



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 02:55 PM EDT

PDB ID : 6M7X  
Title : Structure of human CYP11B1 in complex with fadrozole  
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Deposited on : 2018-08-21  
Resolution : 2.10 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 : 2.35.1  
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) : 2.35.1

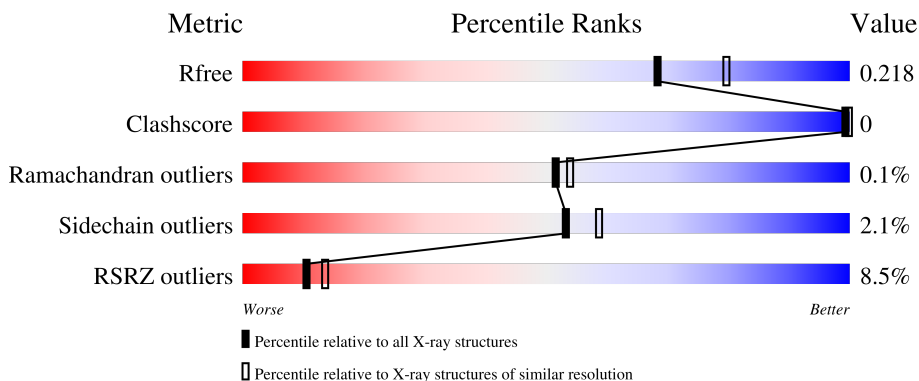
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

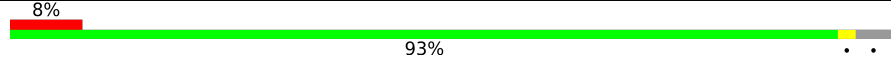
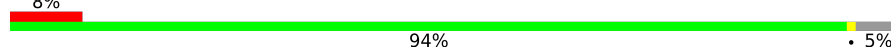
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	484	 8% 93%
1	B	484	 8% 94% 5%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 15684 atoms, of which 7640 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.

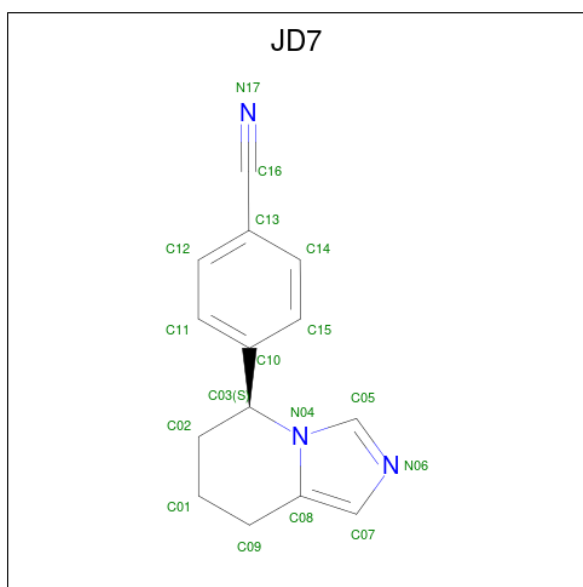
- Molecule 1 is a protein called Cytochrome P450 11B1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	463	7517	2413	3772	663	650	19	0	0	0
1	B	461	7533	2420	3782	664	648	19	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP P15538
A	25	ALA	-	expression tag	UNP P15538
A	26	LYS	-	expression tag	UNP P15538
A	27	LYS	-	expression tag	UNP P15538
A	28	THR	-	expression tag	UNP P15538
A	29	SER	-	expression tag	UNP P15538
A	30	SER	-	expression tag	UNP P15538
A	504	HIS	-	expression tag	UNP P15538
A	505	HIS	-	expression tag	UNP P15538
A	506	HIS	-	expression tag	UNP P15538
A	507	HIS	-	expression tag	UNP P15538
B	24	MET	-	expression tag	UNP P15538
B	25	ALA	-	expression tag	UNP P15538
B	26	LYS	-	expression tag	UNP P15538
B	27	LYS	-	expression tag	UNP P15538
B	28	THR	-	expression tag	UNP P15538
B	29	SER	-	expression tag	UNP P15538
B	30	SER	-	expression tag	UNP P15538
B	504	HIS	-	expression tag	UNP P15538
B	505	HIS	-	expression tag	UNP P15538
B	506	HIS	-	expression tag	UNP P15538
B	507	HIS	-	expression tag	UNP P15538

- Molecule 2 is 4-[(5S)-5,6,7,8-tetrahydroimidazo[1,5-a]pyridin-5-yl]benzotrile (three-letter code: JD7) (formula: C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
2	A	1	30	14	13	3	0	0
2	B	1	30	14	13	3	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
3	A	1	73	34	1	30	4	4	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
3	B	1	73	34	1	30	4	4	0	0

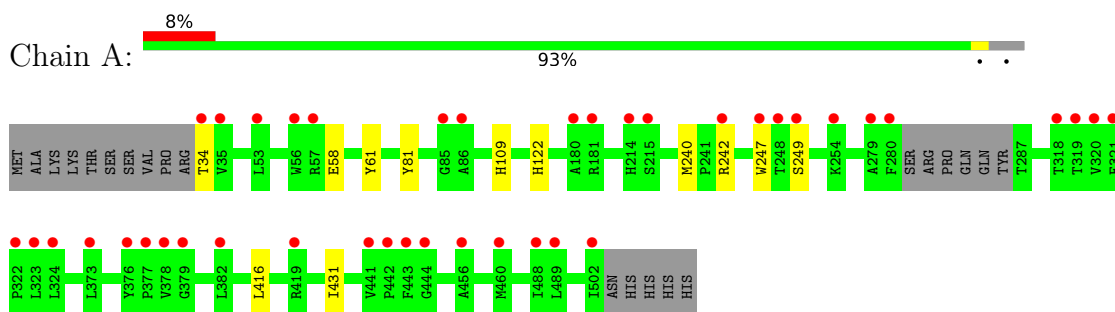
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	204	Total	O	0	0
			204	204		

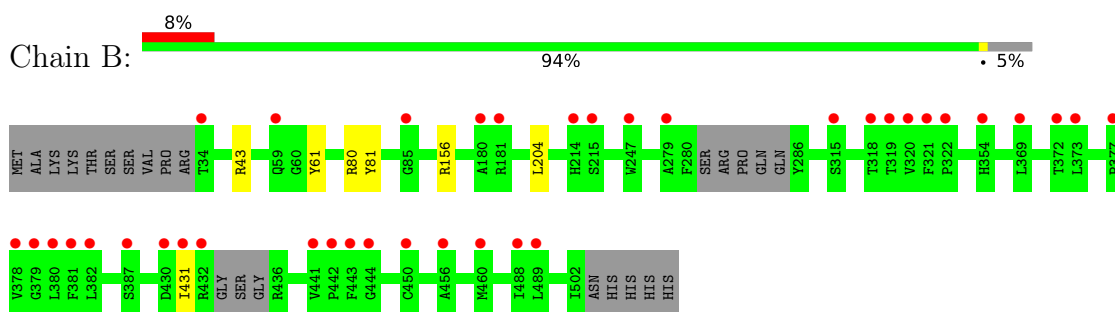
### 3 Residue-property plots [i](#)

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 11B1, mitochondrial



- Molecule 1: Cytochrome P450 11B1, mitochondrial



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.57Å 140.57Å 145.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.45 – 2.10 38.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.45-2.10) 99.0 (38.45-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.189 , 0.218 0.189 , 0.218	Depositor DCC
$R_{free}$ test set	1975 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h 0.008 for -l,-k,-h 0.010 for -h,-l,-k 0.001 for -h,l,k 0.021 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, JD7

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	0.26	0/3842	0.41	0/5213
1	B	0.25	0/3851	0.40	0/5224
All	All	0.26	0/7693	0.40	0/10437

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	3745	3772	3771	0	0
1	B	3751	3782	3781	1	0
2	A	17	13	0	0	0
2	B	17	13	0	0	0
3	A	43	30	30	0	0
3	B	43	30	30	0	0
4	A	224	0	0	0	0
4	B	204	0	0	1	0
All	All	8044	7640	7612	1	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 0.



All (1) 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:B:43:ARG:NH1	4:B:718:HOH:O	2.49	0.46

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	459/484 (95%)	442 (96%)	17 (4%)	0	100	100
1	B	456/484 (94%)	439 (96%)	16 (4%)	1 (0%)	47	49
All	All	915/968 (94%)	881 (96%)	33 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	431	ILE

### 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	406/426 (95%)	394 (97%)	12 (3%)	41	44
1	B	407/426 (96%)	402 (99%)	5 (1%)	71	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	813/852 (95%)	796 (98%)	17 (2%)	53 59

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	58	GLU
1	A	61	TYR
1	A	81	TYR
1	A	109	HIS
1	A	122	HIS
1	A	240	MET
1	A	242	ARG
1	A	247	TRP
1	A	249	SER
1	A	416	LEU
1	A	431	ILE
1	B	61	TYR
1	B	80	ARG
1	B	81	TYR
1	B	156	ARG
1	B	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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	HEM	A	602	1,2	41,50,50	1.48	4 (9%)	45,82,82	1.47	7 (15%)
2	JD7	B	601	3	15,19,19	1.01	0	18,26,26	1.75	5 (27%)
3	HEM	B	602	1,2	41,50,50	1.47	4 (9%)	45,82,82	1.46	7 (15%)
2	JD7	A	601	3	15,19,19	0.99	0	18,26,26	1.74	5 (27%)

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	HEM	A	602	1,2	-	0/12/54/54	-
2	JD7	B	601	3	-	0/6/16/16	0/2/3/3
3	HEM	B	602	1,2	-	1/12/54/54	-
2	JD7	A	601	3	-	0/6/16/16	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	C3C-CAC	3.93	1.55	1.47
3	A	602	HEM	C3C-CAC	3.90	1.55	1.47
3	A	602	HEM	C3C-C2C	-3.76	1.35	1.40
3	B	602	HEM	C3C-C2C	-3.63	1.35	1.40
3	A	602	HEM	CAB-C3B	3.04	1.55	1.47
3	B	602	HEM	CAB-C3B	2.95	1.55	1.47
3	A	602	HEM	CMB-C2B	2.21	1.55	1.50
3	B	602	HEM	CMB-C2B	2.07	1.55	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JD7	C15-C10-C11	-3.95	113.37	118.29
2	A	601	JD7	C15-C10-C11	-3.85	113.49	118.29
3	A	602	HEM	CMC-C2C-C3C	3.28	130.82	124.68
2	B	601	JD7	C12-C13-C16	3.22	125.35	119.99
3	B	602	HEM	CMC-C2C-C3C	3.16	130.59	124.68
2	A	601	JD7	C12-C13-C16	3.11	125.17	119.99
3	B	602	HEM	CBA-CAA-C2A	-3.09	107.36	112.62
3	A	602	HEM	C4D-ND-C1D	2.90	108.07	105.07
3	A	602	HEM	C4C-CHD-C1D	2.90	126.38	122.56
3	B	602	HEM	C4B-CHC-C1C	2.84	126.30	122.56
3	A	602	HEM	CBA-CAA-C2A	-2.84	107.78	112.62
3	B	602	HEM	C4C-CHD-C1D	2.83	126.29	122.56
3	B	602	HEM	C4D-ND-C1D	2.77	107.93	105.07
3	A	602	HEM	C4B-CHC-C1C	2.72	126.15	122.56
3	B	602	HEM	C1B-NB-C4B	2.64	107.81	105.07
3	B	602	HEM	CMB-C2B-C1B	-2.40	121.39	125.04
3	A	602	HEM	CMB-C2B-C1B	-2.40	121.39	125.04
3	A	602	HEM	C1B-NB-C4B	2.37	107.53	105.07
2	B	601	JD7	C14-C15-C10	2.35	123.56	121.20
2	A	601	JD7	C14-C15-C10	2.21	123.42	121.20
2	B	601	JD7	C14-C13-C12	-2.12	115.13	118.96
2	A	601	JD7	C14-C13-C12	-2.09	115.19	118.96
2	B	601	JD7	C12-C11-C10	2.06	123.27	121.20
2	A	601	JD7	C12-C11-C10	2.02	123.23	121.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

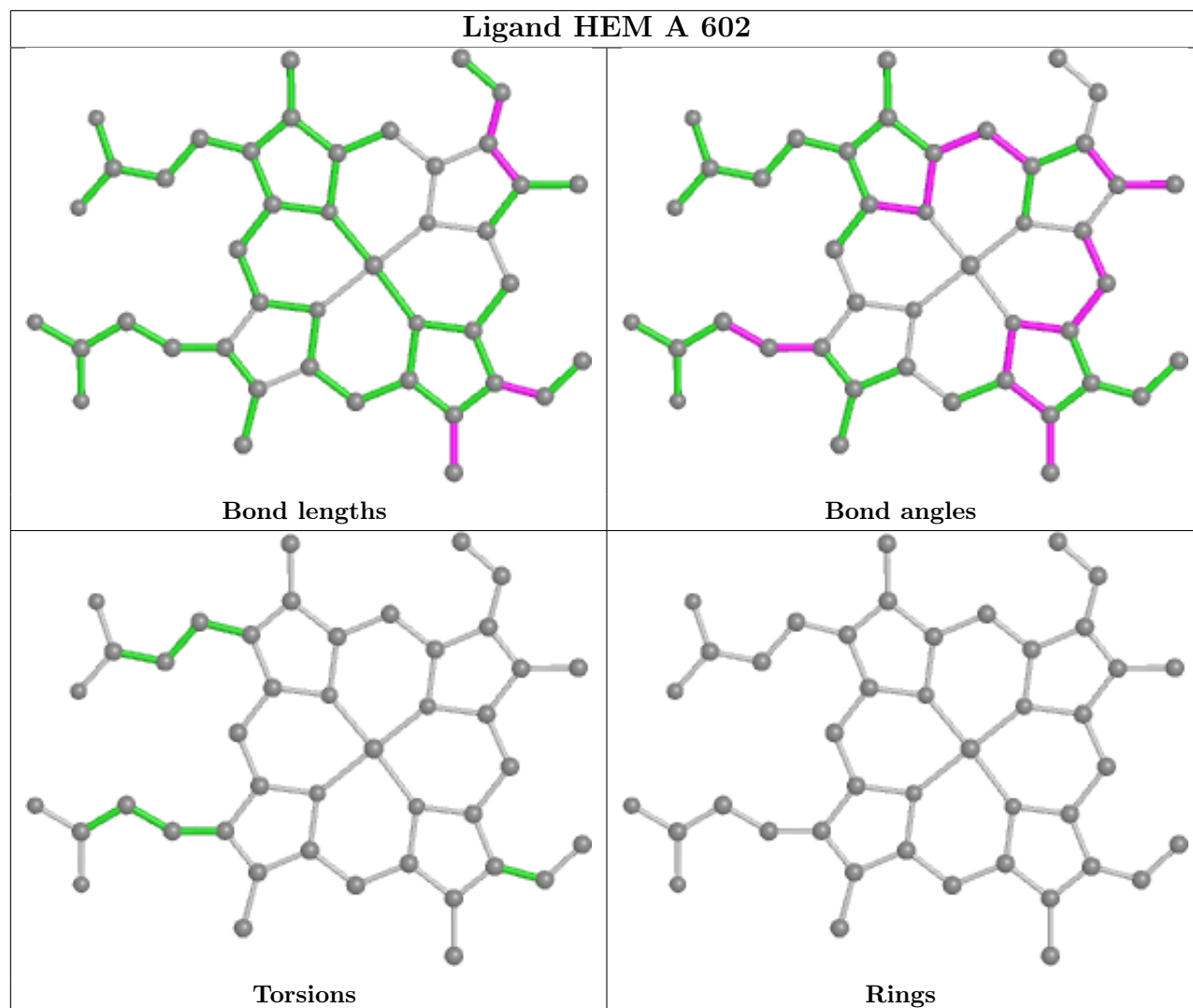
Mol	Chain	Res	Type	Atoms
3	B	602	HEM	CAD-CBD-CGD-O2D

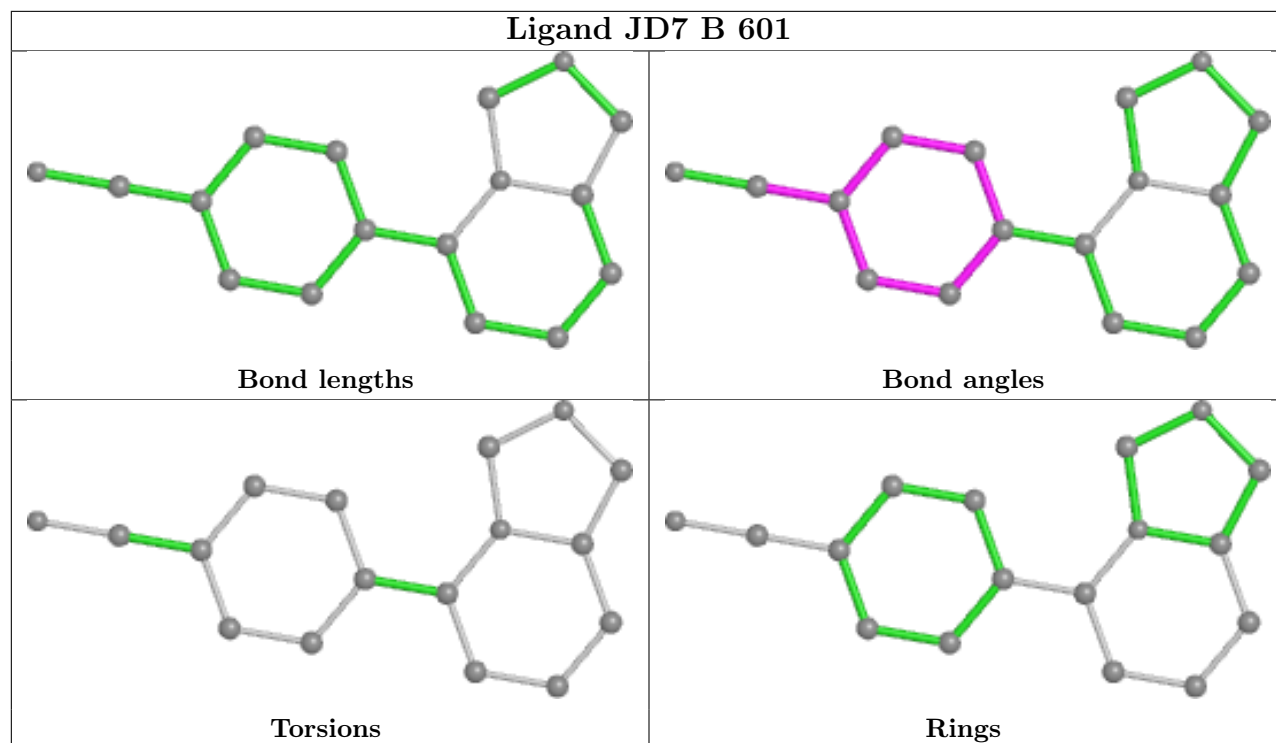
There are no ring outliers.

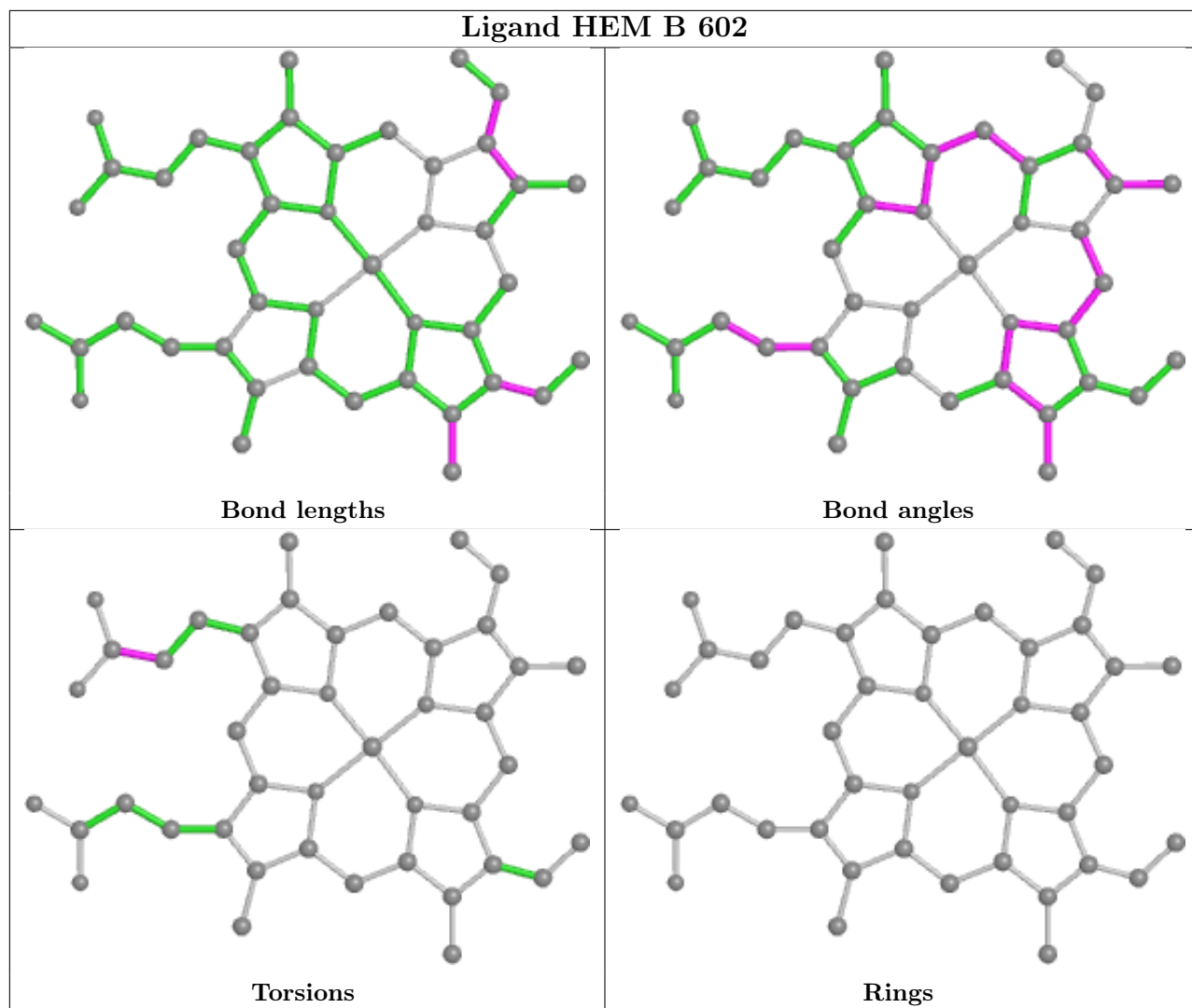
No monomer is involved in short contacts.

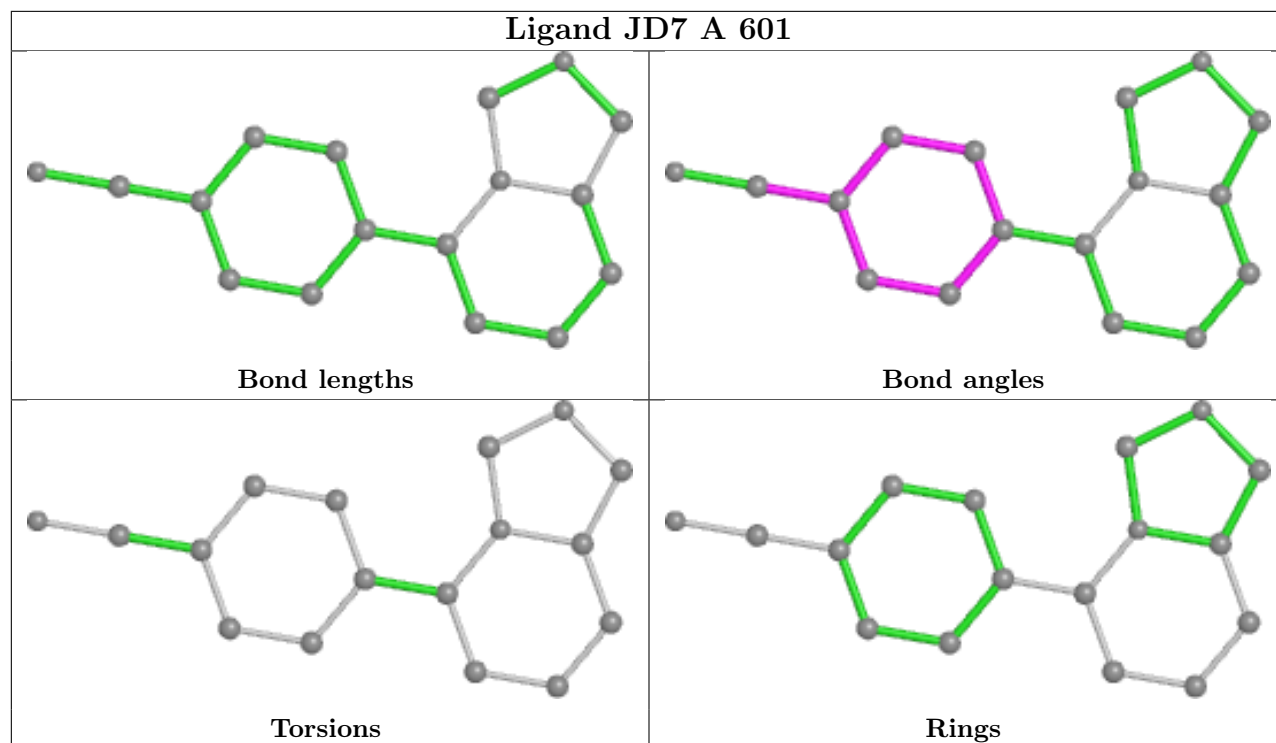
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	463/484 (95%)	0.28	41 (8%) <b>9</b> <b>12</b>	33, 48, 76, 113	0
1	B	461/484 (95%)	0.29	38 (8%) <b>11</b> <b>15</b>	31, 49, 74, 114	0
All	All	924/968 (95%)	0.29	79 (8%) <b>10</b> <b>13</b>	31, 49, 76, 114	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	6.4
1	B	432	ARG	5.6
1	B	247	TRP	5.3
1	A	214	HIS	5.2
1	A	247	TRP	4.9
1	A	280	PHE	4.8
1	A	279	ALA	4.2
1	A	180	ALA	3.9
1	B	443	PHE	3.9
1	B	430	ASP	3.8
1	B	378	VAL	3.8
1	B	180	ALA	3.6
1	A	34	THR	3.6
1	B	214	HIS	3.5
1	A	215	SER	3.2
1	B	279	ALA	3.2
1	A	53	LEU	3.1
1	A	378	VAL	3.1
1	B	377	PRO	3.1
1	A	321	PHE	3.0
1	A	85	GLY	2.9
1	A	318	THR	2.9
1	B	379	GLY	2.9
1	B	373	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	321	PHE	2.8
1	A	248	THR	2.8
1	B	320	VAL	2.8
1	B	456	ALA	2.8
1	A	443	PHE	2.7
1	B	215	SER	2.7
1	B	369	LEU	2.7
1	B	442	PRO	2.7
1	A	56	TRP	2.7
1	B	382	LEU	2.7
1	A	242	ARG	2.7
1	B	181	ARG	2.6
1	B	59	GLN	2.6
1	A	488	ILE	2.6
1	B	444	GLY	2.6
1	B	488	ILE	2.6
1	B	450	CYS	2.6
1	B	85	GLY	2.6
1	A	489	LEU	2.6
1	A	320	VAL	2.5
1	A	323	LEU	2.5
1	A	254	LYS	2.5
1	A	181	ARG	2.5
1	B	318	THR	2.5
1	B	489	LEU	2.4
1	A	322	PRO	2.4
1	A	419	ARG	2.4
1	A	502	ILE	2.4
1	A	319	THR	2.4
1	A	377	PRO	2.4
1	B	460	MET	2.4
1	A	373	LEU	2.3
1	B	319	THR	2.3
1	A	57	ARG	2.3
1	B	380	LEU	2.3
1	A	442	PRO	2.2
1	B	381	PHE	2.2
1	A	35	VAL	2.2
1	B	387	SER	2.2
1	A	324	LEU	2.2
1	A	441	VAL	2.1
1	A	86	ALA	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	34	THR	2.1
1	A	379	GLY	2.1
1	A	444	GLY	2.1
1	A	456	ALA	2.1
1	A	382	LEU	2.1
1	A	376	TYR	2.1
1	B	441	VAL	2.1
1	B	315	SER	2.0
1	B	354	HIS	2.0
1	A	460	MET	2.0
1	B	372	THR	2.0
1	A	249	SER	2.0
1	B	322	PRO	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](#)

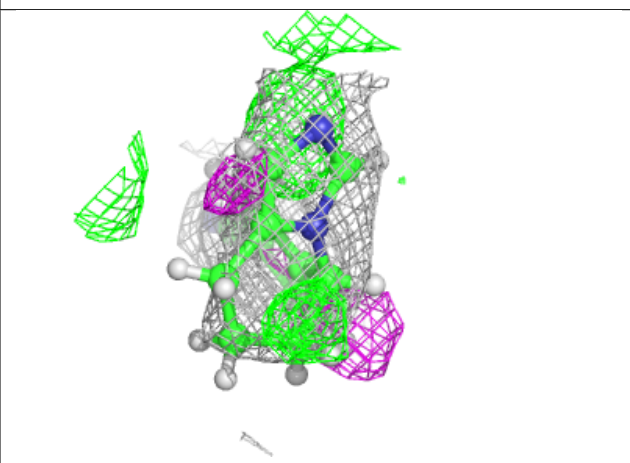
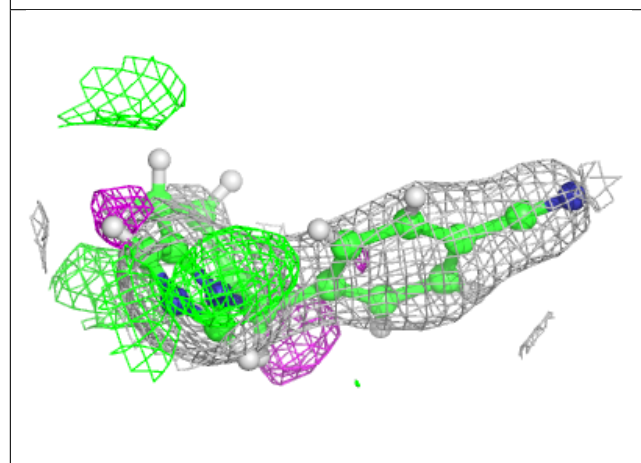
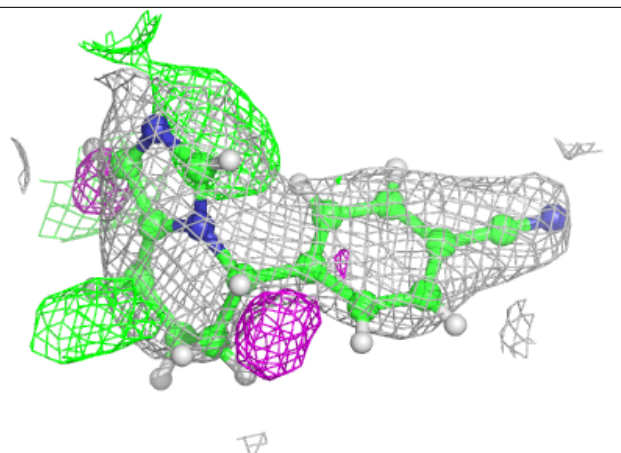
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	JD7	A	601	17/17	0.90	0.25	41,58,78,83	0
2	JD7	B	601	17/17	0.90	0.28	41,55,74,82	0
3	HEM	A	602	43/43	0.98	0.25	28,36,46,53	0
3	HEM	B	602	43/43	0.98	0.24	28,36,45,54	0

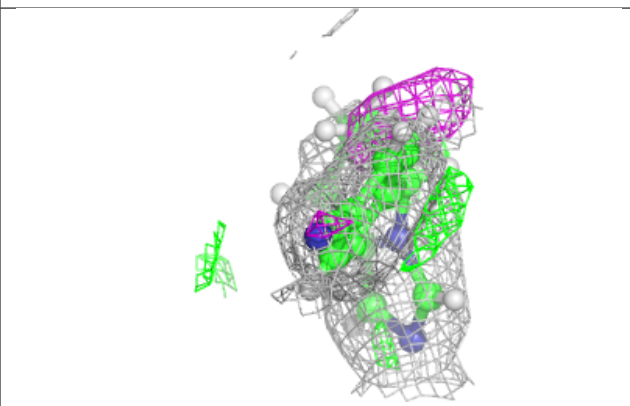
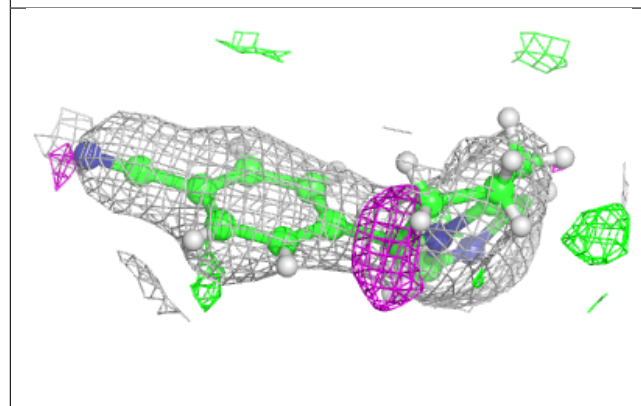
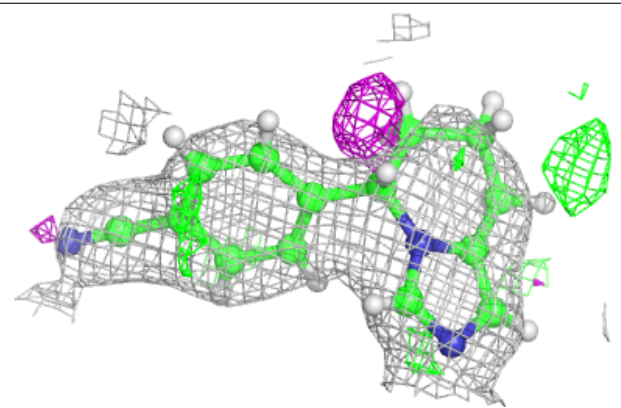
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around JD7 A 601:**

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

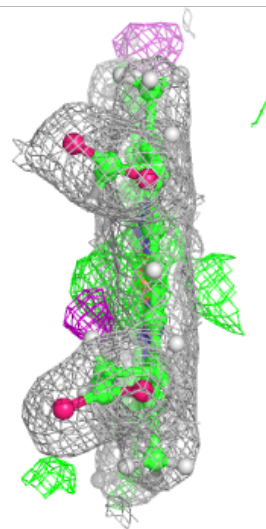
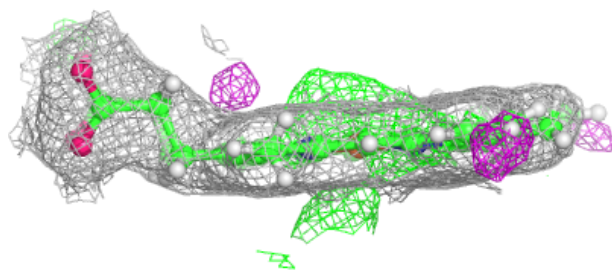
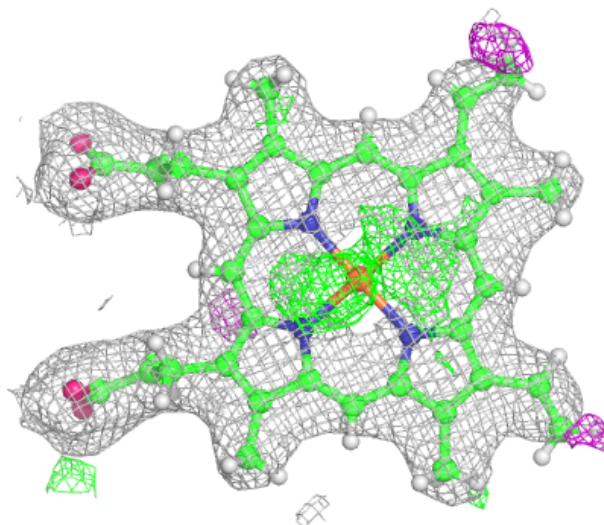
**Electron density around JD7 B 601:**

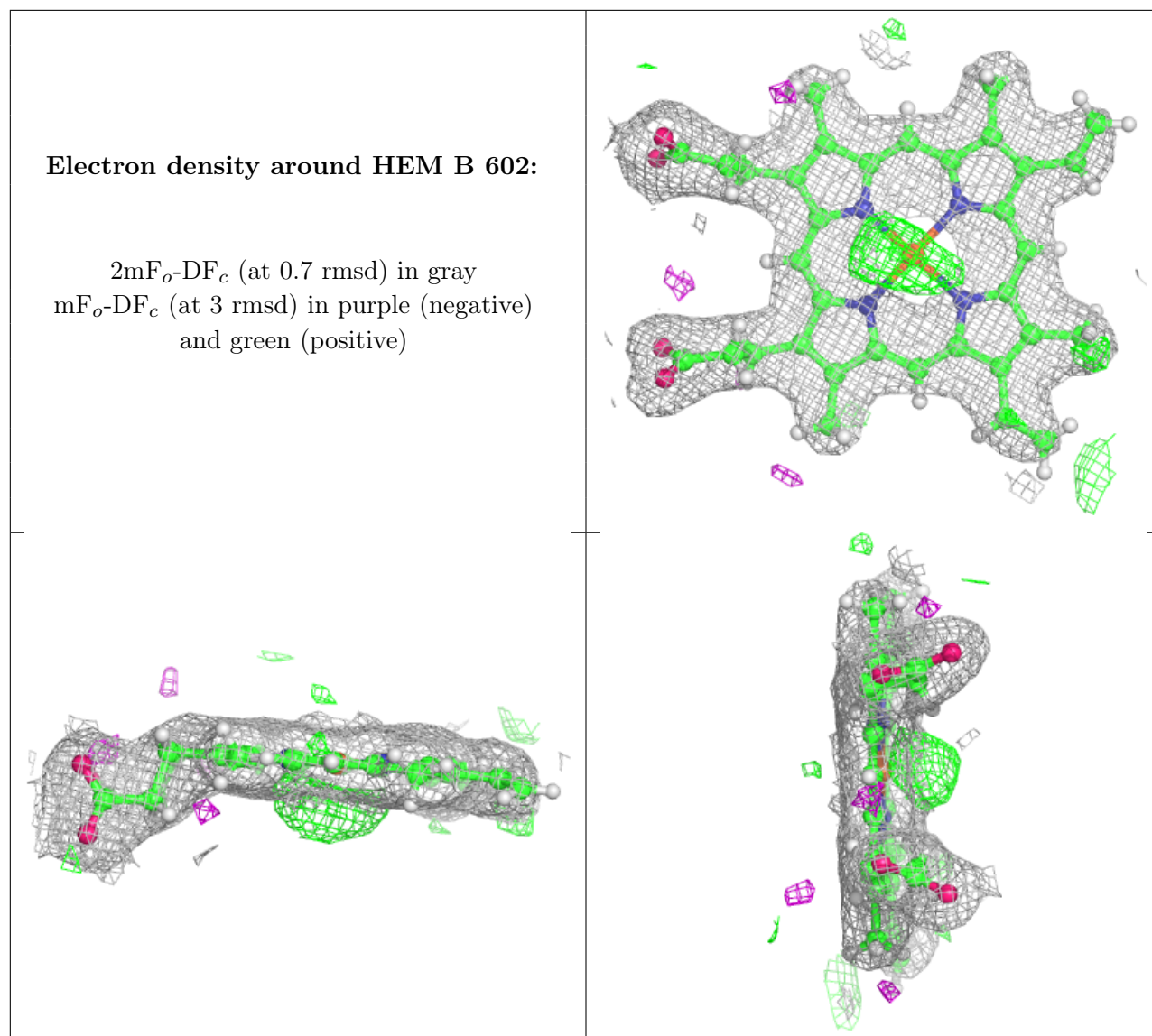
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 602:**

$2mF_o-DF_c$  (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.