ( {S} )-cyclohexyl(imidazo[1,5-a]pyridin-5-yl)methanol (three-letter code: A1H6U) (formula: C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).

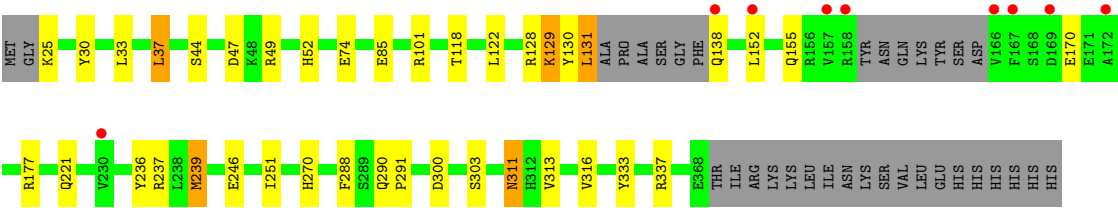


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	14	2	1		
3	B	1	Total	C	N	O	0	0
			17	14	2	1		
3	C	1	Total	C	N	O	0	0
			17	14	2	1		
3	D	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.77Å 143.77Å 141.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 2.50 47.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.06-2.50) 99.9 (47.06-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, $R_{free}$	0.245 , 0.274 0.238 , 0.262	Depositor DCC
$R_{free}$ test set	2882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 17.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.060 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A1H6U

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	0.36	0/2759	0.49	0/3718
1	B	0.36	0/2790	0.49	0/3760
1	C	0.38	0/2791	0.53	1/3766 (0.0%)
1	D	0.36	0/2794	0.49	0/3767
All	All	0.36	0/11134	0.50	1/15011 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	SER	C-N-CA	5.29	134.93	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2706	0	2713	24	0
1	B	2734	0	2734	22	0
1	C	2735	0	2729	26	0
1	D	2741	0	2727	28	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	17	0	0	1	0
3	B	17	0	0	1	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
All	All	11162	0	11023	81	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 4.

The worst 5 of 81 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:D:49:ARG:HH22	1:D:129:LYS:NZ	1.55	1.04
1:C:49:ARG:HH22	1:C:129:LYS:NZ	1.58	1.01
1:A:49:ARG:HH22	1:A:129:LYS:NZ	1.56	1.01
1:C:49:ARG:HH22	1:C:129:LYS:HZ2	1.18	0.90
1:A:49:ARG:HH22	1:A:129:LYS:HZ3	1.24	0.82

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	318/365 (87%)	310 (98%)	8 (2%)	0	100	100
1	B	323/365 (88%)	317 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	326/365 (89%)	314 (96%)	11 (3%)	1 (0%)	37	56
1	D	325/365 (89%)	317 (98%)	8 (2%)	0	100	100
All	All	1292/1460 (88%)	1258 (97%)	33 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	ALA

### 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	300/337 (89%)	289 (96%)	11 (4%)	29	55
1	B	301/337 (89%)	288 (96%)	13 (4%)	25	48
1	C	301/337 (89%)	287 (95%)	14 (5%)	22	44
1	D	300/337 (89%)	287 (96%)	13 (4%)	25	48
All	All	1202/1348 (89%)	1151 (96%)	51 (4%)	25	49

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	131	LEU
1	C	311	ASN
1	D	311	ASN
1	C	135	SER
1	C	171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	221	GLN

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Mol	Chain	Res	Type
1	C	311	ASN
1	D	274	GLN
1	C	274	GLN
1	D	52	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 oligosaccharides in this entry.

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

8 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	A1H6U	B	402	2	16,19,19	1.21	2 (12%)	16,26,26	1.08	1 (6%)
3	A1H6U	C	402	2	16,19,19	1.29	2 (12%)	16,26,26	1.23	1 (6%)
3	A1H6U	A	402	2	16,19,19	1.26	2 (12%)	16,26,26	0.94	1 (6%)
2	HEM	D	401	1,3	41,50,50	0.95	2 (4%)	45,82,82	1.15	3 (6%)
3	A1H6U	D	402	2	16,19,19	1.26	2 (12%)	16,26,26	1.13	1 (6%)
2	HEM	B	401	1,3	41,50,50	0.95	2 (4%)	45,82,82	1.08	3 (6%)
2	HEM	A	401	1,3	41,50,50	0.97	2 (4%)	45,82,82	1.13	3 (6%)
2	HEM	C	401	1,3	41,50,50	0.95	1 (2%)	45,82,82	1.12	3 (6%)

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	A1H6U	B	402	2	-	1/8/16/16	0/3/3/3
3	A1H6U	C	402	2	-	1/8/16/16	0/3/3/3
3	A1H6U	A	402	2	-	1/8/16/16	0/3/3/3
2	HEM	D	401	1,3	-	6/12/54/54	-
3	A1H6U	D	402	2	-	1/8/16/16	0/3/3/3
2	HEM	B	401	1,3	-	6/12/54/54	-
2	HEM	A	401	1,3	-	6/12/54/54	-
2	HEM	C	401	1,3	-	6/12/54/54	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	CHB-C1B	3.05	1.42	1.35
3	B	402	A1H6U	C6-CA	-3.04	1.34	1.39
3	C	402	A1H6U	C6-CA	-3.03	1.34	1.39
2	B	401	HEM	CHB-C1B	3.00	1.42	1.35
3	A	402	A1H6U	C6-CA	-2.98	1.34	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C4C-CHD-C1D	3.79	127.56	122.56
2	D	401	HEM	C4C-CHD-C1D	3.71	127.45	122.56
3	D	402	A1H6U	C5-CG2-C3	-3.69	119.16	121.25
3	C	402	A1H6U	C5-CG2-C3	-3.63	119.19	121.25
2	B	401	HEM	C4C-CHD-C1D	3.60	127.31	122.56

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1H6U	O-C1-CA-C6
3	C	402	A1H6U	O-C1-CA-C6
2	A	401	HEM	C2B-C3B-CAB-CBB
2	B	401	HEM	C2B-C3B-CAB-CBB
2	C	401	HEM	C2B-C3B-CAB-CBB

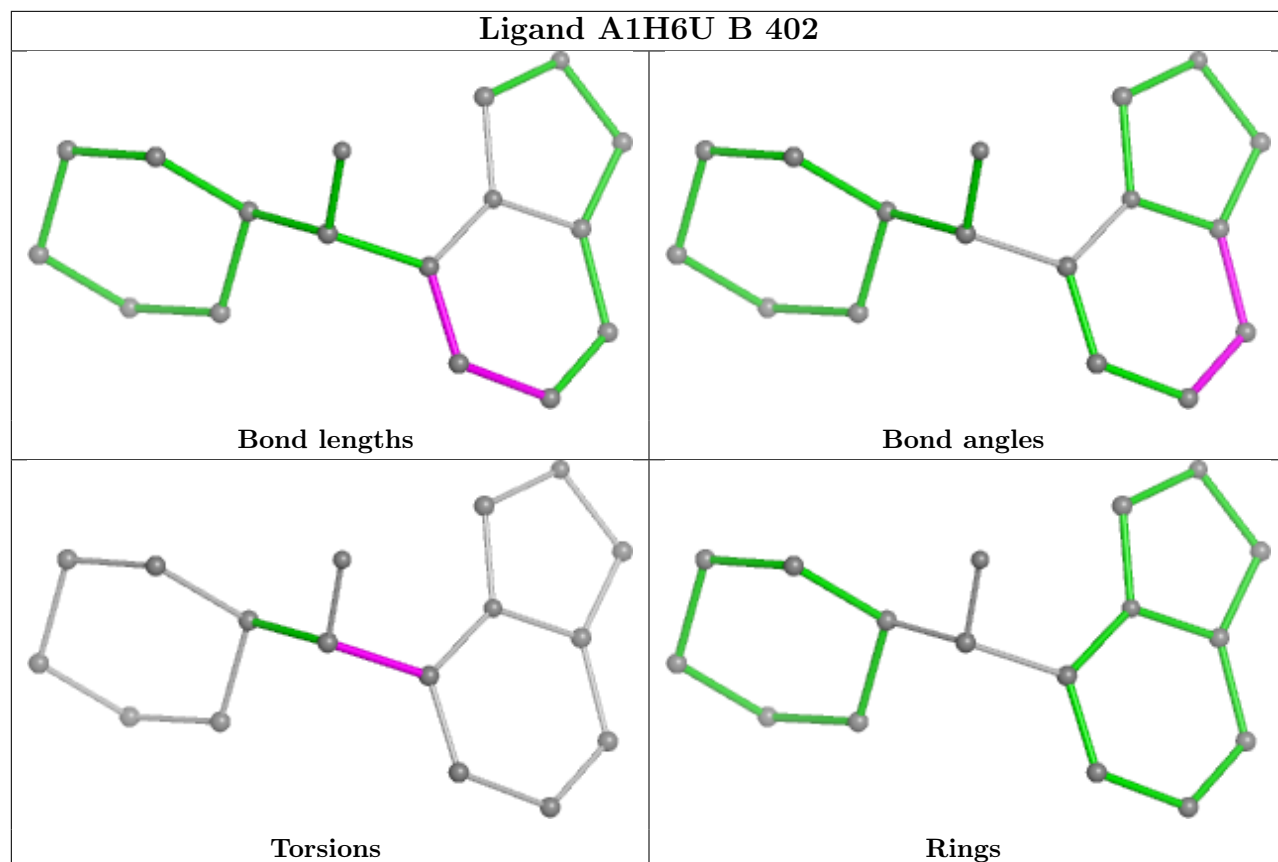
There are no ring outliers.

7 monomers are involved in 7 short contacts:

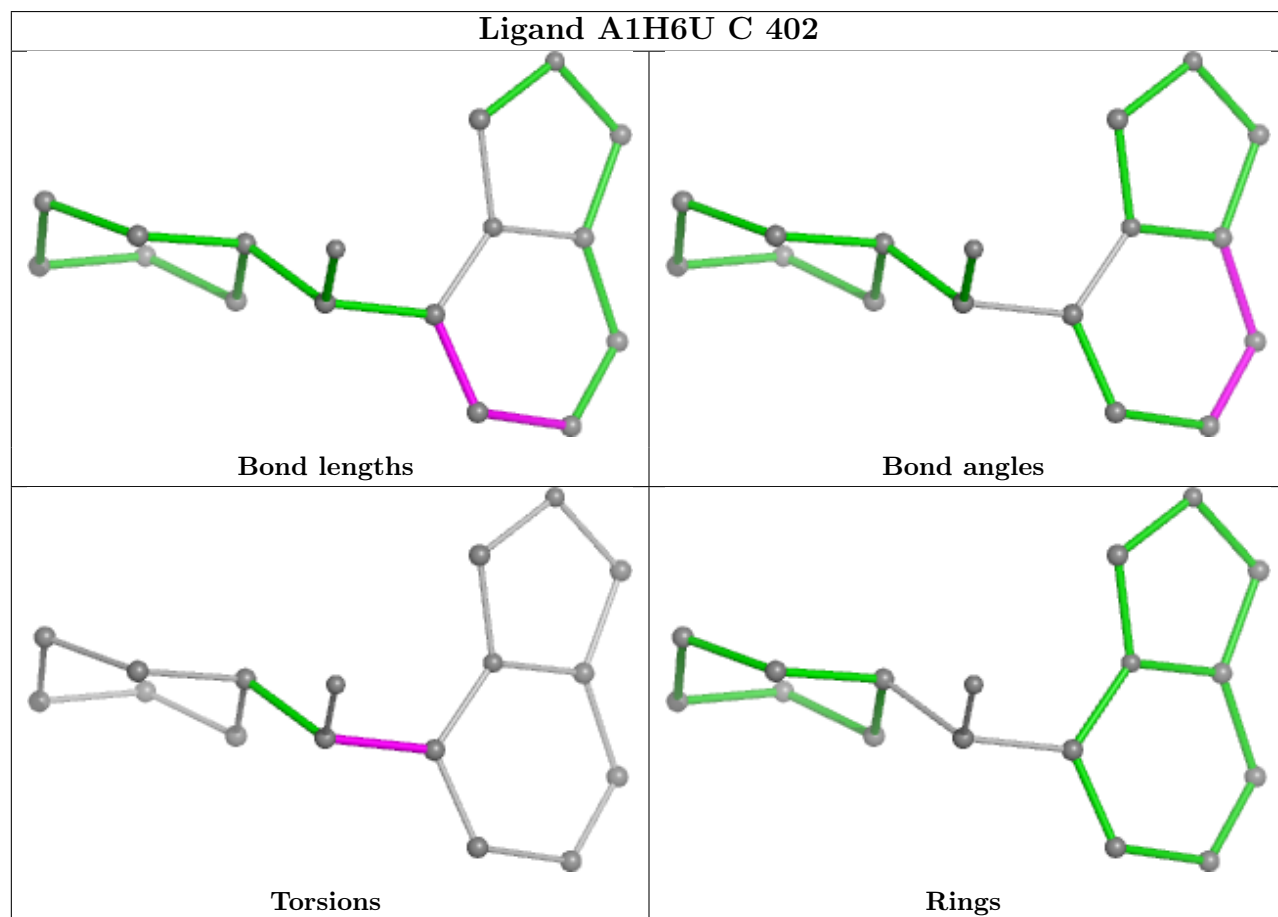
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	A1H6U	1	0
3	A	402	A1H6U	1	0
2	D	401	HEM	1	0
3	D	402	A1H6U	1	0
2	B	401	HEM	1	0
2	A	401	HEM	1	0
2	C	401	HEM	1	0

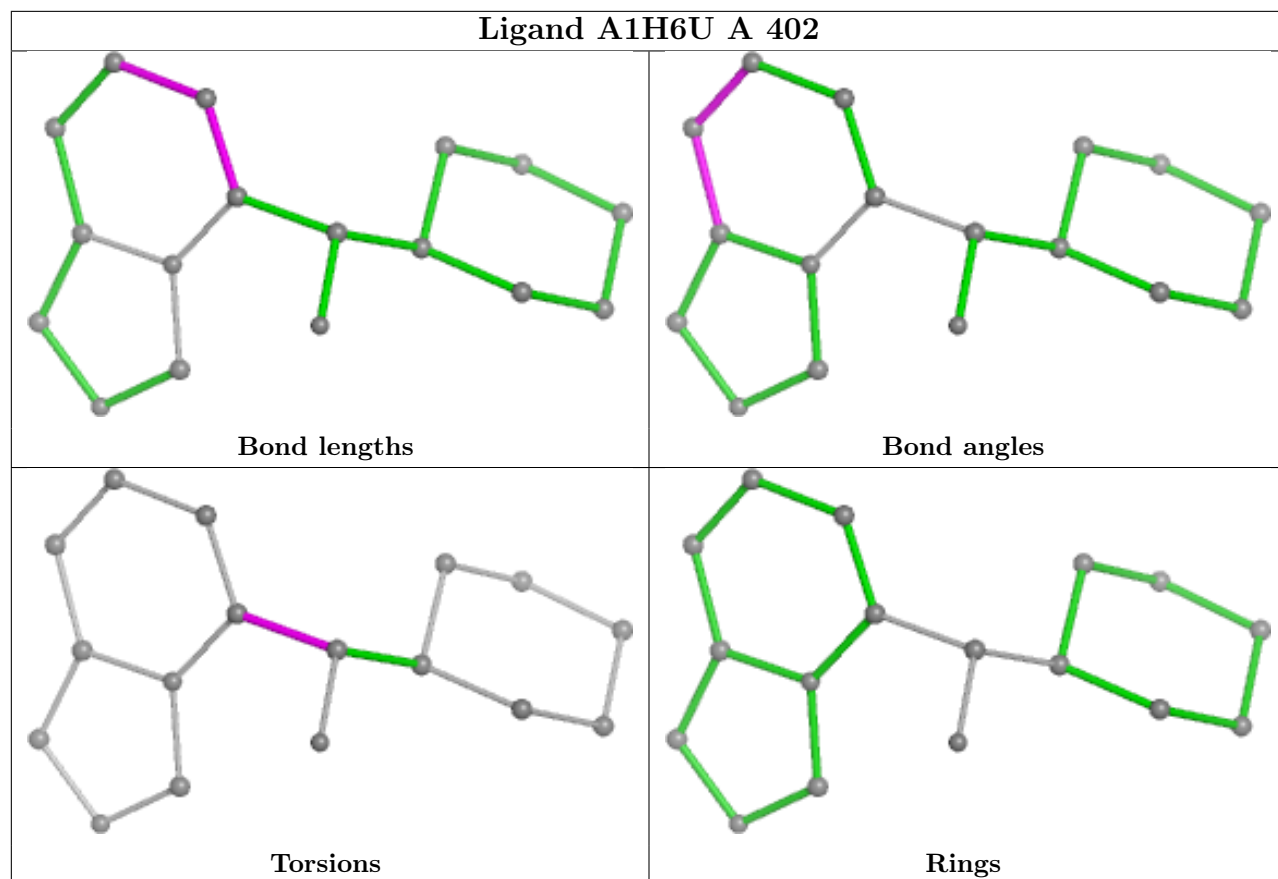
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand A1H6U B 402

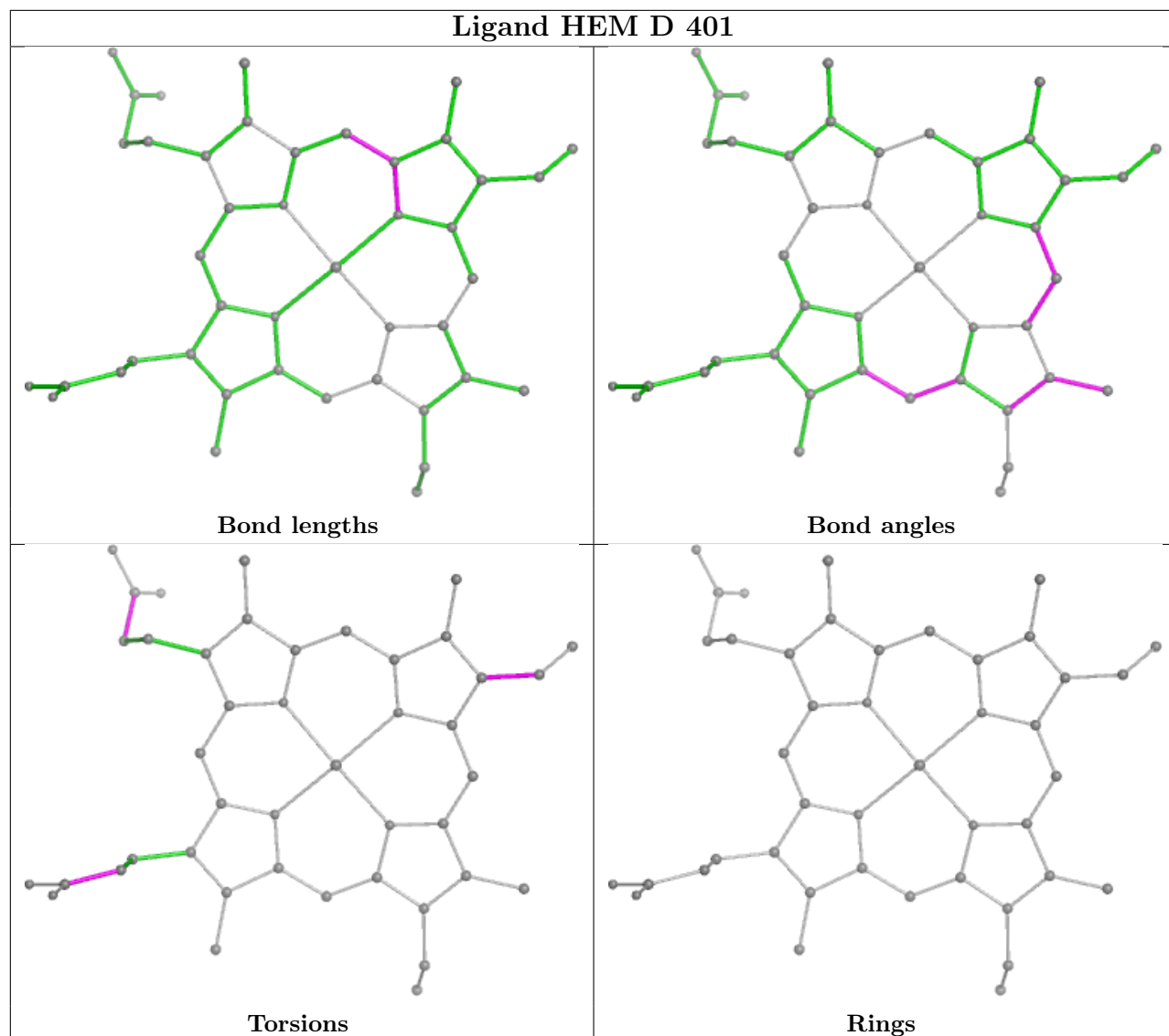


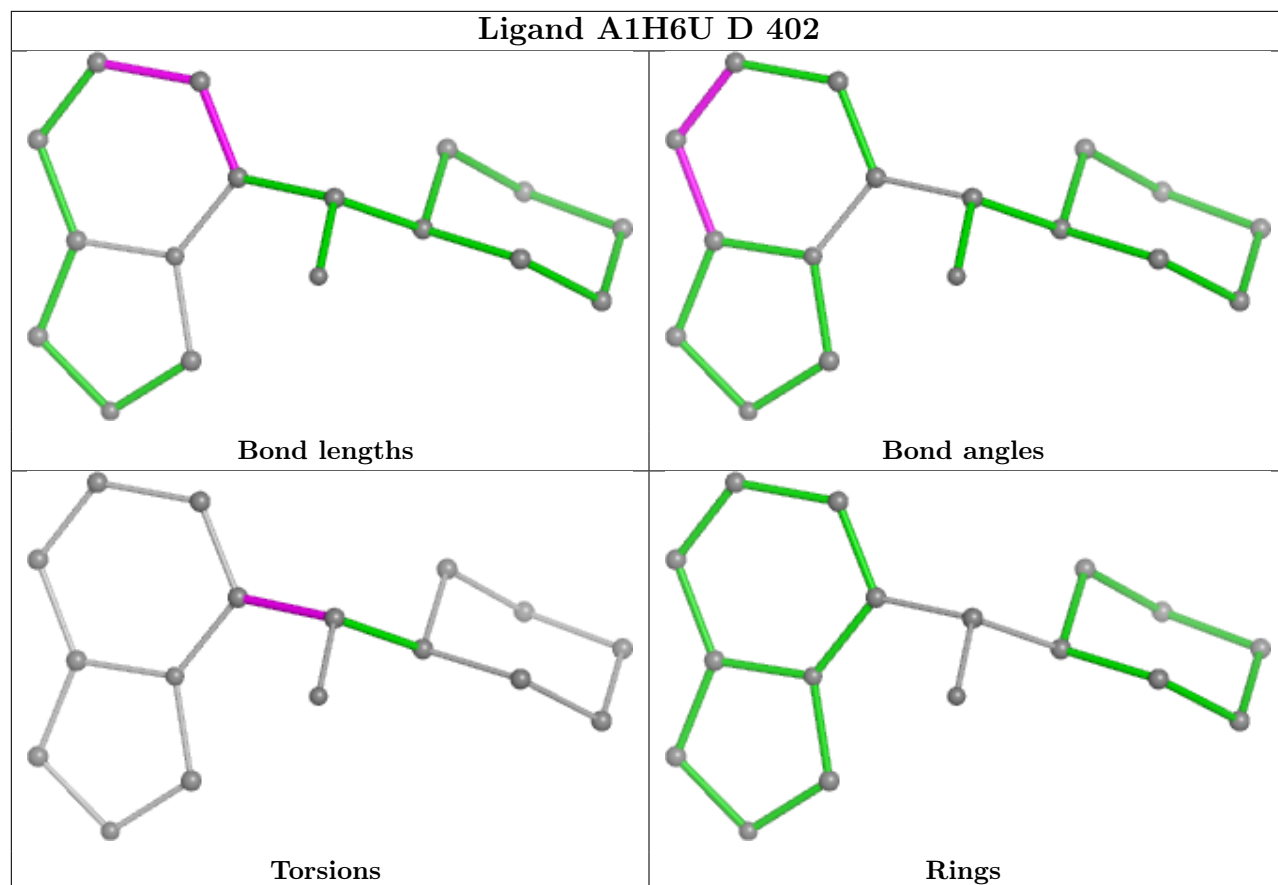
## Ligand A1H6U C 402

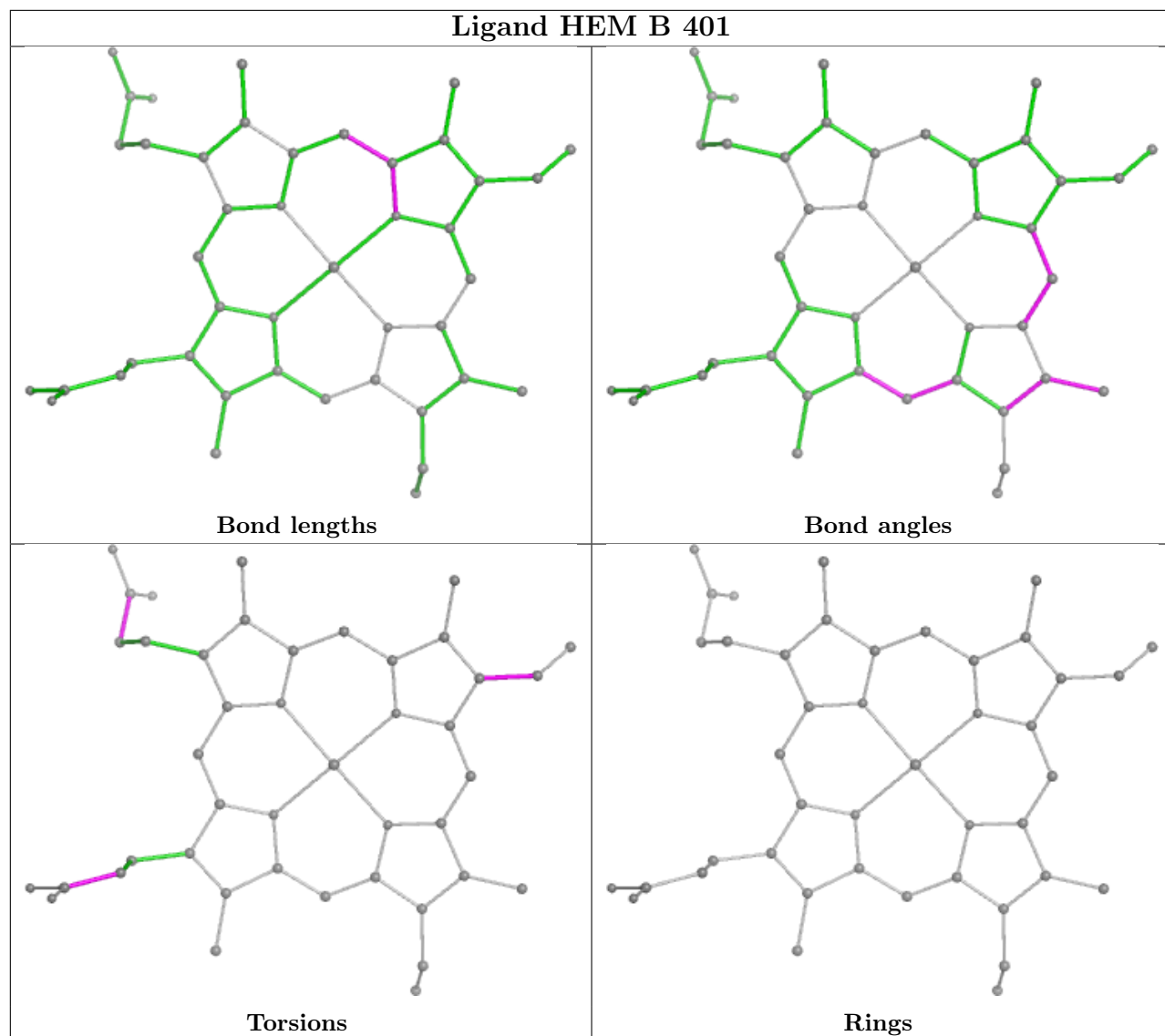


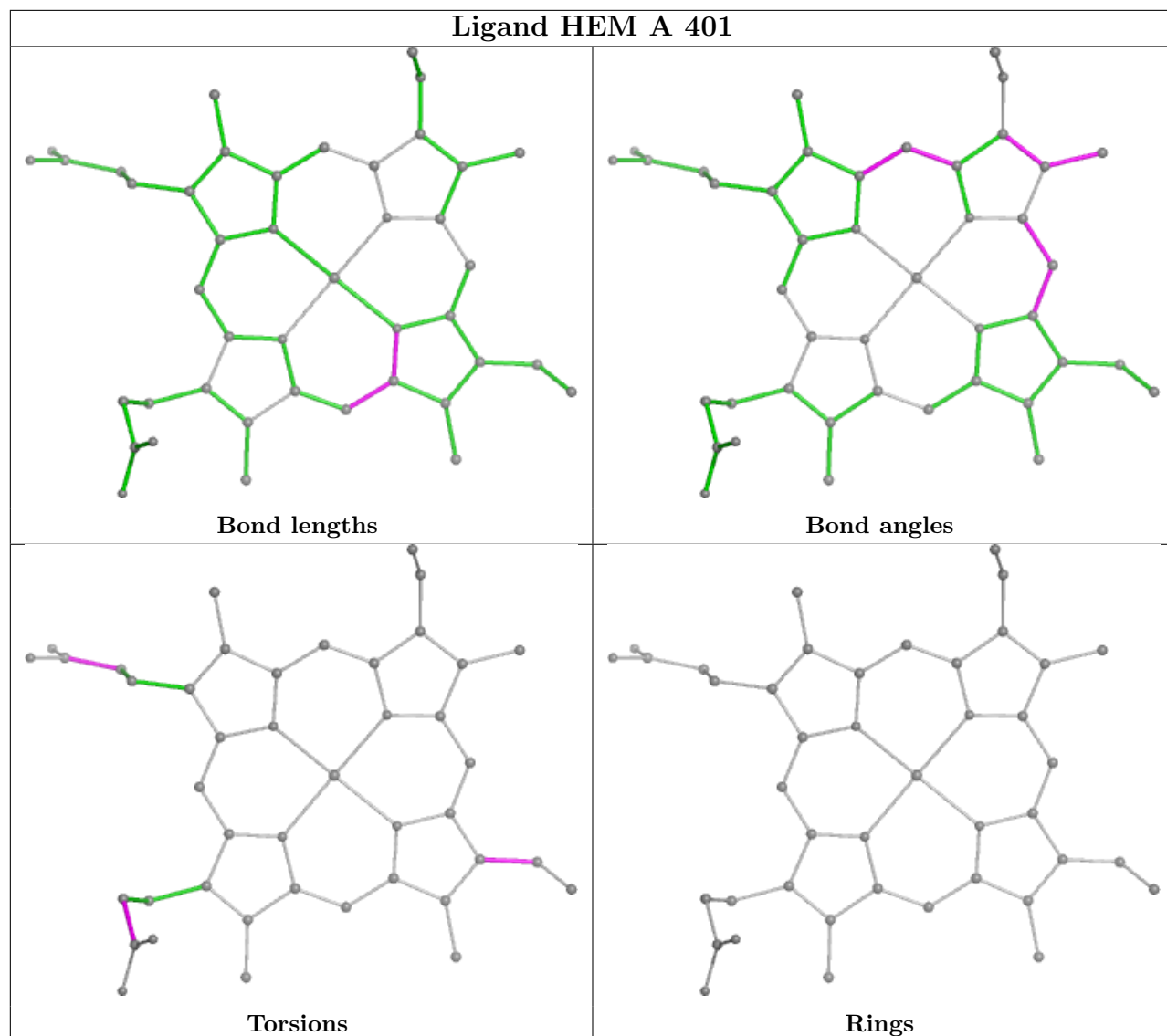


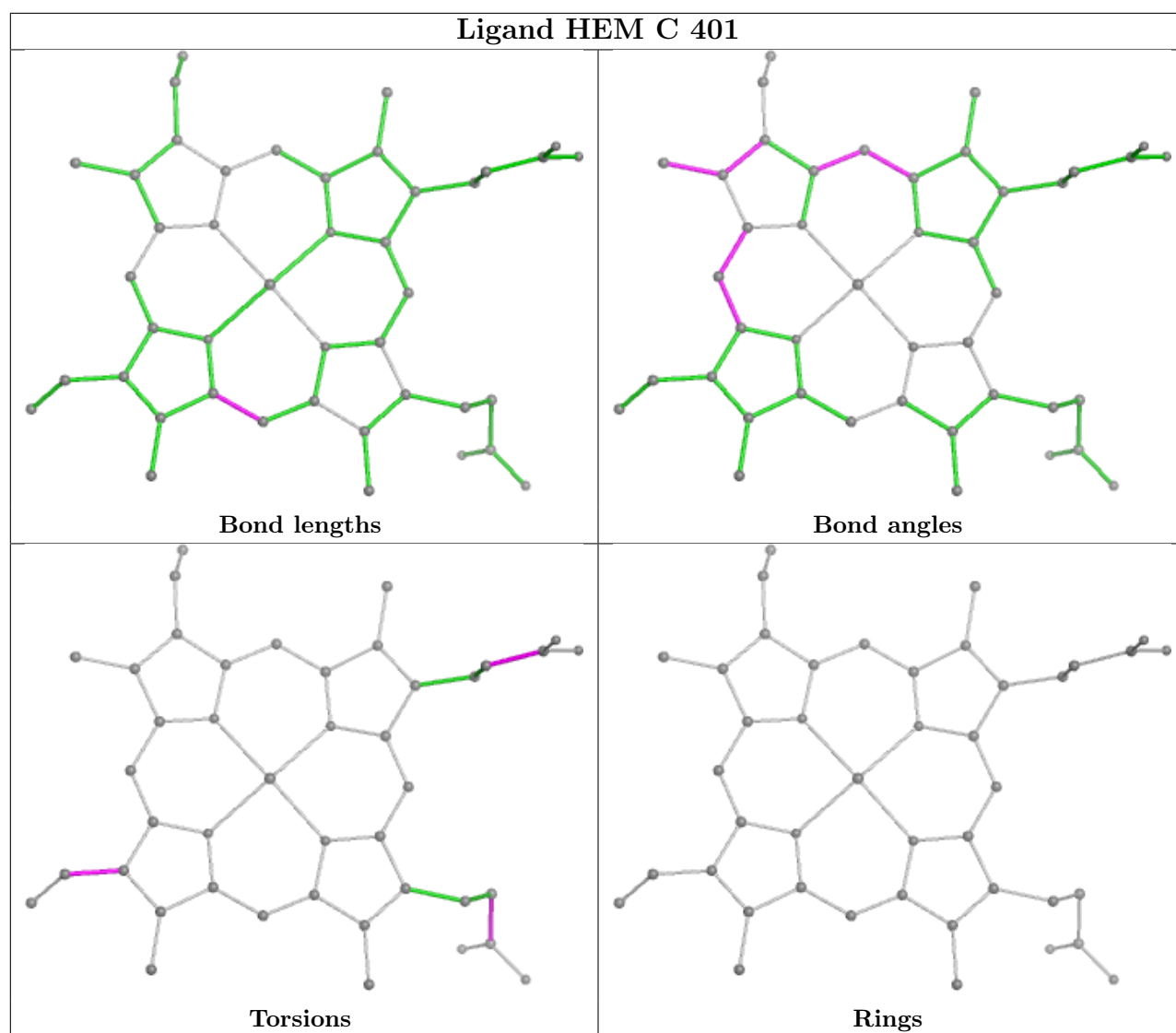












## 5.7 Other polymers [i](#)

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	324/365 (88%)	-0.05	3 (0%) 81 78	34, 54, 77, 92	0
1	B	328/365 (89%)	0.09	10 (3%) 52 49	29, 53, 80, 105	1 (0%)
1	C	330/365 (90%)	0.04	10 (3%) 52 49	33, 51, 73, 95	0
1	D	331/365 (90%)	0.08	9 (2%) 56 52	34, 52, 83, 100	0
All	All	1313/1460 (89%)	0.04	32 (2%) 59 56	29, 52, 79, 105	1 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	4.9
1	C	168	SER	4.6
1	D	166	VAL	4.0
1	B	152	LEU	3.6
1	B	166	VAL	3.6

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

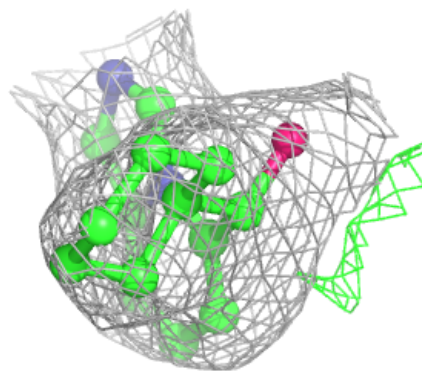
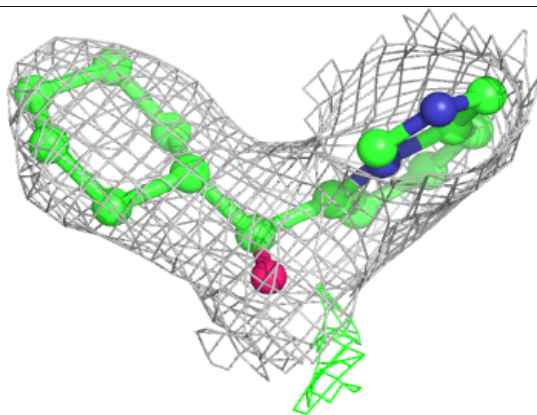
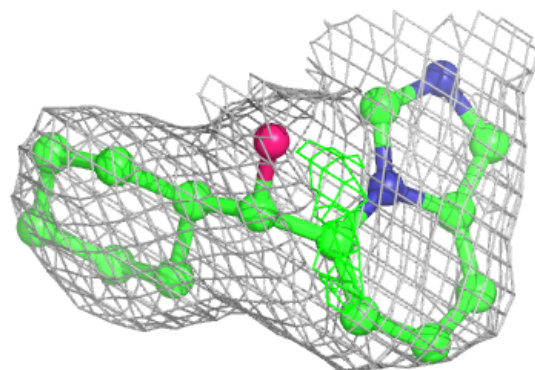
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
3	A1H6U	A	402	17/17	0.91	0.10	53,53,54,54	0
3	A1H6U	D	402	17/17	0.93	0.09	40,42,43,43	0
3	A1H6U	C	402	17/17	0.95	0.09	53,54,54,54	0
2	HEM	C	401	43/43	0.96	0.09	47,48,52,54	0
3	A1H6U	B	402	17/17	0.96	0.06	36,37,37,37	0
2	HEM	B	401	43/43	0.97	0.08	50,51,55,56	0
2	HEM	D	401	43/43	0.97	0.08	49,50,51,52	0
2	HEM	A	401	43/43	0.98	0.07	47,48,51,51	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.

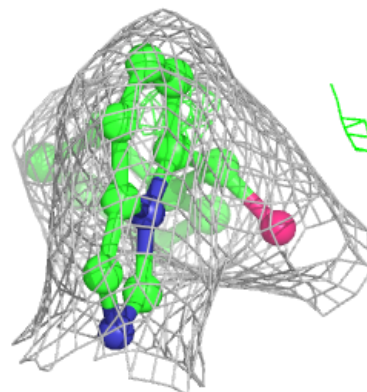
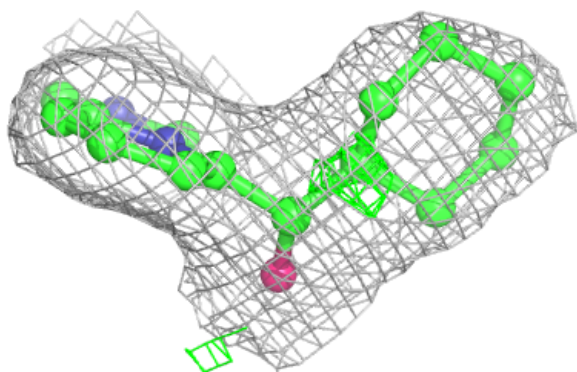
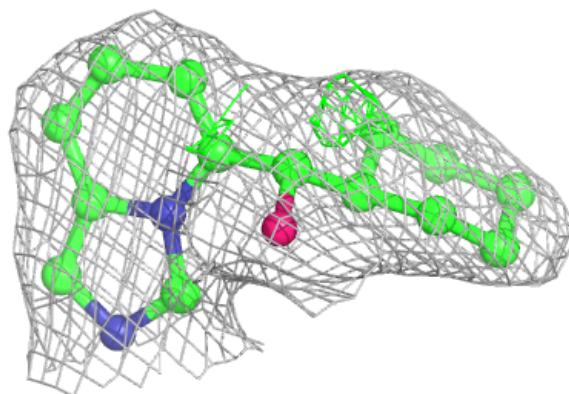
**Electron density around A1H6U A 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

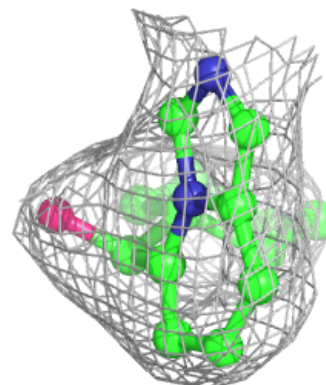
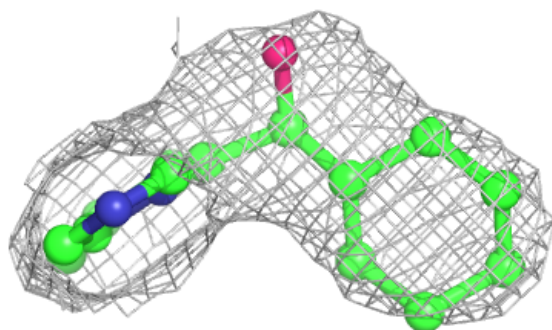
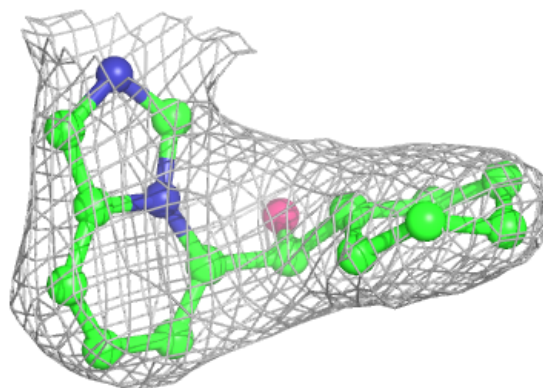


**Electron density around A1H6U D 402:**

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

**Electron density around A1H6U C 402:**

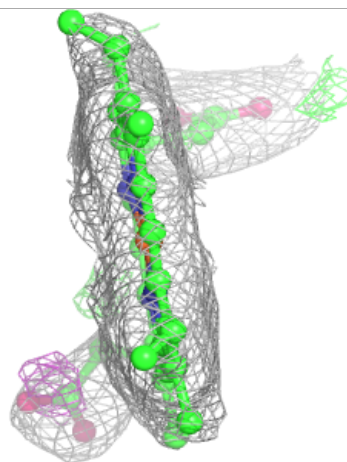
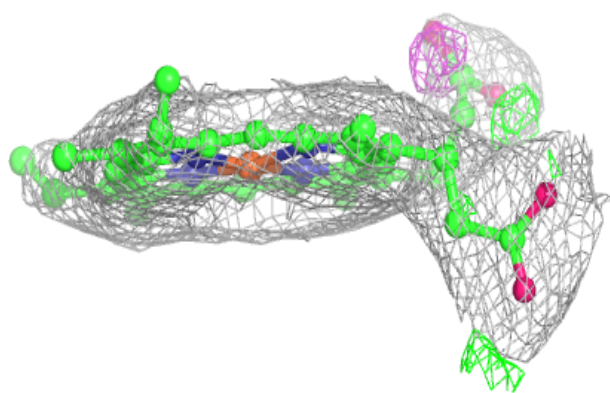
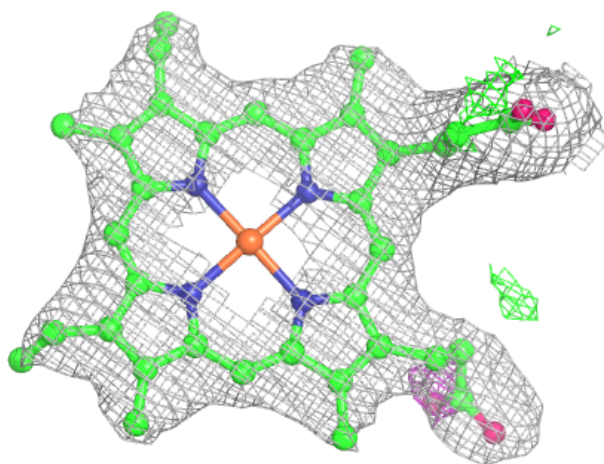
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





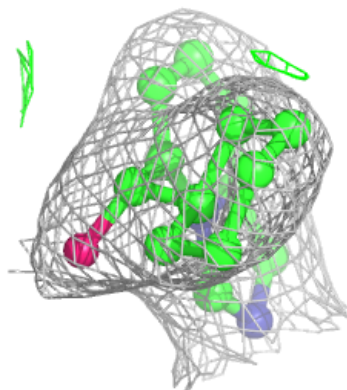
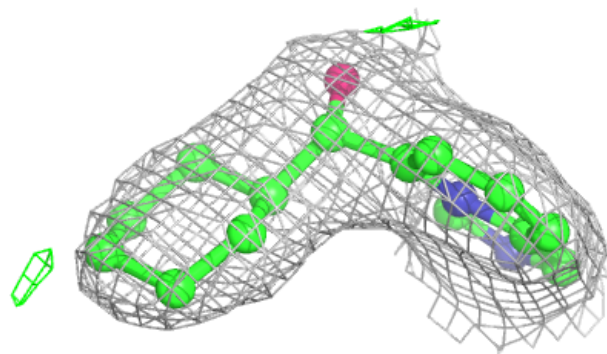
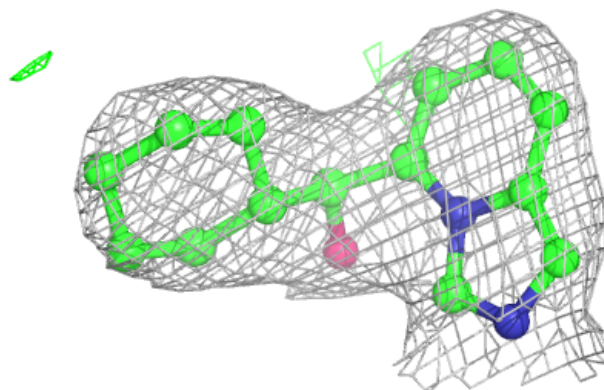
**Electron density around HEM C 401:**

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



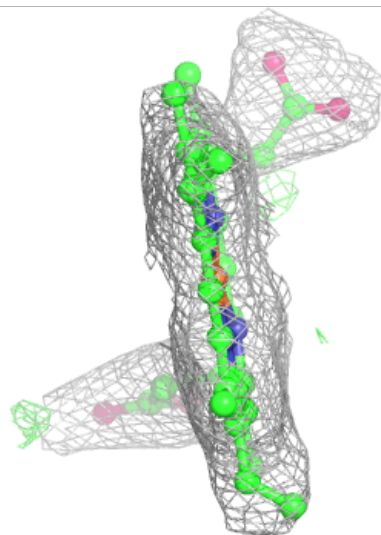
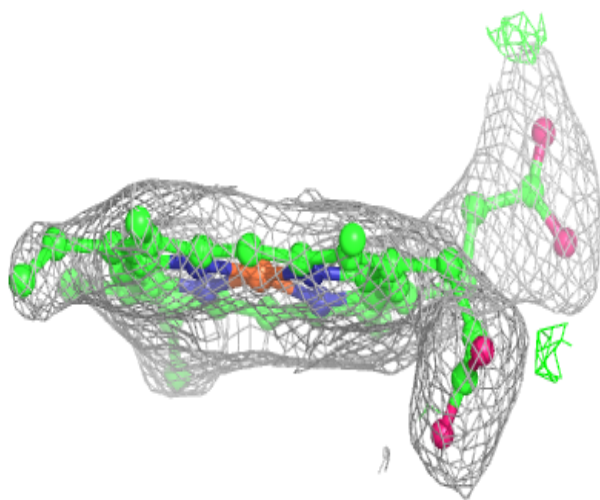
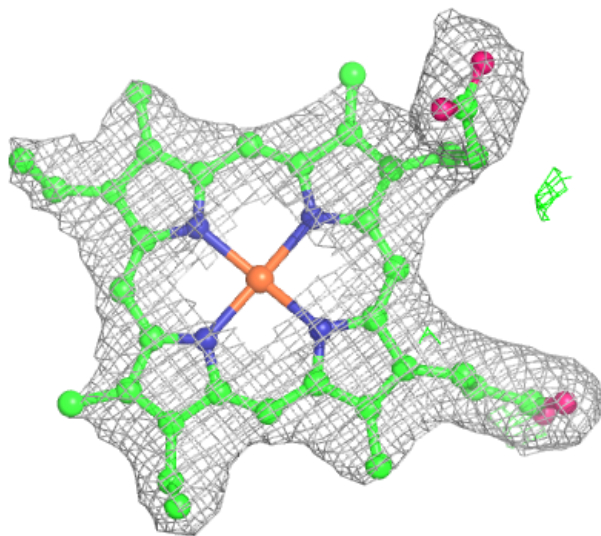
**Electron density around A1H6U B 402:**

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



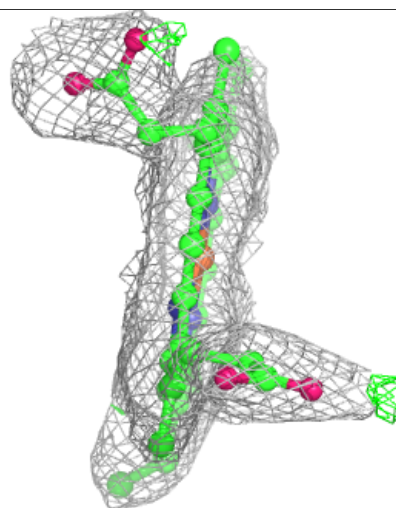
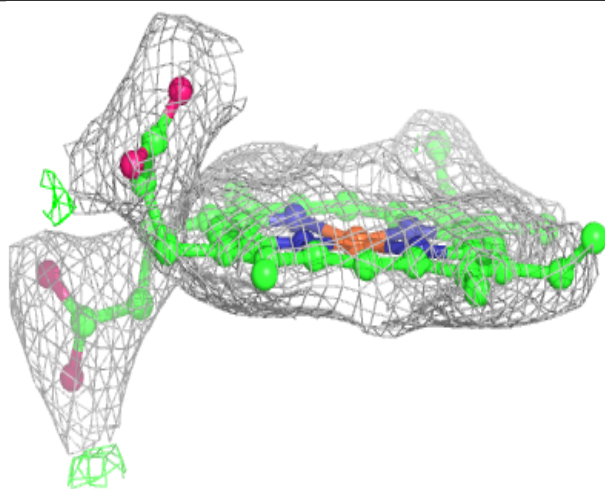
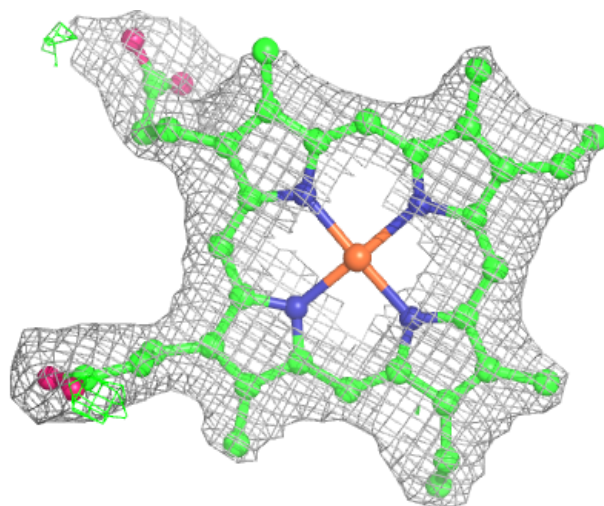
**Electron density around HEM B 401:**

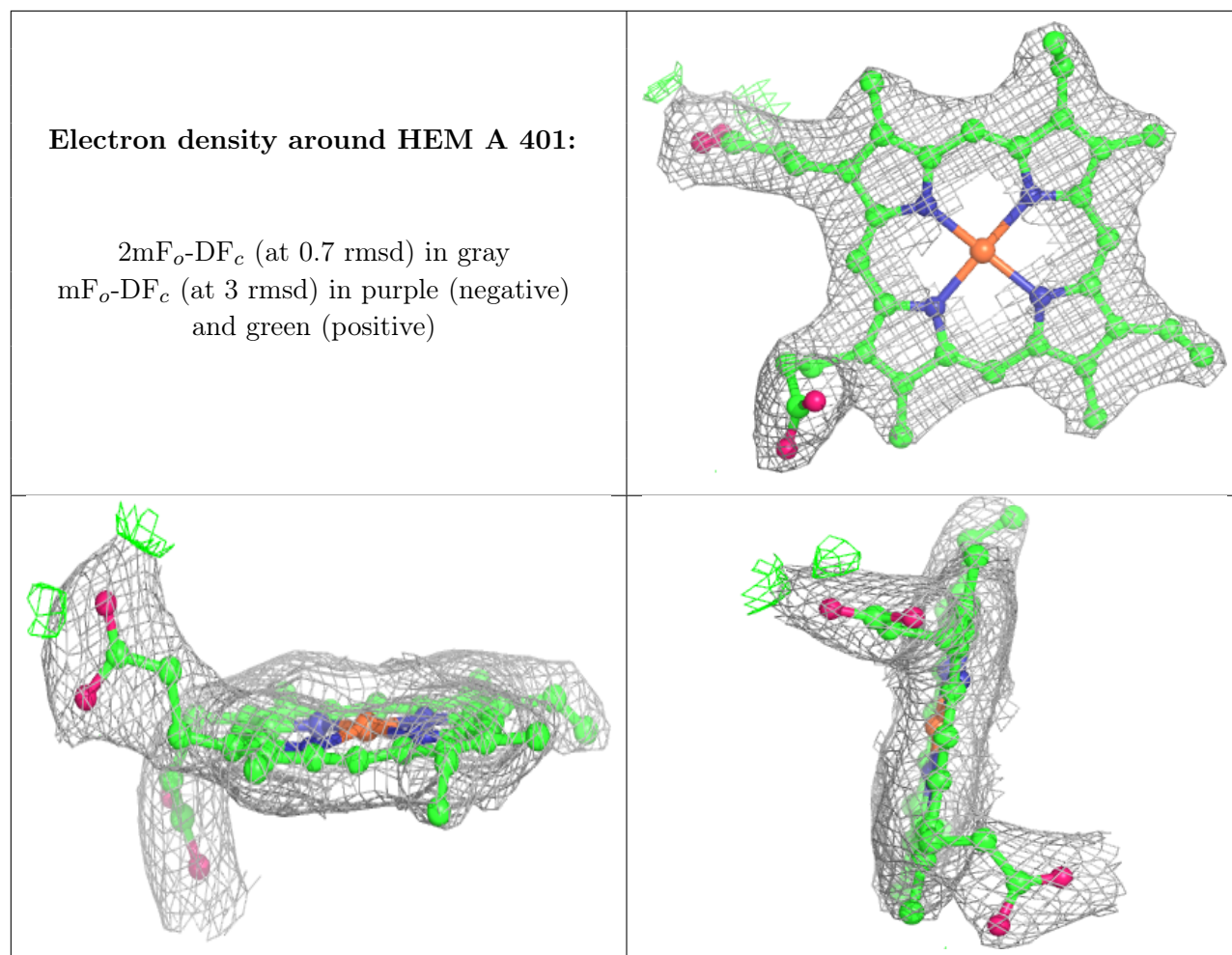
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM D 401:**

$2mF_o-DF_c$  (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.