



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 08:13 AM EST

PDB ID : 4FDH  
Title : Structure of human aldosterone synthase, CYP11B2, in complex with fadrozole  
Authors : Strushkevich, N.; Shen, L.; Tempel, W.; Arrowsmith, C.; Edwards, A.; Usanov, S.A.; Park, H.-W.  
Deposited on : 2012-05-28  
Resolution : 2.71 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 : 1.8.5 (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

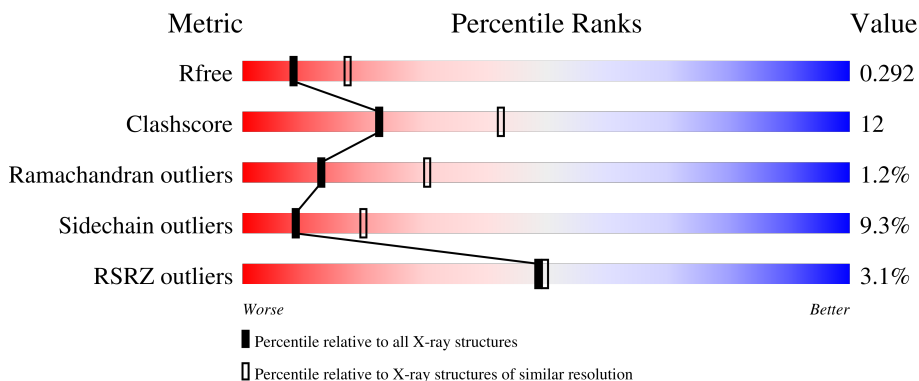
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	483	
1	B	483	
1	C	483	
1	D	483	
1	E	483	

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Mol	Chain	Length	Quality of chain
1	F	483	<p>1% 63% 30% . .</p>
1	G	483	<p>3% 71% 21% . .</p>
1	H	483	<p>4% 67% 26% . .</p>
1	I	483	<p>5% 66% 25% 5% .</p>
1	J	483	<p>7% 65% 27% . .</p>
1	K	483	<p>8% 64% 28% 5% .</p>
1	L	483	<p>2% 69% 21% . 6%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 46075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	3758	2429	663	646	20	0	0	0
1	B	465	3777	2441	668	648	20	0	0	0
1	C	462	3750	2425	661	644	20	0	0	0
1	D	465	3777	2441	668	648	20	0	0	0
1	E	470	3826	2469	683	654	20	0	0	0
1	F	469	3818	2465	681	652	20	0	0	0
1	G	463	3758	2429	663	646	20	0	0	0
1	H	462	3750	2425	661	644	20	0	0	0
1	I	462	3750	2425	661	644	20	0	0	0
1	J	462	3750	2425	661	644	20	0	0	0
1	K	469	3802	2454	675	653	20	0	0	0
1	L	456	3712	2402	654	636	20	0	0	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP P19099
A	28	ALA	-	expression tag	UNP P19099
A	29	LYS	-	expression tag	UNP P19099
A	30	LYS	-	expression tag	UNP P19099
A	31	THR	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	expression tag	UNP P19099
A	33	SER	-	expression tag	UNP P19099
A	504	HIS	-	expression tag	UNP P19099
A	505	HIS	-	expression tag	UNP P19099
A	506	HIS	-	expression tag	UNP P19099
A	507	HIS	-	expression tag	UNP P19099
A	508	HIS	-	expression tag	UNP P19099
A	509	HIS	-	expression tag	UNP P19099
B	27	MET	-	expression tag	UNP P19099
B	28	ALA	-	expression tag	UNP P19099
B	29	LYS	-	expression tag	UNP P19099
B	30	LYS	-	expression tag	UNP P19099
B	31	THR	-	expression tag	UNP P19099
B	32	SER	-	expression tag	UNP P19099
B	33	SER	-	expression tag	UNP P19099
B	504	HIS	-	expression tag	UNP P19099
B	505	HIS	-	expression tag	UNP P19099
B	506	HIS	-	expression tag	UNP P19099
B	507	HIS	-	expression tag	UNP P19099
B	508	HIS	-	expression tag	UNP P19099
B	509	HIS	-	expression tag	UNP P19099
C	27	MET	-	expression tag	UNP P19099
C	28	ALA	-	expression tag	UNP P19099
C	29	LYS	-	expression tag	UNP P19099
C	30	LYS	-	expression tag	UNP P19099
C	31	THR	-	expression tag	UNP P19099
C	32	SER	-	expression tag	UNP P19099
C	33	SER	-	expression tag	UNP P19099
C	504	HIS	-	expression tag	UNP P19099
C	505	HIS	-	expression tag	UNP P19099
C	506	HIS	-	expression tag	UNP P19099
C	507	HIS	-	expression tag	UNP P19099
C	508	HIS	-	expression tag	UNP P19099
C	509	HIS	-	expression tag	UNP P19099
D	27	MET	-	expression tag	UNP P19099
D	28	ALA	-	expression tag	UNP P19099
D	29	LYS	-	expression tag	UNP P19099
D	30	LYS	-	expression tag	UNP P19099
D	31	THR	-	expression tag	UNP P19099
D	32	SER	-	expression tag	UNP P19099
D	33	SER	-	expression tag	UNP P19099
D	504	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	expression tag	UNP P19099
D	506	HIS	-	expression tag	UNP P19099
D	507	HIS	-	expression tag	UNP P19099
D	508	HIS	-	expression tag	UNP P19099
D	509	HIS	-	expression tag	UNP P19099
E	27	MET	-	expression tag	UNP P19099
E	28	ALA	-	expression tag	UNP P19099
E	29	LYS	-	expression tag	UNP P19099
E	30	LYS	-	expression tag	UNP P19099
E	31	THR	-	expression tag	UNP P19099
E	32	SER	-	expression tag	UNP P19099
E	33	SER	-	expression tag	UNP P19099
E	504	HIS	-	expression tag	UNP P19099
E	505	HIS	-	expression tag	UNP P19099
E	506	HIS	-	expression tag	UNP P19099
E	507	HIS	-	expression tag	UNP P19099
E	508	HIS	-	expression tag	UNP P19099
E	509	HIS	-	expression tag	UNP P19099
F	27	MET	-	expression tag	UNP P19099
F	28	ALA	-	expression tag	UNP P19099
F	29	LYS	-	expression tag	UNP P19099
F	30	LYS	-	expression tag	UNP P19099
F	31	THR	-	expression tag	UNP P19099
F	32	SER	-	expression tag	UNP P19099
F	33	SER	-	expression tag	UNP P19099
F	504	HIS	-	expression tag	UNP P19099
F	505	HIS	-	expression tag	UNP P19099
F	506	HIS	-	expression tag	UNP P19099
F	507	HIS	-	expression tag	UNP P19099
F	508	HIS	-	expression tag	UNP P19099
F	509	HIS	-	expression tag	UNP P19099
G	27	MET	-	expression tag	UNP P19099
G	28	ALA	-	expression tag	UNP P19099
G	29	LYS	-	expression tag	UNP P19099
G	30	LYS	-	expression tag	UNP P19099
G	31	THR	-	expression tag	UNP P19099
G	32	SER	-	expression tag	UNP P19099
G	33	SER	-	expression tag	UNP P19099
G	504	HIS	-	expression tag	UNP P19099
G	505	HIS	-	expression tag	UNP P19099
G	506	HIS	-	expression tag	UNP P19099
G	507	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
G	508	HIS	-	expression tag	UNP P19099
G	509	HIS	-	expression tag	UNP P19099
H	27	MET	-	expression tag	UNP P19099
H	28	ALA	-	expression tag	UNP P19099
H	29	LYS	-	expression tag	UNP P19099
H	30	LYS	-	expression tag	UNP P19099
H	31	THR	-	expression tag	UNP P19099
H	32	SER	-	expression tag	UNP P19099
H	33	SER	-	expression tag	UNP P19099
H	504	HIS	-	expression tag	UNP P19099
H	505	HIS	-	expression tag	UNP P19099
H	506	HIS	-	expression tag	UNP P19099
H	507	HIS	-	expression tag	UNP P19099
H	508	HIS	-	expression tag	UNP P19099
H	509	HIS	-	expression tag	UNP P19099
I	27	MET	-	expression tag	UNP P19099
I	28	ALA	-	expression tag	UNP P19099
I	29	LYS	-	expression tag	UNP P19099
I	30	LYS	-	expression tag	UNP P19099
I	31	THR	-	expression tag	UNP P19099
I	32	SER	-	expression tag	UNP P19099
I	33	SER	-	expression tag	UNP P19099
I	504	HIS	-	expression tag	UNP P19099
I	505	HIS	-	expression tag	UNP P19099
I	506	HIS	-	expression tag	UNP P19099
I	507	HIS	-	expression tag	UNP P19099
I	508	HIS	-	expression tag	UNP P19099
I	509	HIS	-	expression tag	UNP P19099
J	27	MET	-	expression tag	UNP P19099
J	28	ALA	-	expression tag	UNP P19099
J	29	LYS	-	expression tag	UNP P19099
J	30	LYS	-	expression tag	UNP P19099
J	31	THR	-	expression tag	UNP P19099
J	32	SER	-	expression tag	UNP P19099
J	33	SER	-	expression tag	UNP P19099
J	504	HIS	-	expression tag	UNP P19099
J	505	HIS	-	expression tag	UNP P19099
J	506	HIS	-	expression tag	UNP P19099
J	507	HIS	-	expression tag	UNP P19099
J	508	HIS	-	expression tag	UNP P19099
J	509	HIS	-	expression tag	UNP P19099
K	27	MET	-	expression tag	UNP P19099

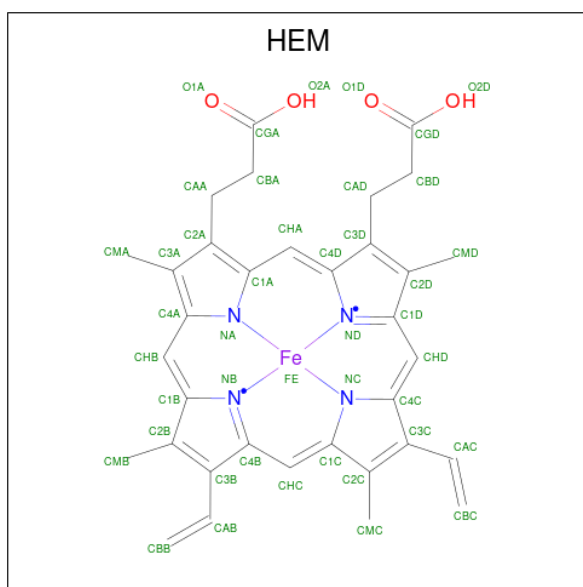
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Chain	Residue	Modelled	Actual	Comment	Reference
K	28	ALA	-	expression tag	UNP P19099
K	29	LYS	-	expression tag	UNP P19099
K	30	LYS	-	expression tag	UNP P19099
K	31	THR	-	expression tag	UNP P19099
K	32	SER	-	expression tag	UNP P19099
K	33	SER	-	expression tag	UNP P19099
K	504	HIS	-	expression tag	UNP P19099
K	505	HIS	-	expression tag	UNP P19099
K	506	HIS	-	expression tag	UNP P19099
K	507	HIS	-	expression tag	UNP P19099
K	508	HIS	-	expression tag	UNP P19099
K	509	HIS	-	expression tag	UNP P19099
L	27	MET	-	expression tag	UNP P19099
L	28	ALA	-	expression tag	UNP P19099
L	29	LYS	-	expression tag	UNP P19099
L	30	LYS	-	expression tag	UNP P19099
L	31	THR	-	expression tag	UNP P19099
L	32	SER	-	expression tag	UNP P19099
L	33	SER	-	expression tag	UNP P19099
L	504	HIS	-	expression tag	UNP P19099
L	505	HIS	-	expression tag	UNP P19099
L	506	HIS	-	expression tag	UNP P19099
L	507	HIS	-	expression tag	UNP P19099
L	508	HIS	-	expression tag	UNP P19099
L	509	HIS	-	expression tag	UNP P19099

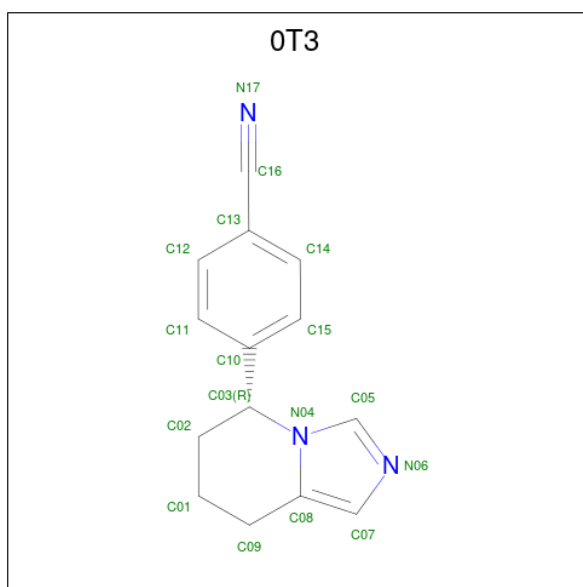
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	C	1	43	34	1	4	4	0	0
2	D	1	43	34	1	4	4	0	0
2	E	1	43	34	1	4	4	0	0
2	F	1	43	34	1	4	4	0	0
2	G	1	43	34	1	4	4	0	0
2	H	1	43	34	1	4	4	0	0
2	I	1	43	34	1	4	4	0	0
2	J	1	43	34	1	4	4	0	0
2	K	1	43	34	1	4	4	0	0
2	L	1	43	34	1	4	4	0	0

- Molecule 3 is 4-[(5R)-5,6,7,8-tetrahydroimidazo[1,5-a]pyridin-5-yl]benzotrile (three-letter code: 0T3) (formula: C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			17	14	3		
3	B	1	Total	C	N	0	0
			17	14	3		
3	C	1	Total	C	N	0	0
			17	14	3		
3	D	1	Total	C	N	0	0
			17	14	3		
3	E	1	Total	C	N	0	0
			17	14	3		
3	F	1	Total	C	N	0	0
			17	14	3		
3	G	1	Total	C	N	0	0
			17	14	3		
3	H	1	Total	C	N	0	0
			17	14	3		
3	I	1	Total	C	N	0	0
			17	14	3		
3	J	1	Total	C	N	0	0
			17	14	3		
3	K	1	Total	C	N	0	0
			17	14	3		
3	L	1	Total	C	N	0	0
			17	14	3		

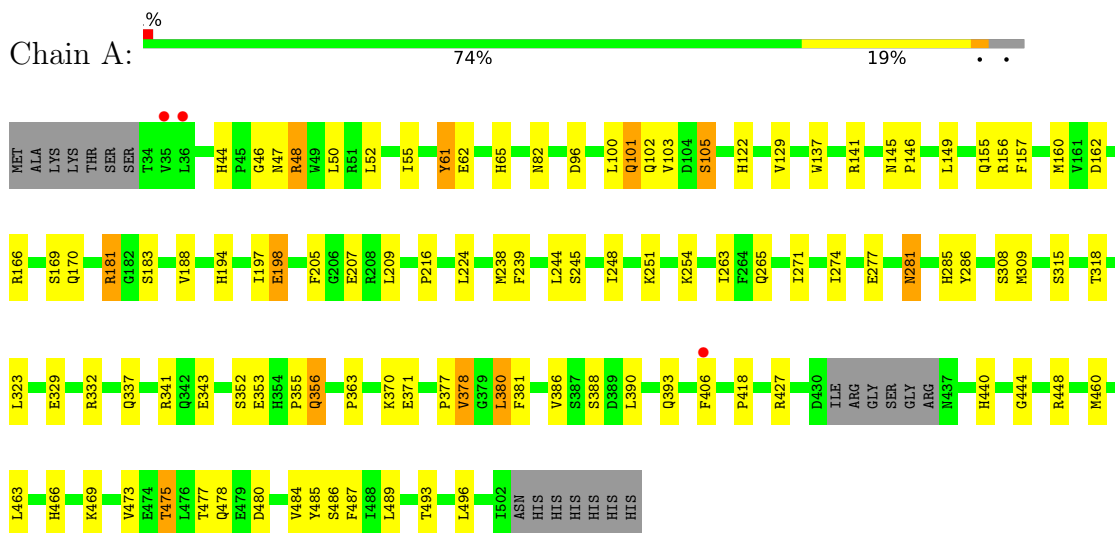
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	6	Total O 6 6	0	0
4	C	17	Total O 17 17	0	0
4	D	9	Total O 9 9	0	0
4	E	12	Total O 12 12	0	0
4	F	17	Total O 17 17	0	0
4	G	3	Total O 3 3	0	0
4	H	13	Total O 13 13	0	0
4	I	9	Total O 9 9	0	0
4	J	3	Total O 3 3	0	0
4	K	4	Total O 4 4	0	0
4	L	20	Total O 20 20	0	0

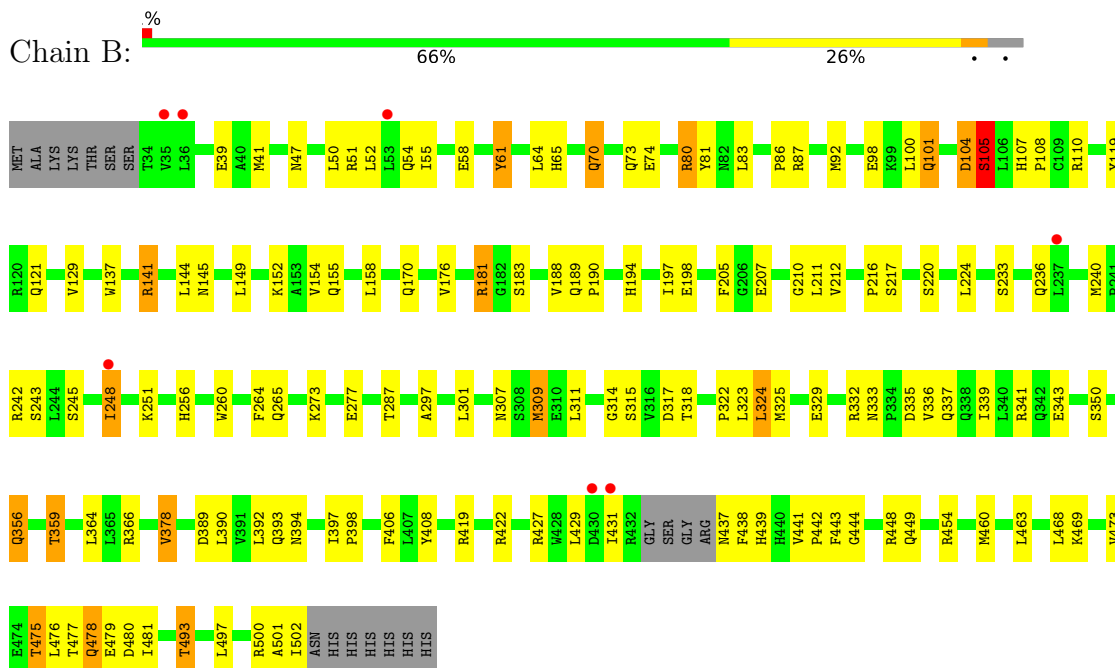
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

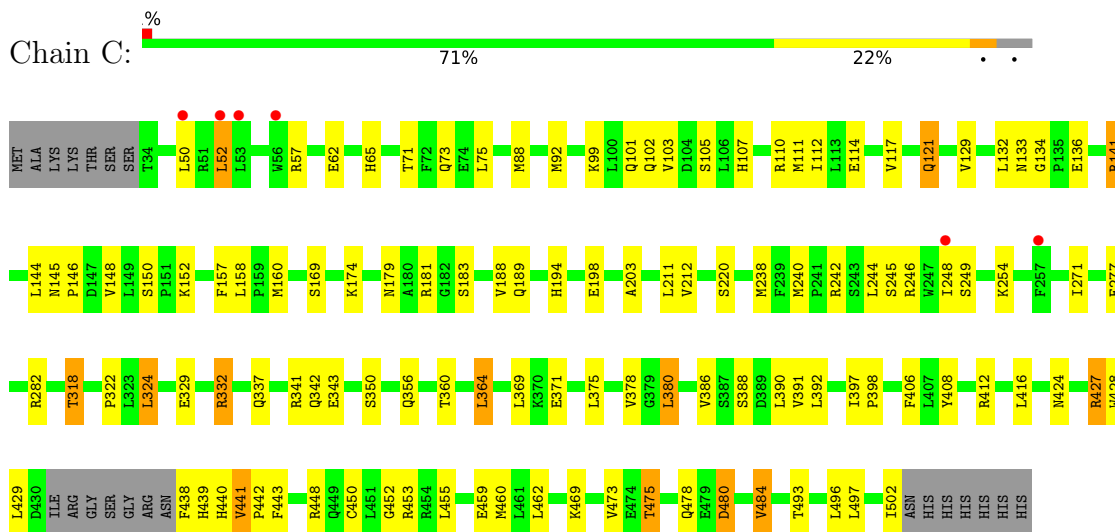
- Molecule 1: Cytochrome P450 11B2, mitochondrial



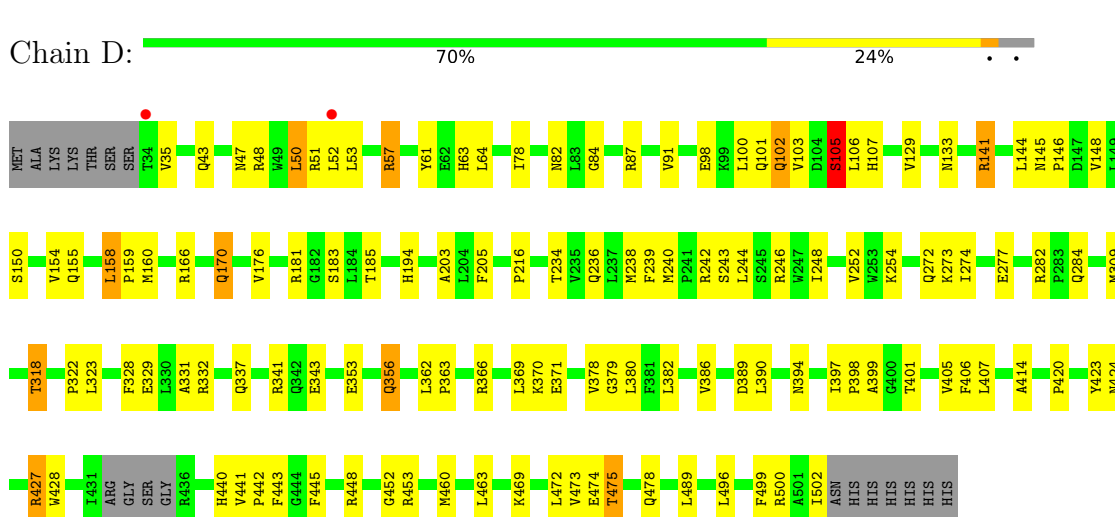
- Molecule 1: Cytochrome P450 11B2, mitochondrial



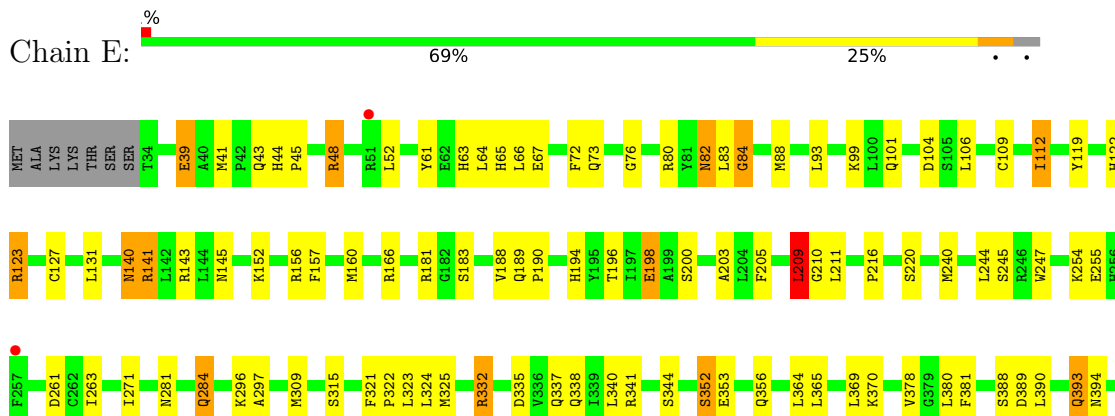
- Molecule 1: Cytochrome P450 11B2, mitochondrial

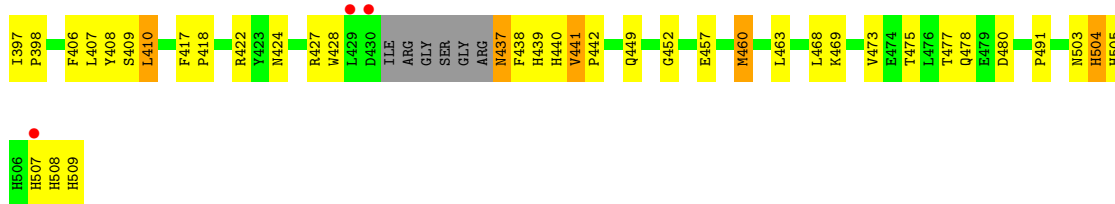


- Molecule 1: Cytochrome P450 11B2, mitochondrial

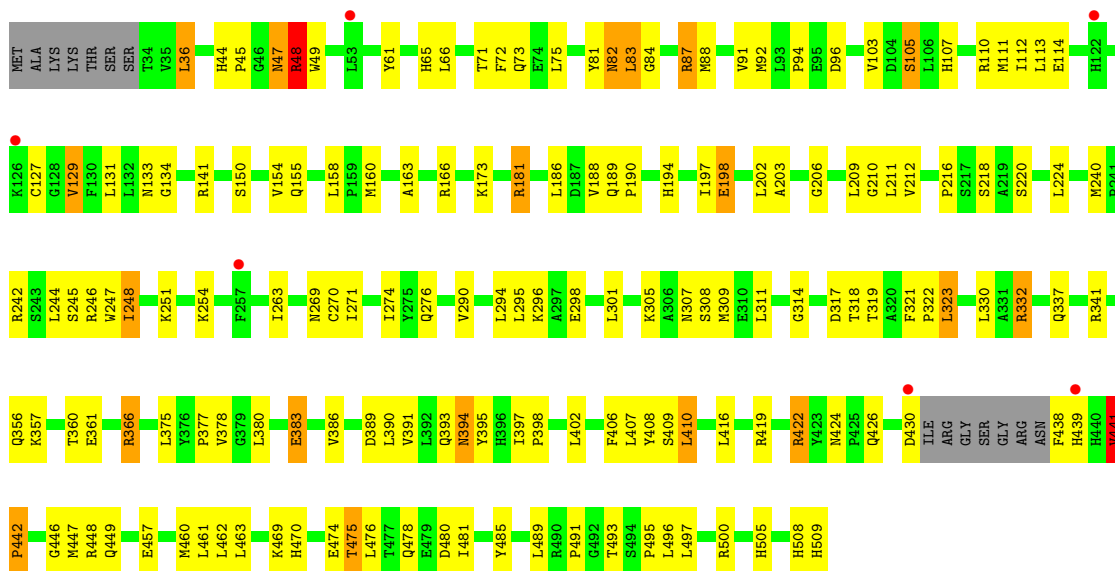


- Molecule 1: Cytochrome P450 11B2, mitochondrial

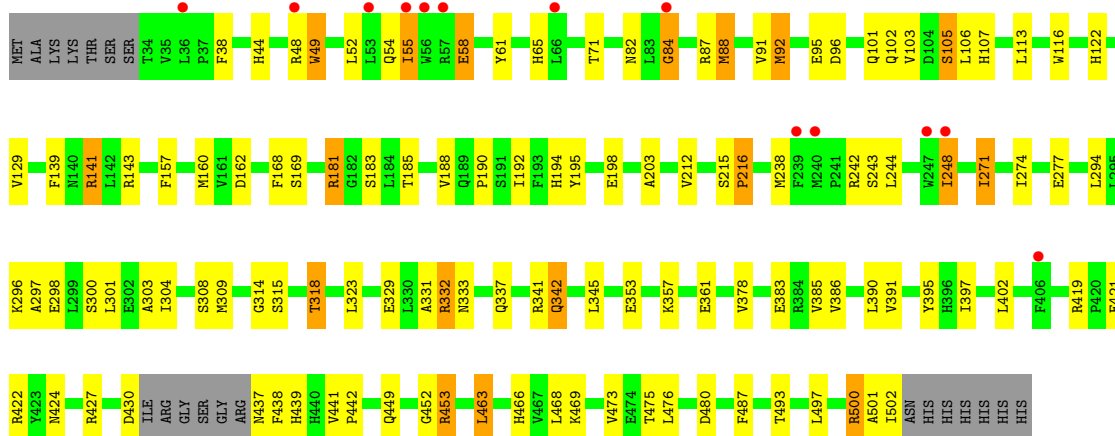




• Molecule 1: Cytochrome P450 11B2, mitochondrial

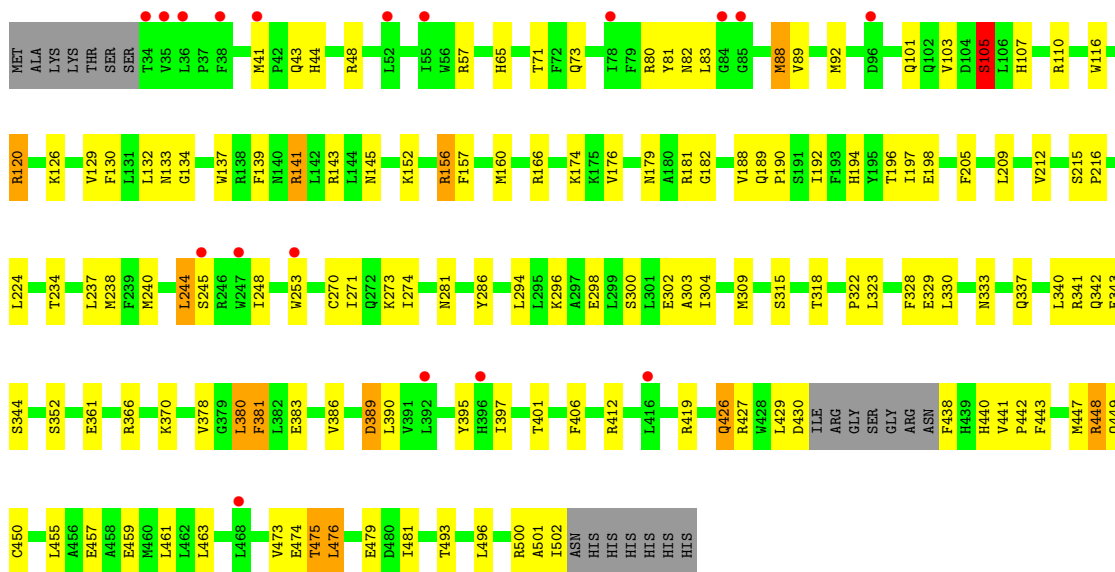


• Molecule 1: Cytochrome P450 11B2, mitochondrial

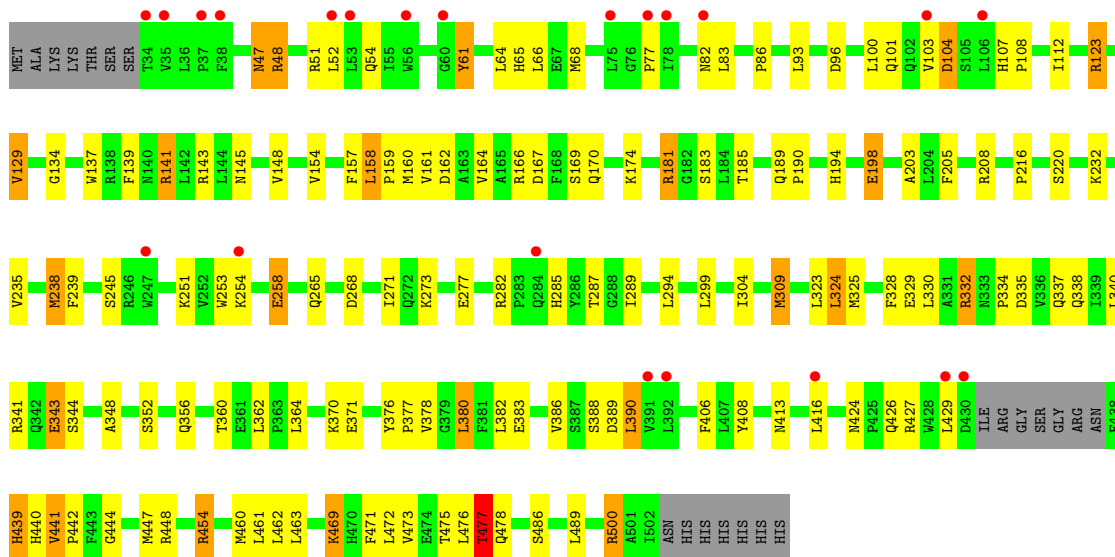


• Molecule 1: Cytochrome P450 11B2, mitochondrial

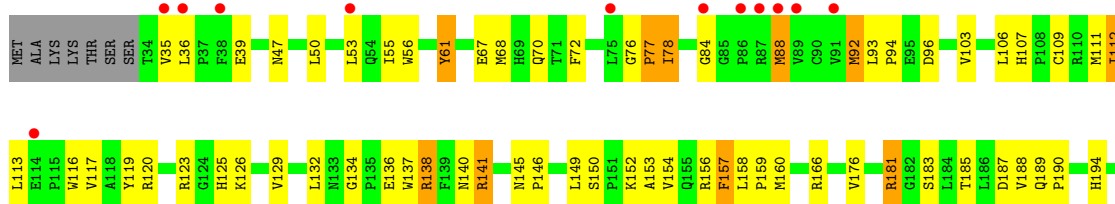


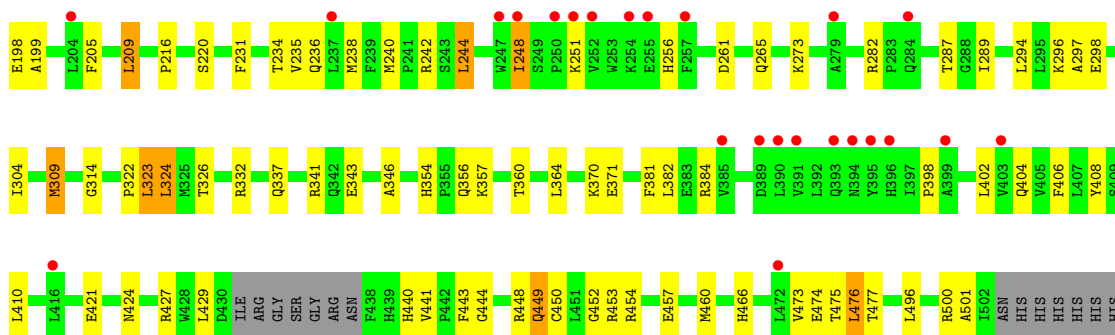


• Molecule 1: Cytochrome P450 11B2, mitochondrial

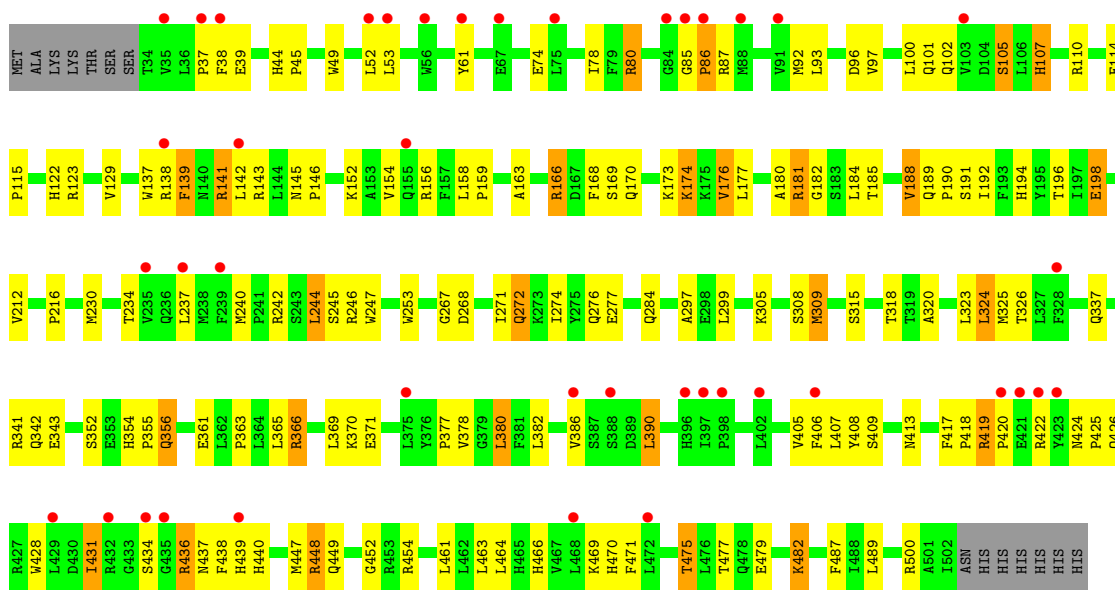


• Molecule 1: Cytochrome P450 11B2, mitochondrial

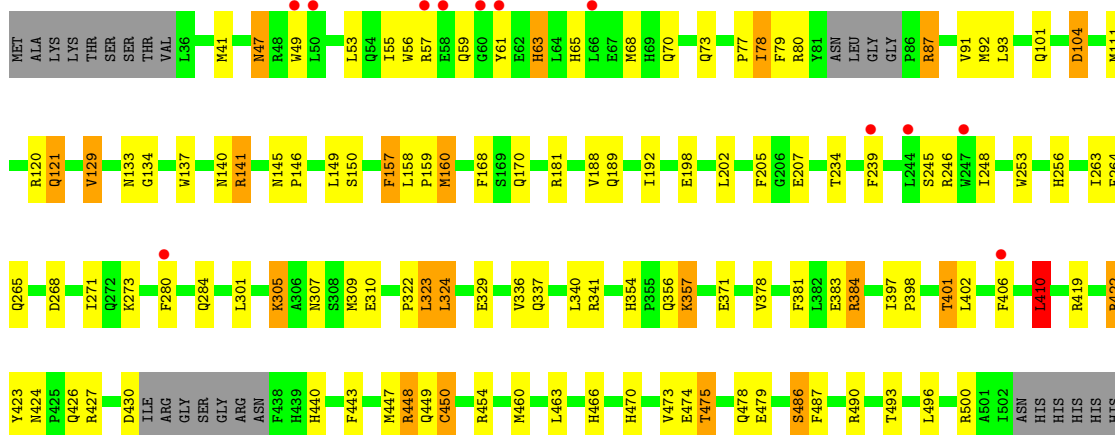




• Molecule 1: Cytochrome P450 11B2, mitochondrial



• Molecule 1: Cytochrome P450 11B2, mitochondrial





HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.75Å 199.09Å 150.02Å 90.00° 112.08° 90.00°	Depositor
Resolution (Å)	48.89 – 2.71 48.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.89-2.71) 98.9 (48.00-2.71)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.73Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.224 , 0.300 0.221 , 0.292	Depositor DCC
$R_{free}$ test set	9381 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	46075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9437e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0T3

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	0.58	0/3858	0.70	1/5235 (0.0%)
1	B	0.53	0/3877	0.67	0/5260
1	C	0.57	0/3850	0.71	0/5224
1	D	0.56	0/3877	0.69	0/5260
1	E	0.56	0/3932	0.68	1/5336 (0.0%)
1	F	0.54	1/3924 (0.0%)	0.67	0/5325
1	G	0.52	0/3858	0.65	0/5235
1	H	0.55	1/3850 (0.0%)	0.69	1/5224 (0.0%)
1	I	0.51	0/3850	0.65	0/5224
1	J	0.50	0/3850	0.64	0/5224
1	K	0.49	0/3903	0.64	0/5295
1	L	0.55	0/3811	0.68	1/5168 (0.0%)
All	All	0.54	2/46440 (0.0%)	0.67	4/63010 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	270	CYS	CB-SG	-6.33	1.71	1.82
1	F	270	CYS	CB-SG	-5.89	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	LEU	CA-CB-CG	5.45	127.83	115.30
1	L	410	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	149	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	E	209	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	501	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3758	0	3791	66	0
1	B	3777	0	3815	93	0
1	C	3750	0	3785	74	0
1	D	3777	0	3815	88	0
1	E	3826	0	3839	85	0
1	F	3818	0	3833	111	0
1	G	3758	0	3791	95	0
1	H	3750	0	3785	92	0
1	I	3750	0	3785	98	0
1	J	3750	0	3785	95	0
1	K	3802	0	3840	99	0
1	L	3712	0	3746	85	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
2	C	43	0	30	6	0
2	D	43	0	30	3	0
2	E	43	0	30	5	0
2	F	43	0	30	9	0
2	G	43	0	30	5	0
2	H	43	0	30	2	0
2	I	43	0	30	6	0
2	J	43	0	30	2	0
2	K	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	43	0	30	7	0
3	A	17	0	13	2	0
3	B	17	0	13	3	0
3	C	17	0	13	2	0
3	D	17	0	13	1	0
3	E	17	0	13	2	0
3	F	17	0	13	3	0
3	G	17	0	13	2	0
3	H	17	0	13	2	0
3	I	17	0	13	2	0
3	J	17	0	13	1	0
3	K	17	0	13	1	0
3	L	17	0	13	5	0
4	A	14	0	0	1	0
4	B	6	0	0	0	0
4	C	17	0	0	1	0
4	D	9	0	0	0	0
4	E	12	0	0	0	0
4	F	17	0	0	2	0
4	G	3	0	0	0	0
4	H	13	0	0	1	0
4	I	9	0	0	0	0
4	J	3	0	0	0	0
4	K	4	0	0	0	0
4	L	20	0	0	1	0
All	All	46075	0	46126	1065	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 12.

The worst 5 of 1065 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:G:181:ARG:HH21	1:K:274:ILE:HG13	1.03	1.13
1:G:183:SER:HB3	1:G:500:ARG:HG2	1.35	1.09
1:L:55:ILE:HD11	1:L:239:PHE:HD1	1.17	1.08
1:L:55:ILE:HD11	1:L:239:PHE:CD1	1.89	1.07
1:G:181:ARG:NH2	1:K:274:ILE:HG13	1.72	1.05

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	459/483 (95%)	436 (95%)	21 (5%)	2 (0%)	34	58
1	B	461/483 (95%)	422 (92%)	33 (7%)	6 (1%)	12	28
1	C	458/483 (95%)	436 (95%)	17 (4%)	5 (1%)	14	32
1	D	461/483 (95%)	433 (94%)	26 (6%)	2 (0%)	34	58
1	E	466/483 (96%)	433 (93%)	23 (5%)	10 (2%)	7	16
1	F	465/483 (96%)	424 (91%)	33 (7%)	8 (2%)	9	21
1	G	459/483 (95%)	422 (92%)	32 (7%)	5 (1%)	14	32
1	H	458/483 (95%)	429 (94%)	24 (5%)	5 (1%)	14	32
1	I	458/483 (95%)	422 (92%)	30 (7%)	6 (1%)	12	28
1	J	458/483 (95%)	418 (91%)	31 (7%)	9 (2%)	7	17
1	K	467/483 (97%)	418 (90%)	43 (9%)	6 (1%)	12	28
1	L	450/483 (93%)	418 (93%)	31 (7%)	1 (0%)	47	72
All	All	5520/5796 (95%)	5111 (93%)	344 (6%)	65 (1%)	13	30

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	THR
1	C	427	ARG
1	D	427	ARG
1	E	210	GLY
1	E	297	ALA

### 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	408/425 (96%)	376 (92%)	32 (8%)	12	28
1	B	410/425 (96%)	369 (90%)	41 (10%)	7	17
1	C	407/425 (96%)	370 (91%)	37 (9%)	9	21
1	D	410/425 (96%)	384 (94%)	26 (6%)	18	38
1	E	415/425 (98%)	374 (90%)	41 (10%)	8	17
1	F	414/425 (97%)	372 (90%)	42 (10%)	7	17
1	G	408/425 (96%)	371 (91%)	37 (9%)	9	21
1	H	407/425 (96%)	369 (91%)	38 (9%)	9	20
1	I	407/425 (96%)	366 (90%)	41 (10%)	7	17
1	J	407/425 (96%)	369 (91%)	38 (9%)	9	20
1	K	412/425 (97%)	364 (88%)	48 (12%)	5	12
1	L	403/425 (95%)	366 (91%)	37 (9%)	9	20
All	All	4908/5100 (96%)	4450 (91%)	458 (9%)	9	20

5 of 458 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	188	VAL
1	L	324	LEU
1	H	430	ASP
1	L	198	GLU
1	K	308	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	121	GLN
1	K	337	GLN
1	L	140	ASN
1	E	393	GLN
1	E	356	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](#)

24 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	OT3	E	602	2	15,19,19	0.44	0	18,26,26	0.43	0
3	OT3	G	602	2	15,19,19	0.47	0	18,26,26	0.41	0
3	OT3	F	602	2	15,19,19	0.39	0	18,26,26	0.38	0
2	HEM	A	601	3,1	41,50,50	1.85	7 (17%)	45,82,82	1.75	12 (26%)
2	HEM	G	601	3,1	41,50,50	1.94	10 (24%)	45,82,82	1.82	10 (22%)
3	OT3	K	602	2	15,19,19	0.38	0	18,26,26	0.39	0
2	HEM	K	601	3,1	41,50,50	1.90	5 (12%)	45,82,82	1.84	8 (17%)
2	HEM	J	601	3,1	41,50,50	1.85	4 (9%)	45,82,82	1.60	8 (17%)
2	HEM	L	601	3,1	41,50,50	1.99	7 (17%)	45,82,82	1.61	8 (17%)
3	OT3	A	602	2	15,19,19	0.38	0	18,26,26	0.44	0
3	OT3	D	602	2	15,19,19	0.39	0	18,26,26	0.39	0
2	HEM	C	601	3,1	41,50,50	1.87	7 (17%)	45,82,82	1.73	9 (20%)
3	OT3	H	602	2	15,19,19	0.48	0	18,26,26	0.38	0
3	OT3	J	602	2	15,19,19	0.39	0	18,26,26	0.35	0
3	OT3	L	602	2	15,19,19	0.49	0	18,26,26	0.41	0
3	OT3	C	602	2	15,19,19	0.40	0	18,26,26	0.42	0
2	HEM	F	601	3,1	41,50,50	1.92	8 (19%)	45,82,82	1.87	11 (24%)
2	HEM	B	601	3,1	41,50,50	1.89	5 (12%)	45,82,82	1.74	11 (24%)
2	HEM	D	601	3,1	41,50,50	1.89	7 (17%)	45,82,82	1.68	10 (22%)
2	HEM	H	601	3,1	41,50,50	2.02	7 (17%)	45,82,82	1.79	10 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OT3	B	602	2	15,19,19	0.35	0	18,26,26	0.42	0
2	HEM	I	601	3,1	41,50,50	1.97	6 (14%)	45,82,82	1.57	8 (17%)
3	OT3	I	602	2	15,19,19	0.39	0	18,26,26	0.40	0
2	HEM	E	601	3,1	41,50,50	1.90	6 (14%)	45,82,82	1.88	8 (17%)

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	OT3	E	602	2	-	0/6/16/16	0/2/3/3
3	OT3	G	602	2	-	0/6/16/16	0/2/3/3
3	OT3	F	602	2	-	0/6/16/16	0/2/3/3
2	HEM	A	601	3,1	-	2/12/54/54	-
2	HEM	G	601	3,1	-	1/12/54/54	-
3	OT3	K	602	2	-	0/6/16/16	0/2/3/3
2	HEM	K	601	3,1	-	6/12/54/54	-
2	HEM	J	601	3,1	-	5/12/54/54	-
2	HEM	L	601	3,1	-	2/12/54/54	-
3	OT3	A	602	2	-	0/6/16/16	0/2/3/3
3	OT3	D	602	2	-	0/6/16/16	0/2/3/3
2	HEM	C	601	3,1	-	1/12/54/54	-
3	OT3	H	602	2	-	1/6/16/16	0/2/3/3
3	OT3	J	602	2	-	0/6/16/16	0/2/3/3
3	OT3	L	602	2	-	0/6/16/16	0/2/3/3
3	OT3	C	602	2	-	0/6/16/16	0/2/3/3
2	HEM	F	601	3,1	-	3/12/54/54	-
2	HEM	B	601	3,1	-	2/12/54/54	-
2	HEM	D	601	3,1	-	2/12/54/54	-
2	HEM	H	601	3,1	-	2/12/54/54	-
3	OT3	B	602	2	-	0/6/16/16	0/2/3/3
2	HEM	I	601	3,1	-	2/12/54/54	-
3	OT3	I	602	2	-	0/6/16/16	0/2/3/3
2	HEM	E	601	3,1	-	1/12/54/54	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	HEM	C3D-C2D	8.51	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3D-C2D	8.14	1.54	1.36
2	D	601	HEM	C3D-C2D	7.87	1.53	1.36
2	L	601	HEM	C3D-C2D	7.78	1.53	1.36
2	I	601	HEM	C3D-C2D	7.65	1.53	1.36

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	C4D-ND-C1D	6.85	112.14	105.07
2	F	601	HEM	C4D-ND-C1D	6.37	111.66	105.07
2	G	601	HEM	C4D-ND-C1D	6.12	111.40	105.07
2	K	601	HEM	C4D-ND-C1D	5.99	111.25	105.07
2	L	601	HEM	C4D-ND-C1D	5.98	111.25	105.07

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	601	HEM	C2B-C3B-CAB-CBB
2	K	601	HEM	C4B-C3B-CAB-CBB
2	K	601	HEM	C2D-C3D-CAD-CBD
2	K	601	HEM	C4D-C3D-CAD-CBD
2	F	601	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

24 monomers are involved in 73 short contacts:

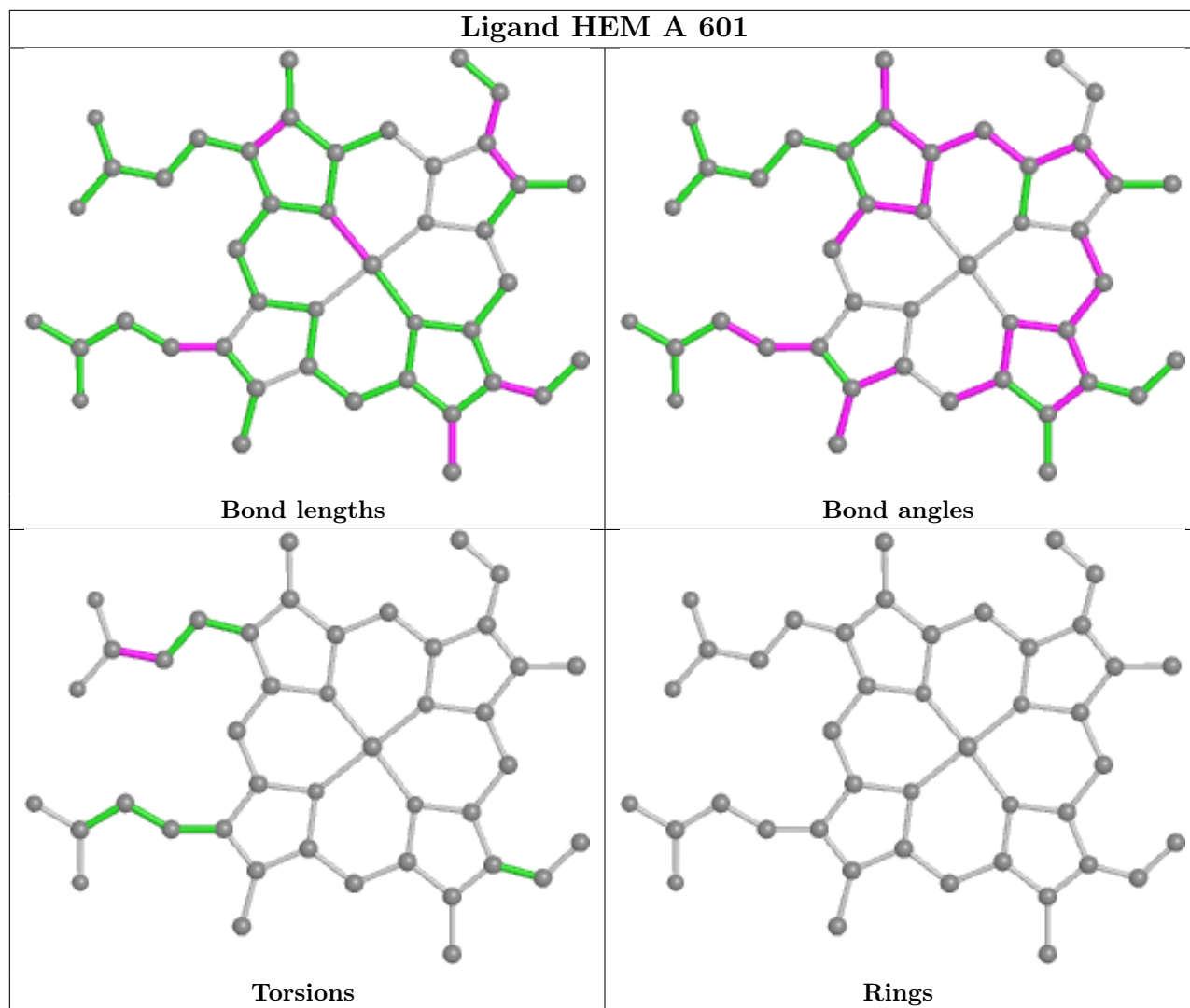
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	OT3	2	0
3	G	602	OT3	2	0
3	F	602	OT3	3	0
2	A	601	HEM	6	0
2	G	601	HEM	5	0
3	K	602	OT3	1	0
2	K	601	HEM	4	0
2	J	601	HEM	2	0
2	L	601	HEM	7	0
3	A	602	OT3	2	0
3	D	602	OT3	1	0
2	C	601	HEM	6	0
3	H	602	OT3	2	0

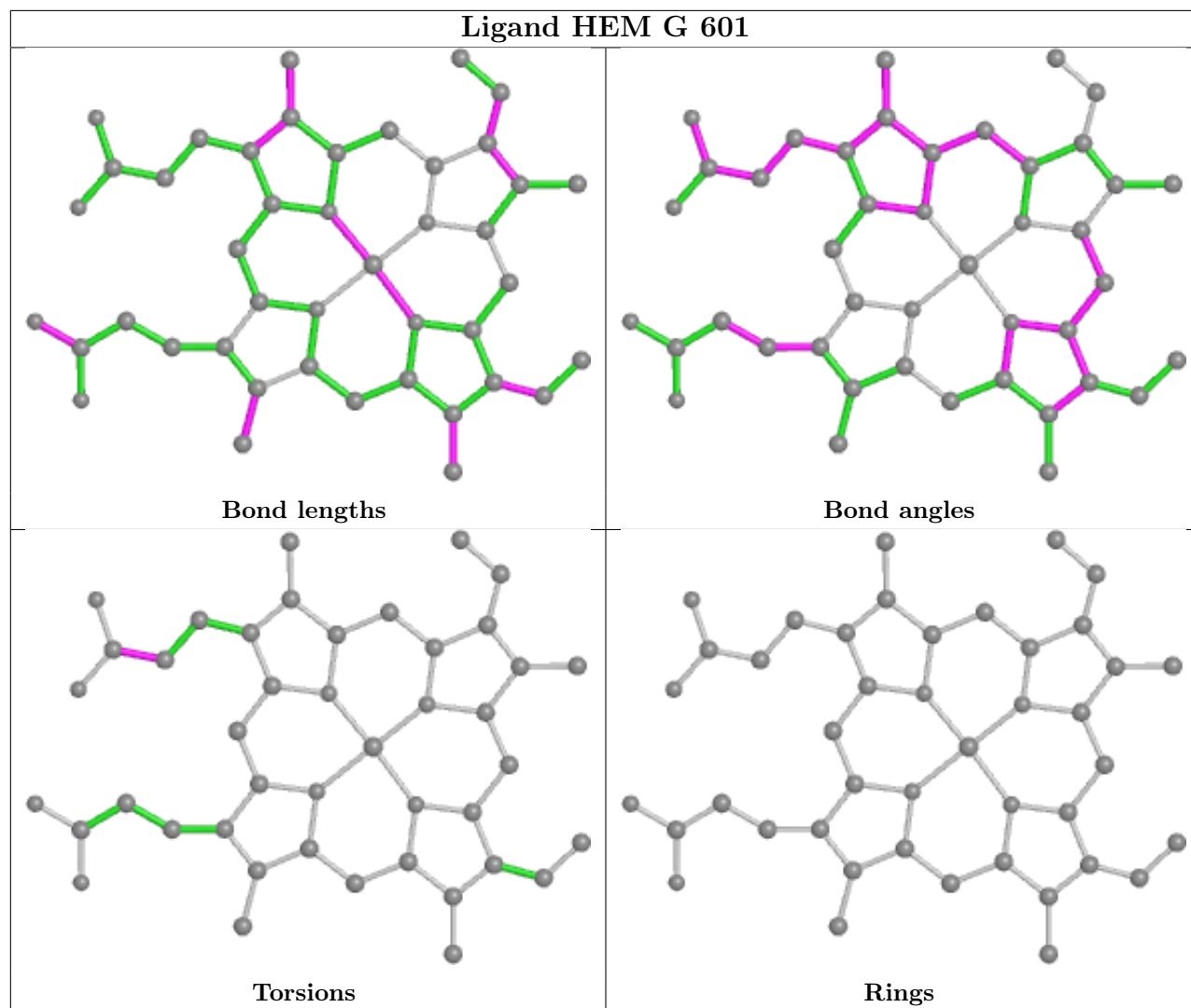
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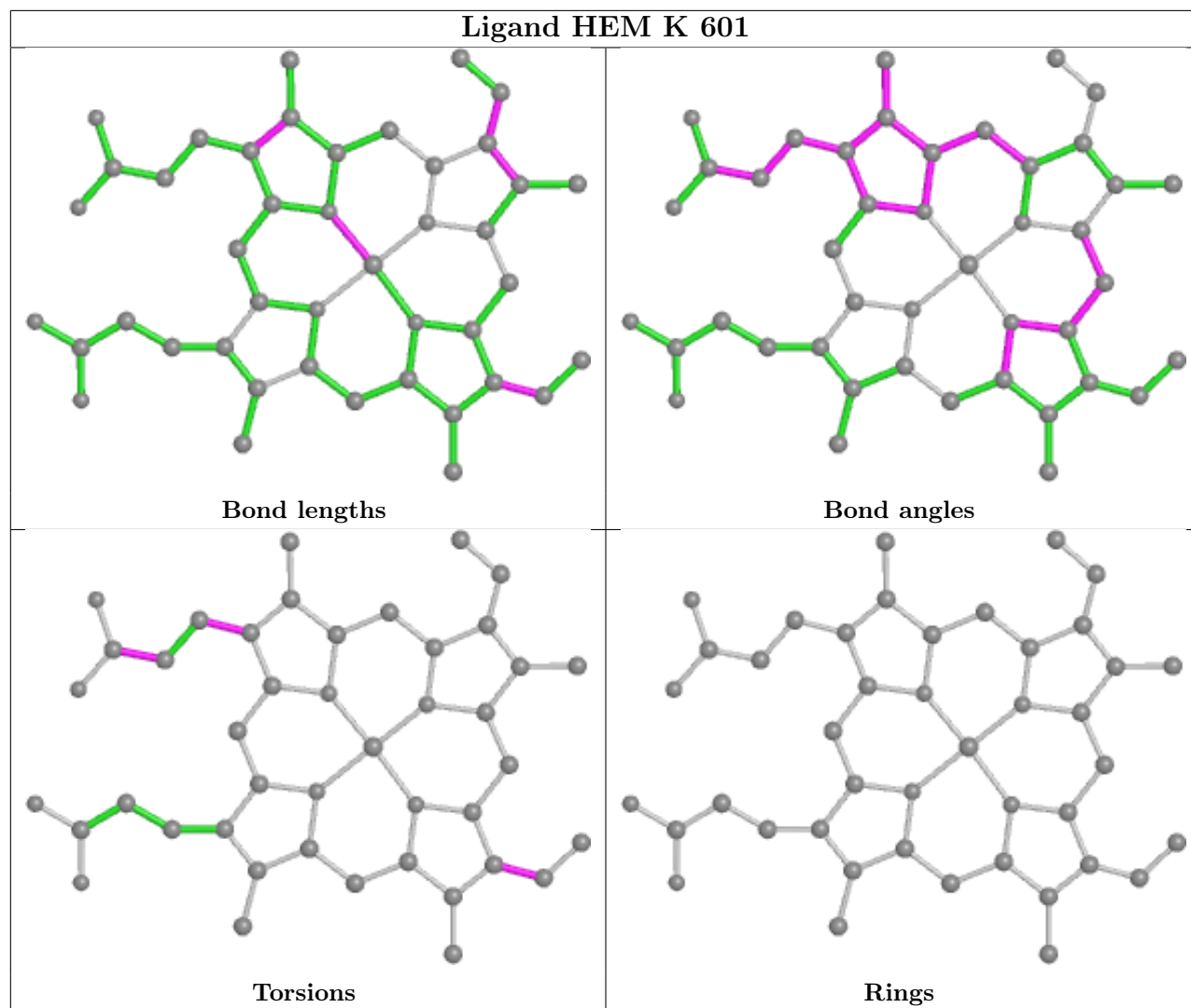
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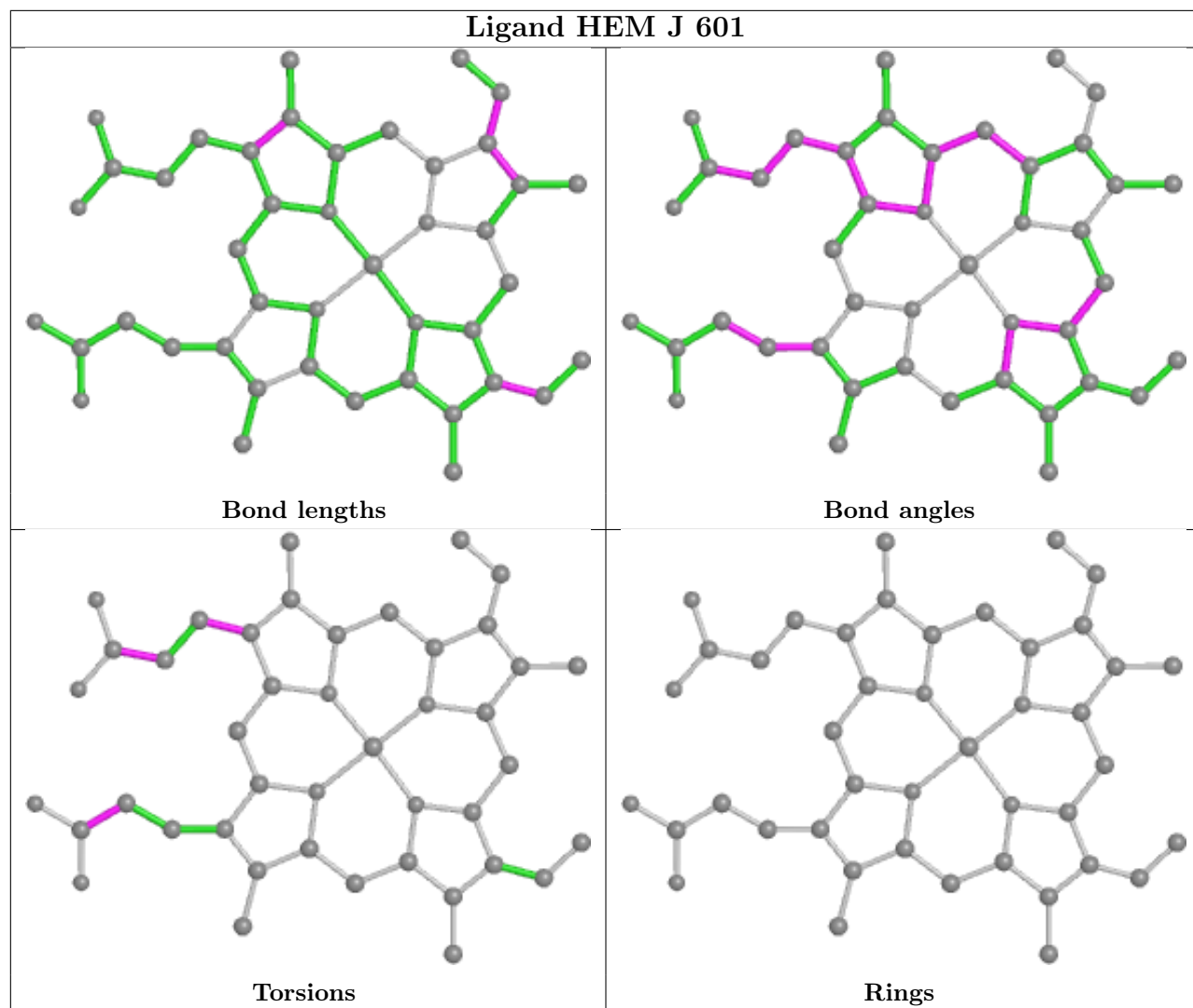
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	602	OT3	1	0
3	L	602	OT3	5	0
3	C	602	OT3	2	0
2	F	601	HEM	9	0
2	B	601	HEM	9	0
2	D	601	HEM	3	0
2	H	601	HEM	2	0
3	B	602	OT3	3	0
2	I	601	HEM	6	0
3	I	602	OT3	2	0
2	E	601	HEM	5	0

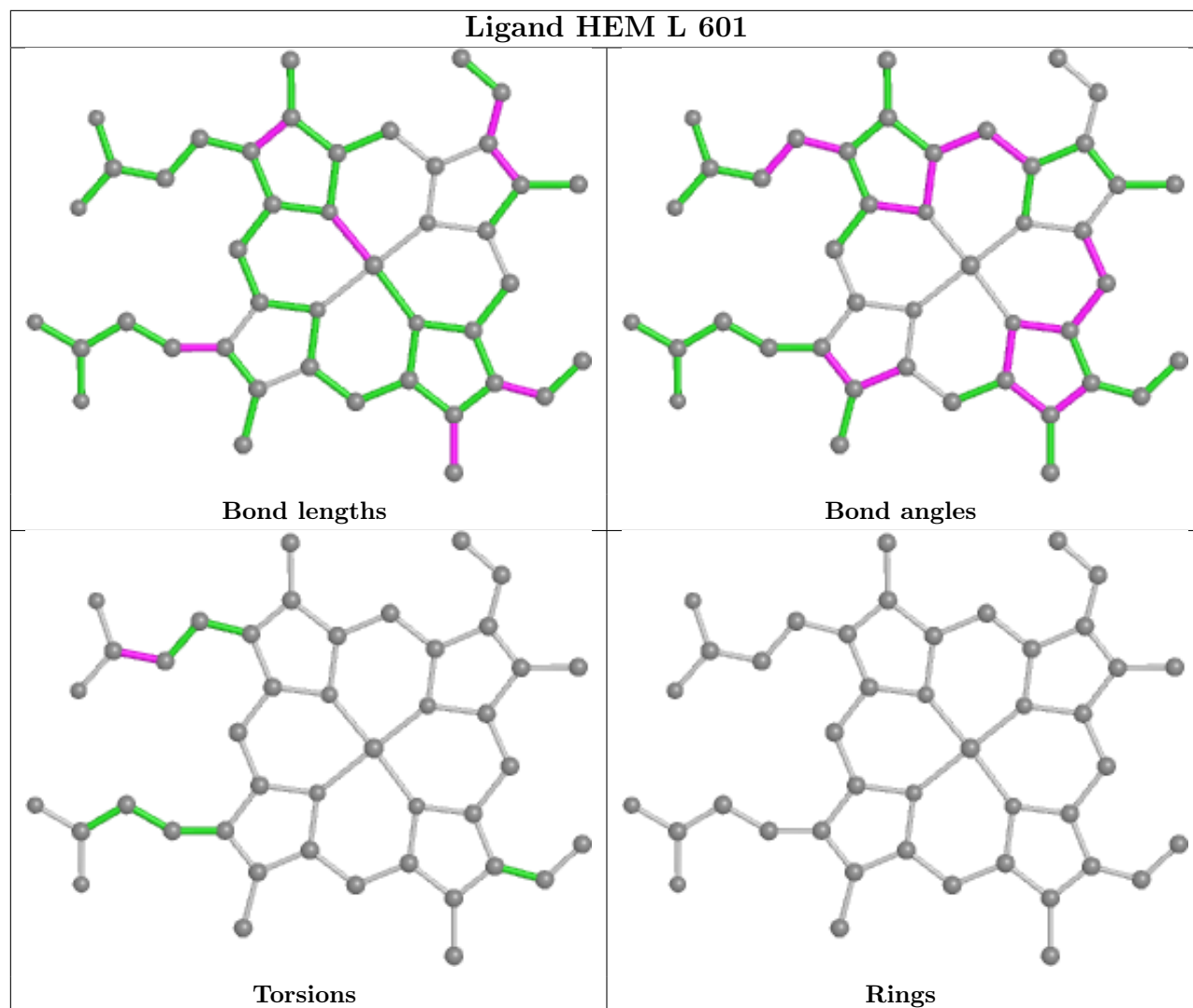
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



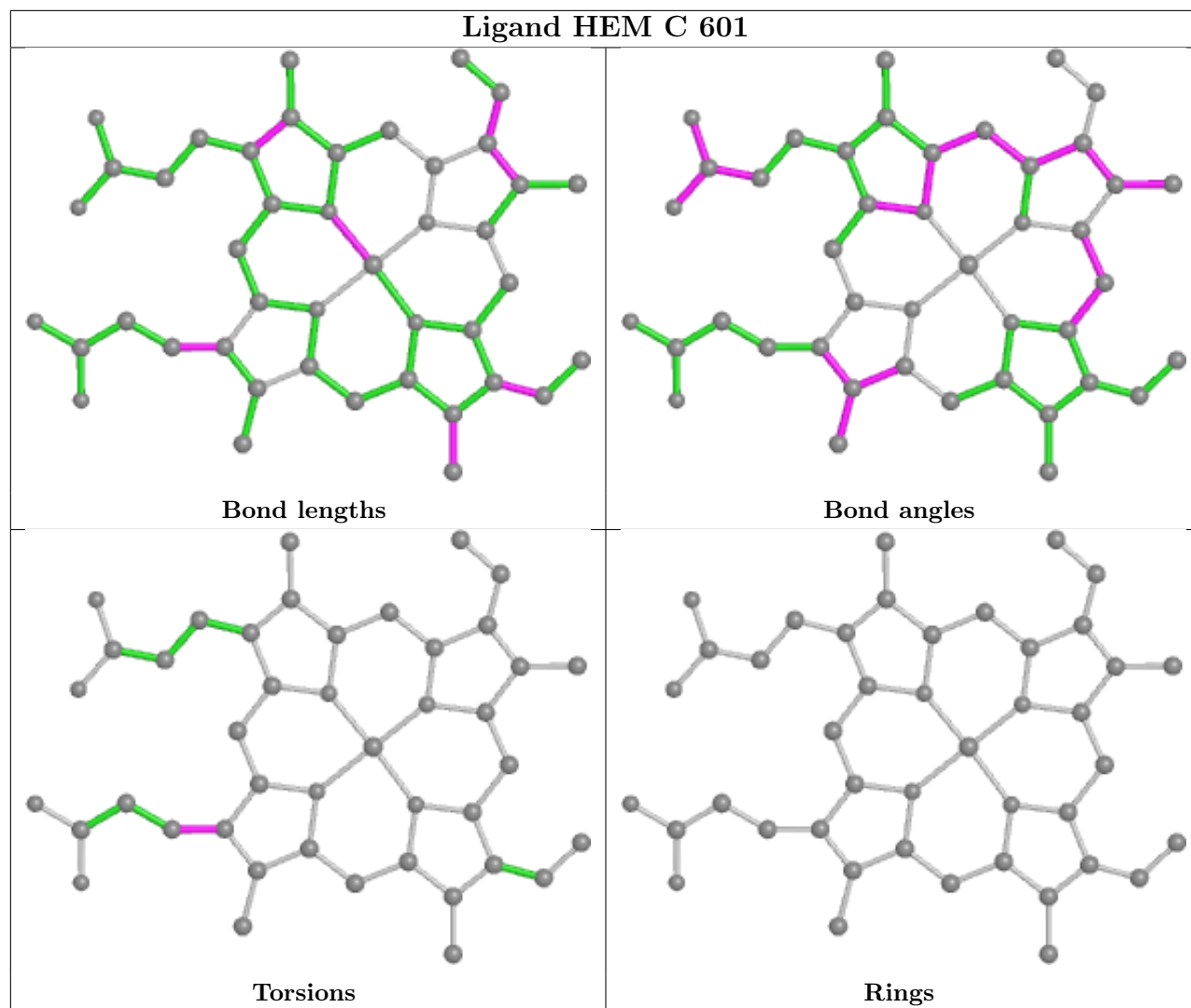


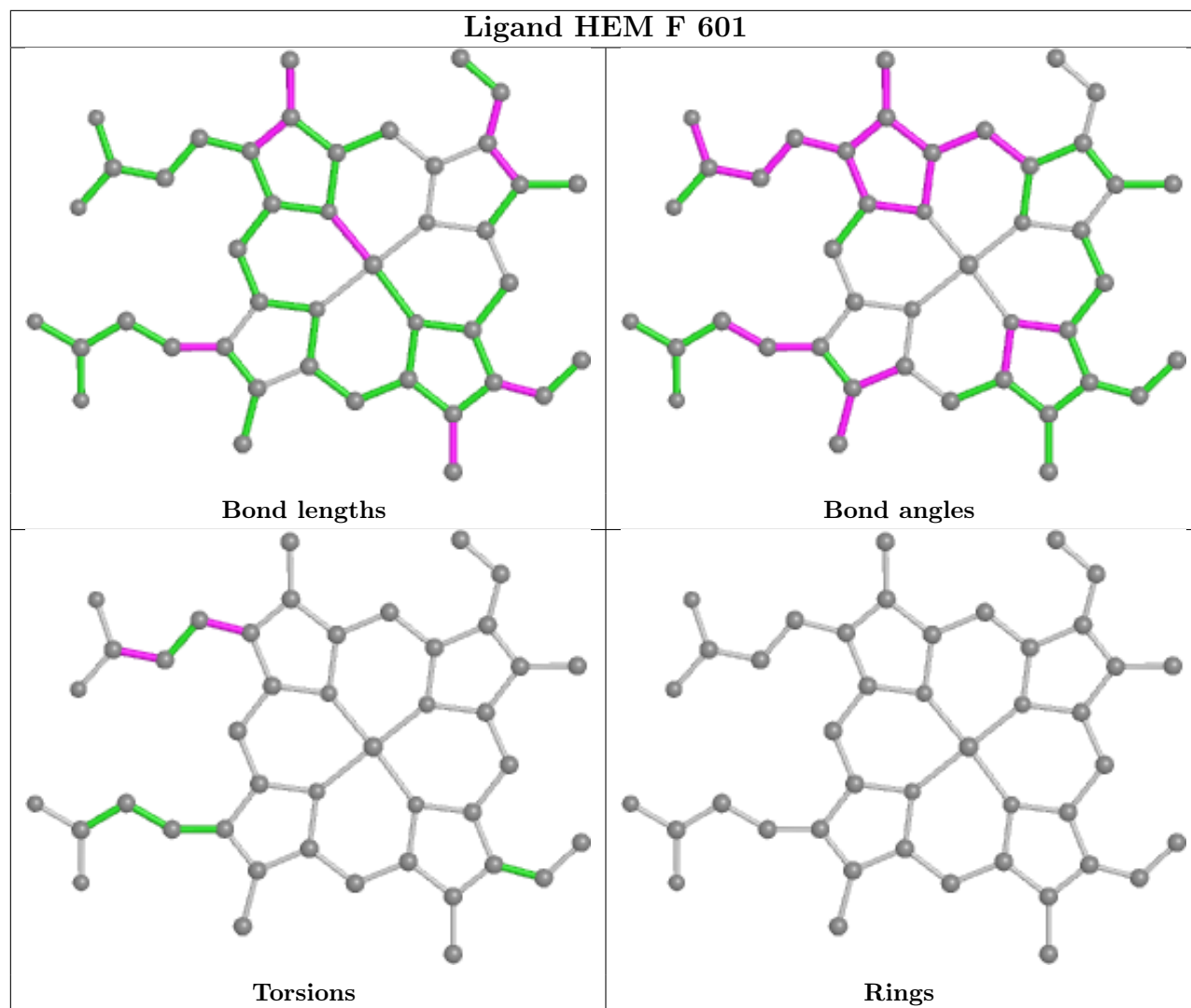


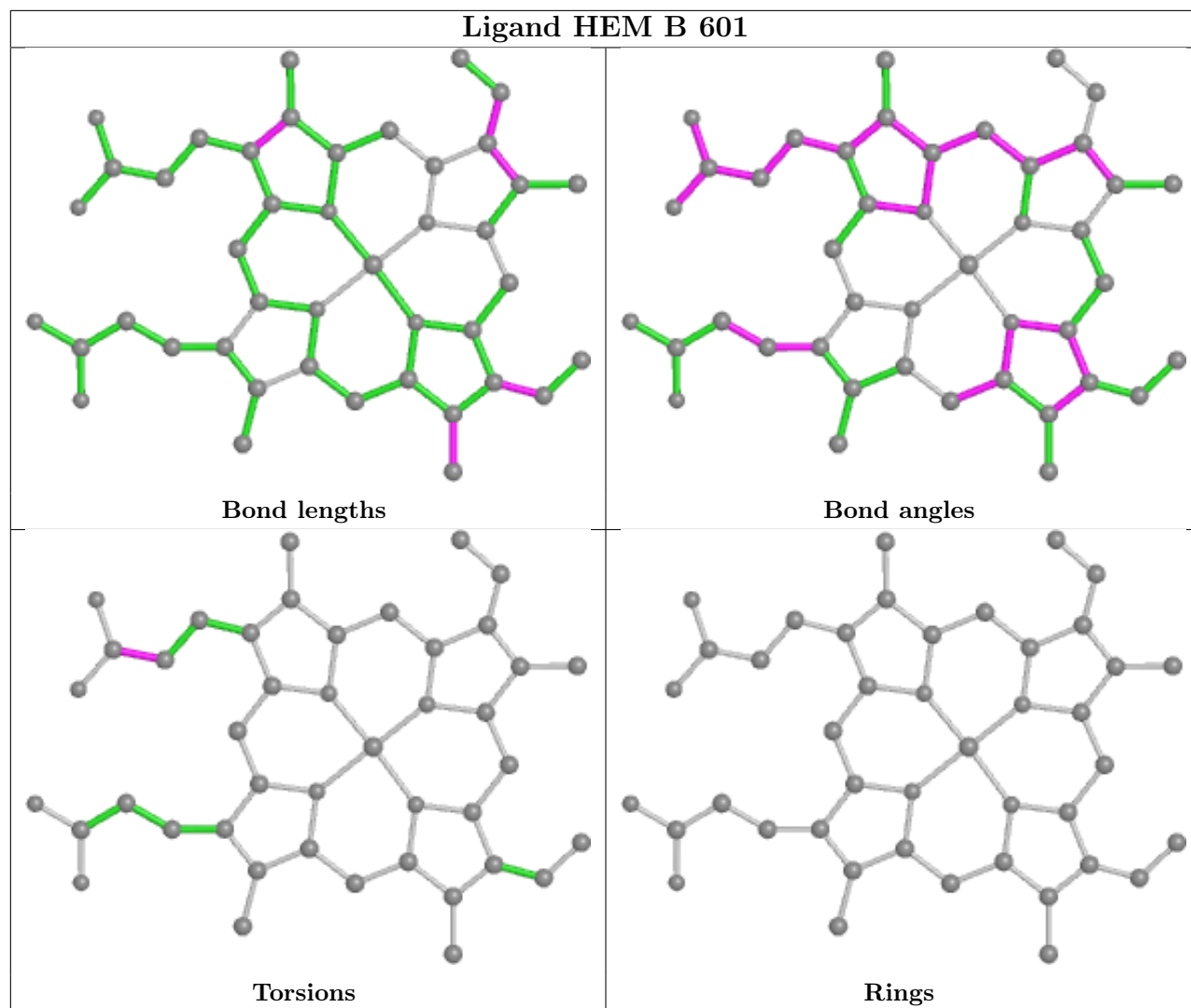


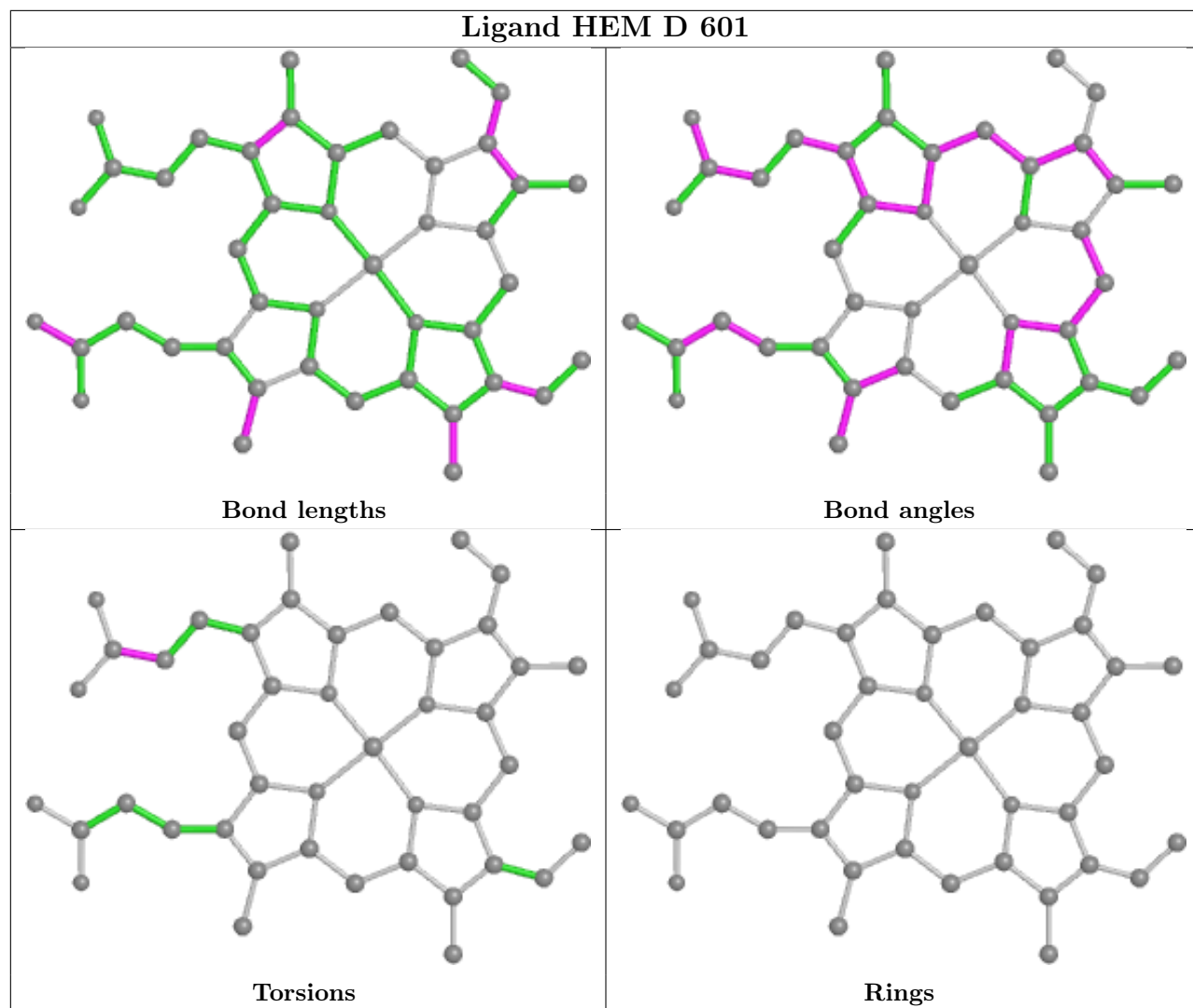


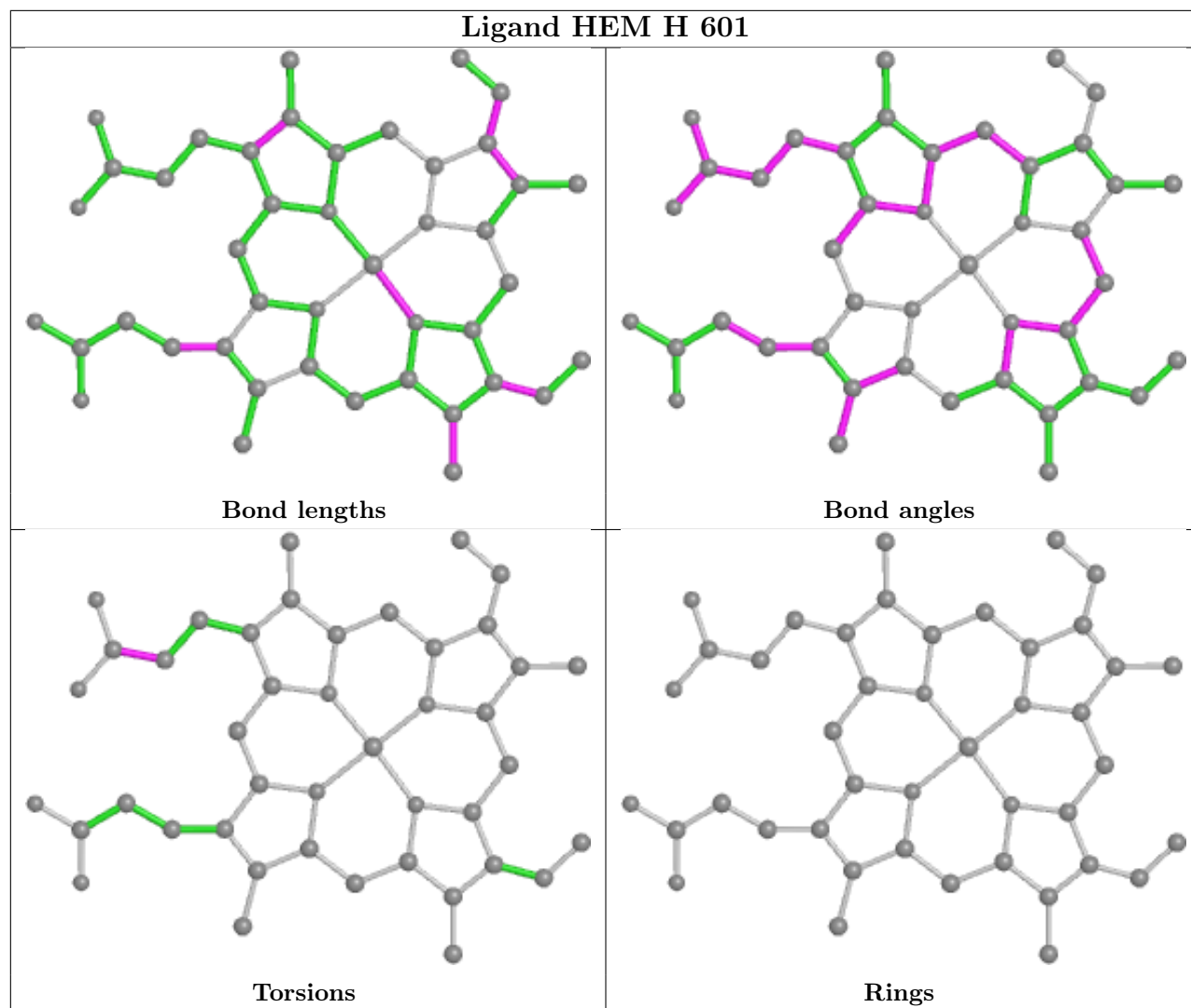


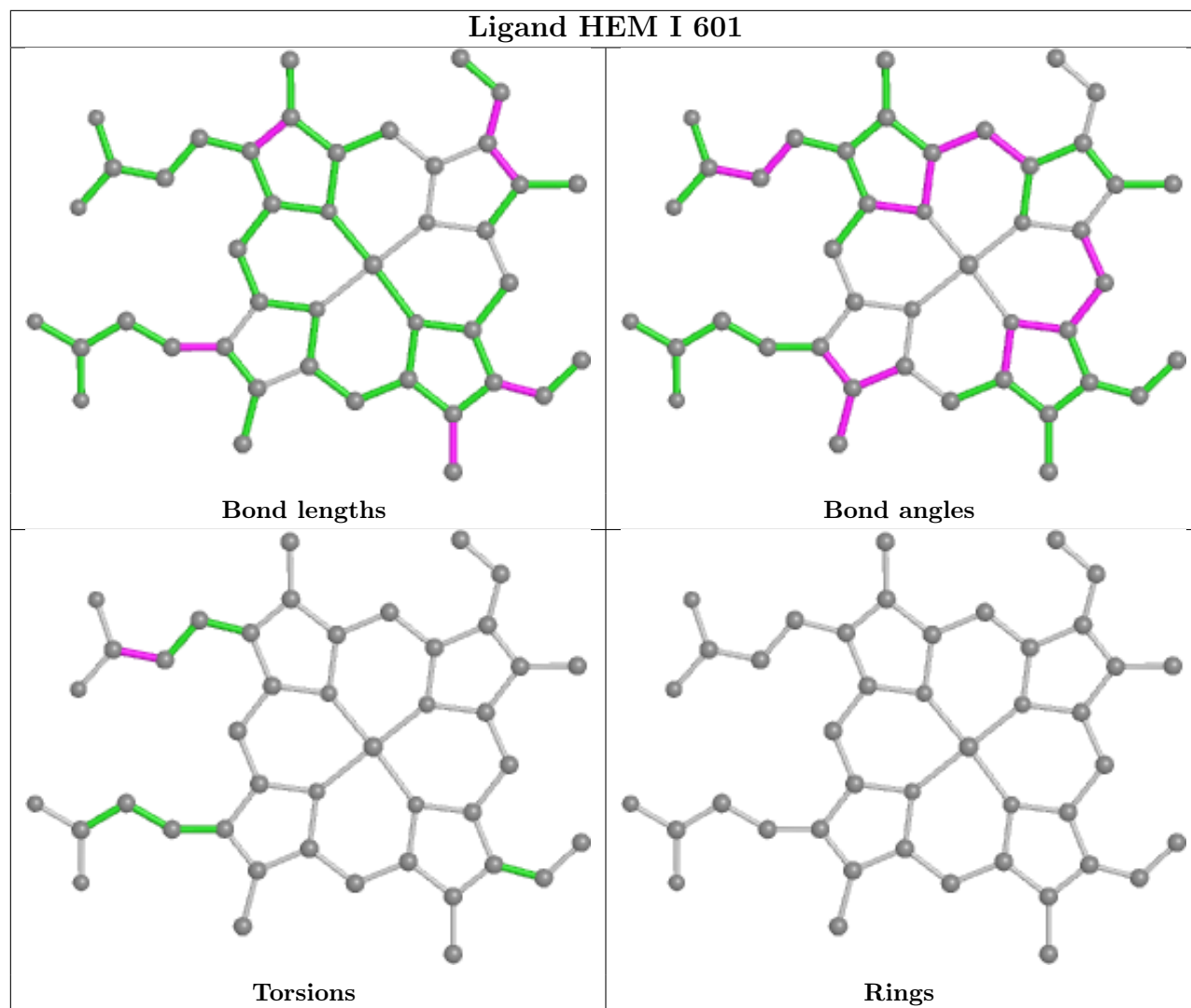


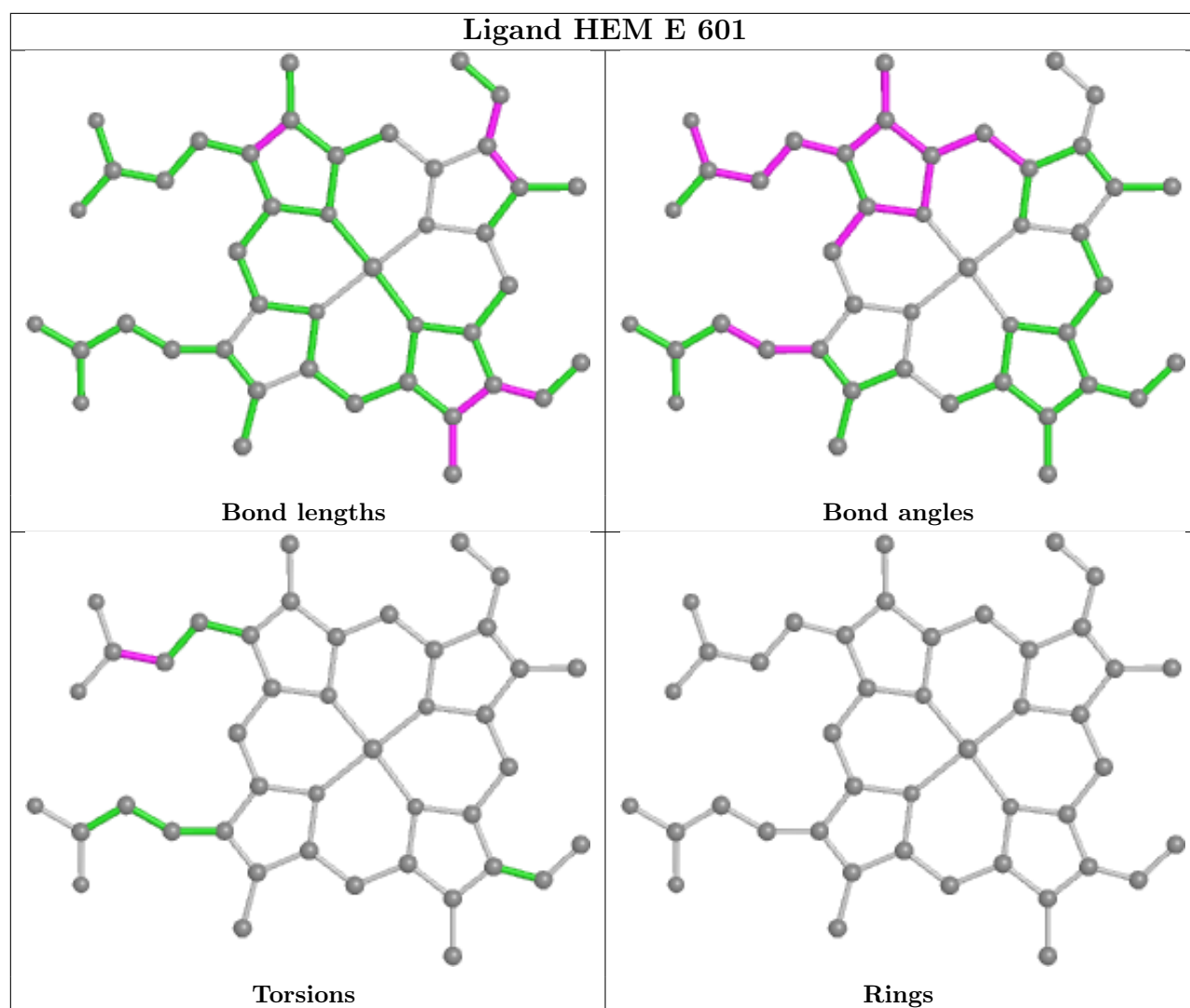












## 5.7 Other polymers [i](#)

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, 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	463/483 (95%)	0.03	3 (0%) 89 90	37, 54, 71, 79	0
1	B	465/483 (96%)	0.10	7 (1%) 73 76	46, 63, 84, 103	0
1	C	462/483 (95%)	0.05	6 (1%) 77 78	42, 56, 77, 88	0
1	D	465/483 (96%)	-0.04	2 (0%) 92 93	41, 57, 75, 90	0
1	E	470/483 (97%)	0.12	5 (1%) 80 82	38, 58, 75, 86	0
1	F	469/483 (97%)	0.17	6 (1%) 77 78	41, 64, 88, 103	0
1	G	463/483 (95%)	0.19	13 (2%) 53 54	47, 67, 96, 115	0
1	H	462/483 (95%)	0.18	18 (3%) 39 39	40, 61, 94, 112	0
1	I	462/483 (95%)	0.31	22 (4%) 30 29	49, 68, 96, 118	0
1	J	462/483 (95%)	0.44	36 (7%) 13 11	52, 78, 101, 120	0
1	K	469/483 (97%)	0.54	41 (8%) 10 8	63, 83, 113, 123	0
1	L	456/483 (94%)	0.21	12 (2%) 56 57	47, 65, 93, 118	0
All	All	5568/5796 (96%)	0.19	171 (3%) 49 50	37, 64, 96, 123	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	37	PRO	5.6
1	J	35	VAL	5.5
1	K	103	VAL	4.8
1	L	49	TRP	4.6
1	F	53	LEU	4.5

### 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](#)

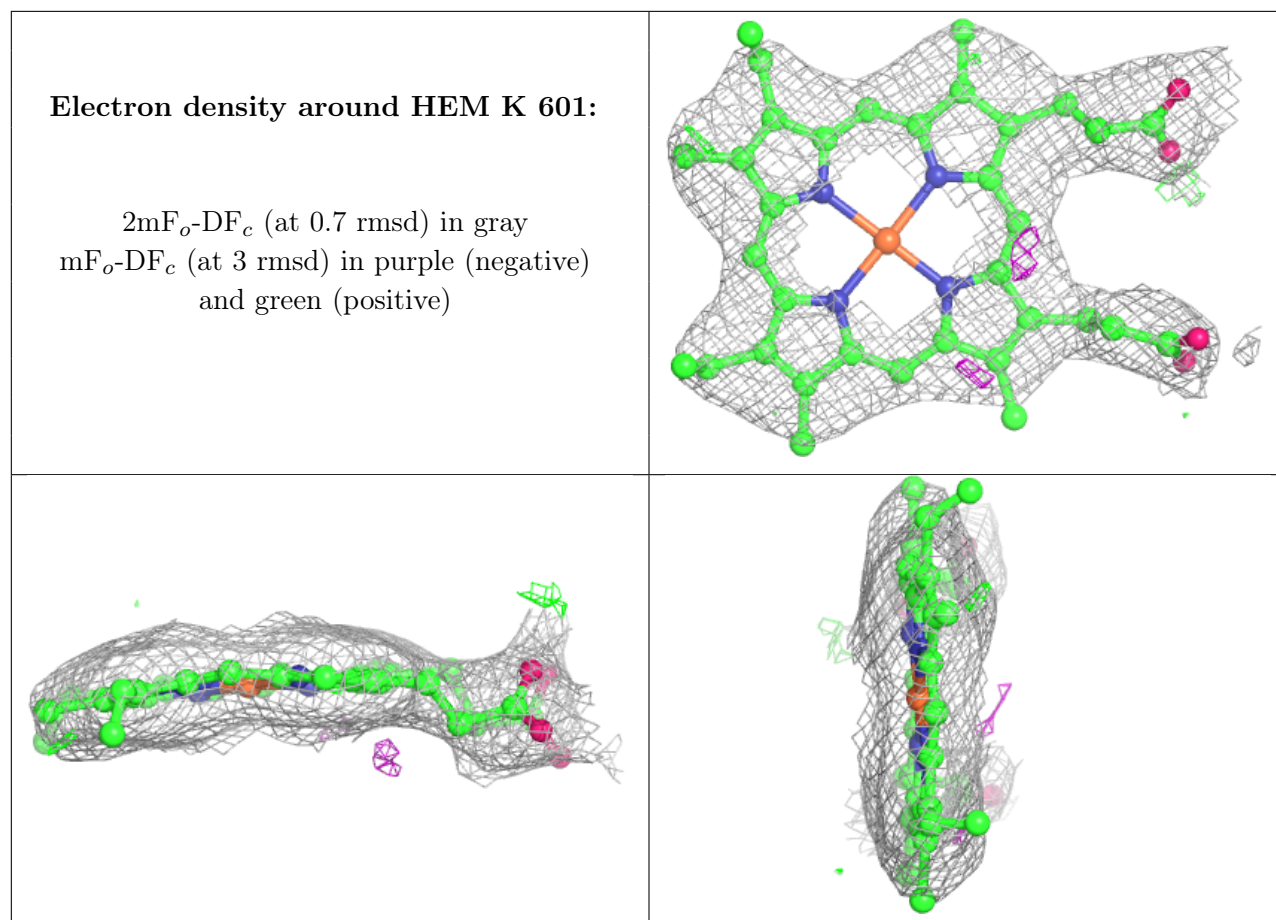
There are no monosaccharides in this entry.

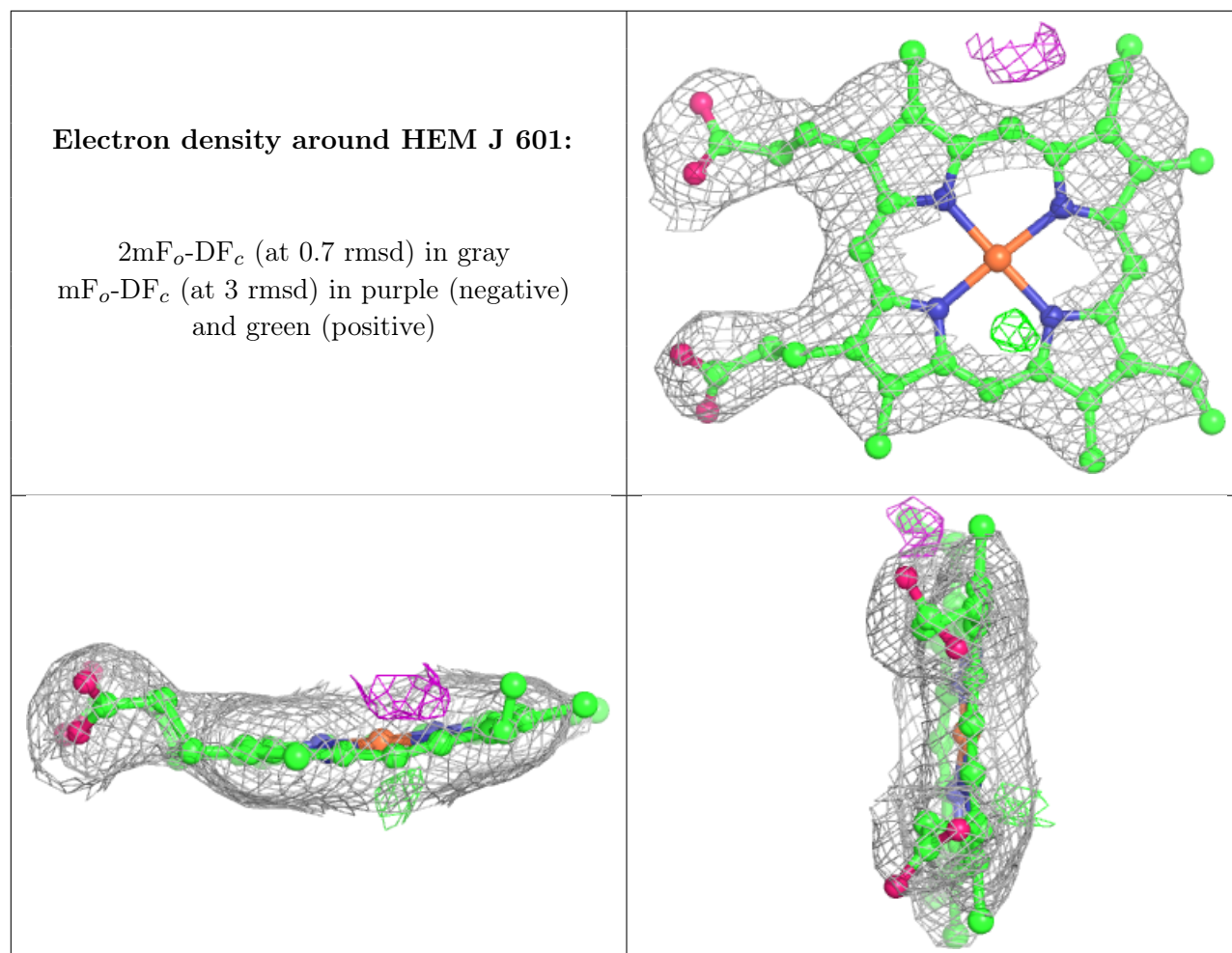
### 6.4 Ligands [i](#)

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	OT3	I	602	17/17	0.95	0.23	58,61,64,66	0
3	OT3	J	602	17/17	0.95	0.23	61,62,64,66	0
2	HEM	K	601	43/43	0.96	0.20	60,64,72,77	0
3	OT3	K	602	17/17	0.96	0.17	67,70,72,72	0
3	OT3	D	602	17/17	0.97	0.22	48,50,54,54	0
3	OT3	E	602	17/17	0.97	0.21	51,53,56,57	0
3	OT3	F	602	17/17	0.97	0.19	46,49,51,51	0
3	OT3	G	602	17/17	0.97	0.21	46,49,53,54	0
3	OT3	H	602	17/17	0.97	0.22	48,50,52,53	0
2	HEM	J	601	43/43	0.97	0.22	55,58,64,68	0
2	HEM	I	601	43/43	0.97	0.20	49,53,58,60	0
3	OT3	B	602	17/17	0.97	0.19	49,51,52,53	0
3	OT3	L	602	17/17	0.97	0.19	53,54,56,57	0
2	HEM	F	601	43/43	0.98	0.18	36,40,52,54	0
2	HEM	G	601	43/43	0.98	0.19	41,46,49,50	0
2	HEM	H	601	43/43	0.98	0.19	38,43,50,52	0
2	HEM	B	601	43/43	0.98	0.19	42,48,56,62	0
2	HEM	C	601	43/43	0.98	0.17	37,42,50,54	0
2	HEM	D	601	43/43	0.98	0.18	38,43,53,59	0
2	HEM	L	601	43/43	0.98	0.21	55,58,65,67	0
2	HEM	E	601	43/43	0.98	0.19	32,36,44,48	0
3	OT3	C	602	17/17	0.98	0.20	48,51,52,52	0
3	OT3	A	602	17/17	0.99	0.17	41,42,44,45	0
2	HEM	A	601	43/43	0.99	0.19	37,42,45,48	0

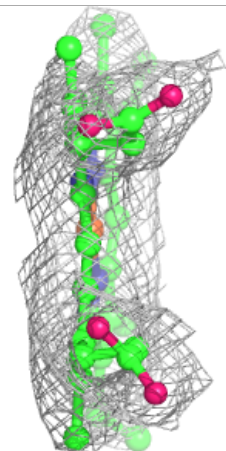
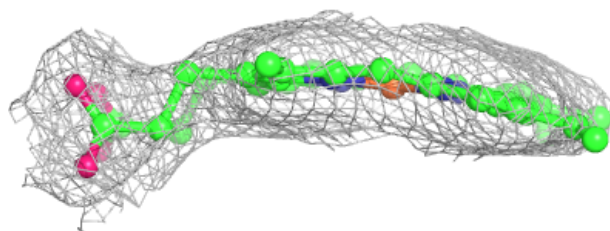
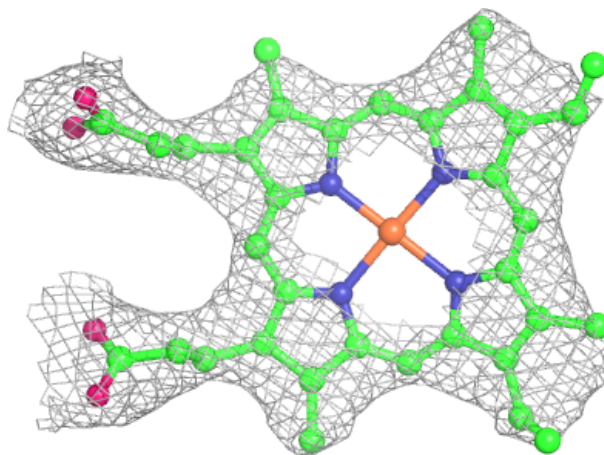
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





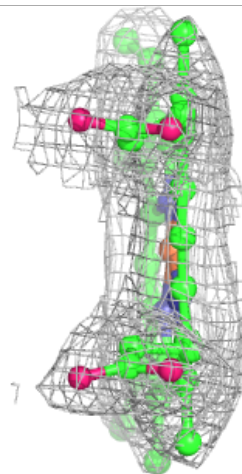
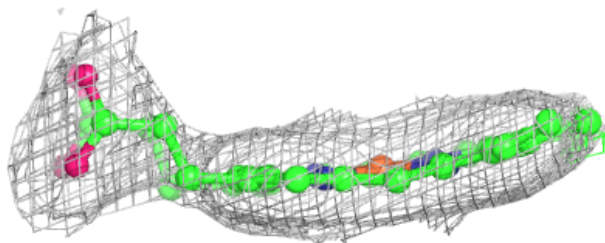
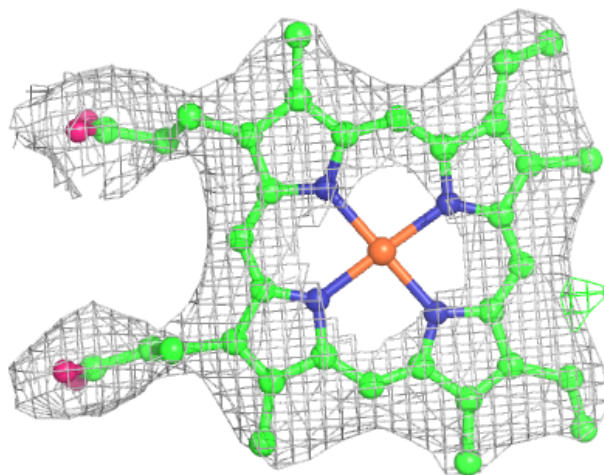
**Electron density around HEM I 601:**

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



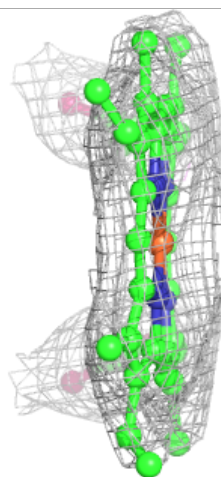
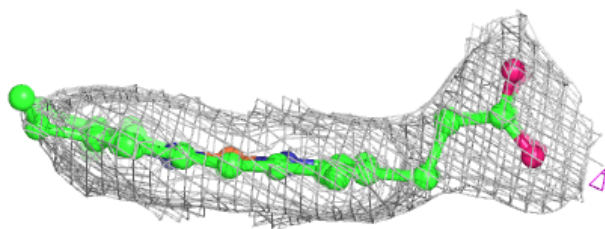
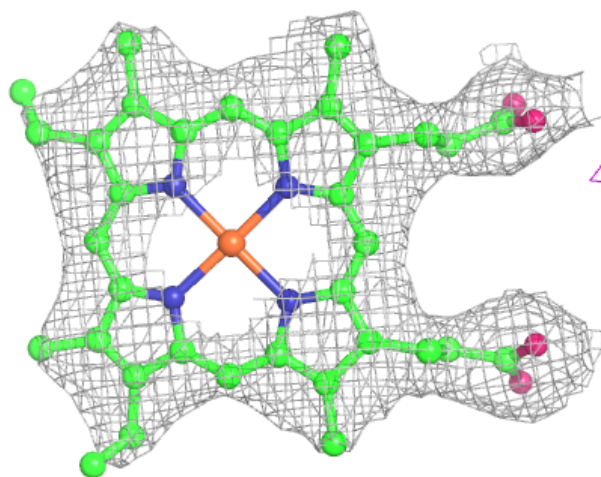
**Electron density around HEM F 601:**

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



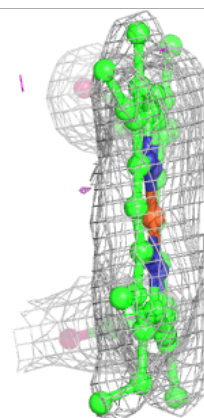
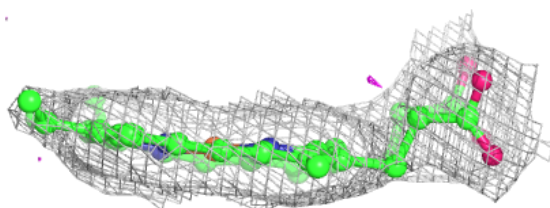
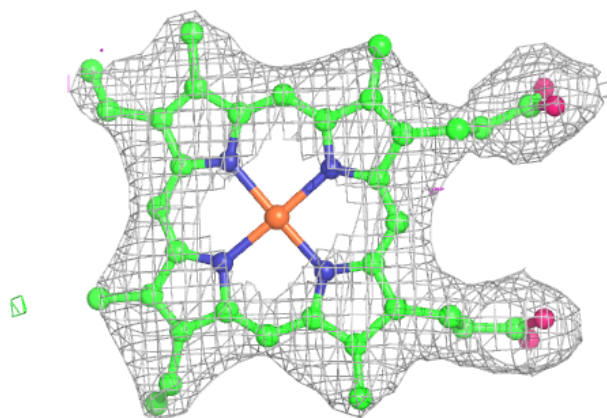
**Electron density around HEM G 601:**

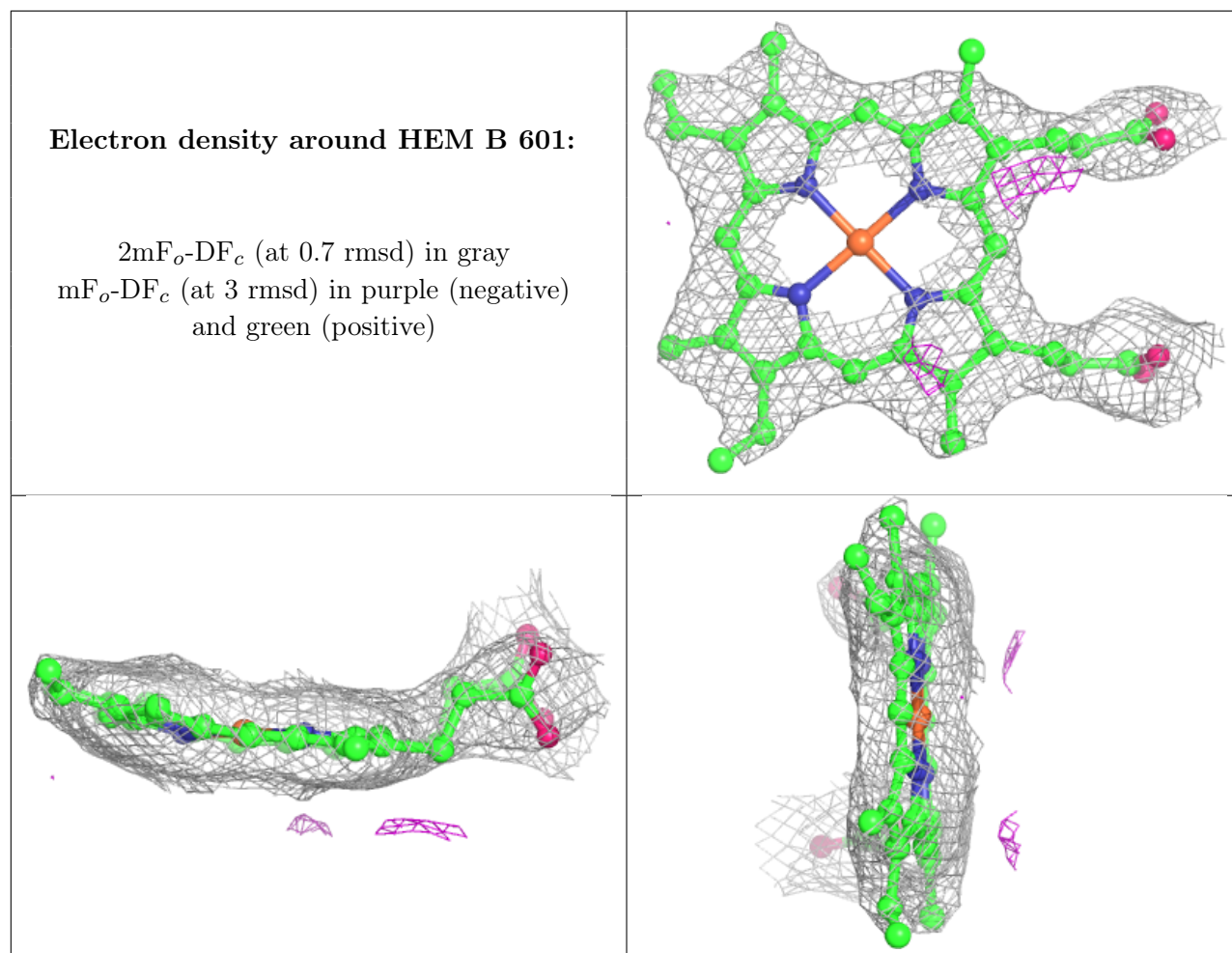
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM H 601:**

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

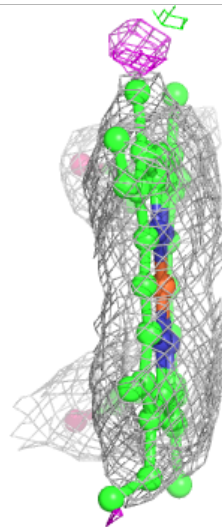
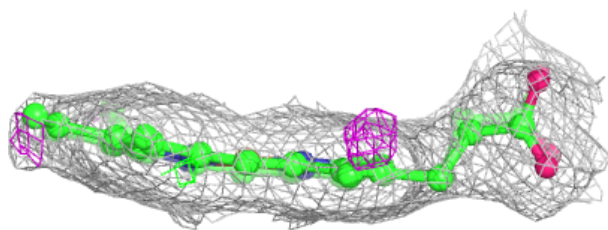
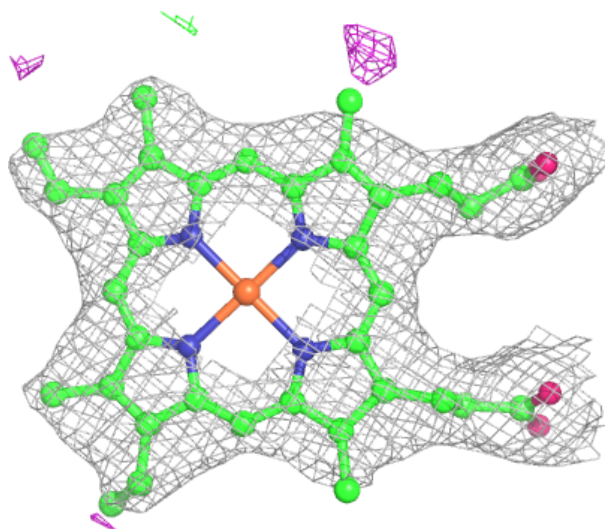






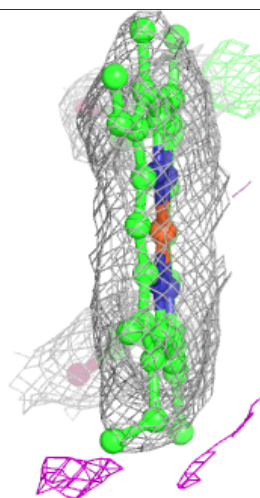
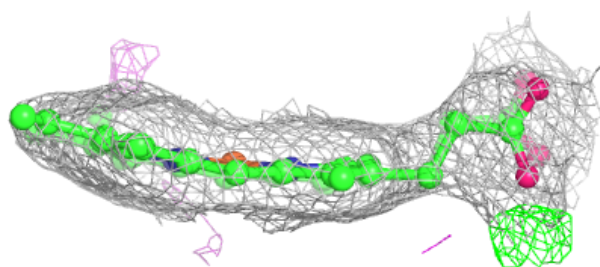
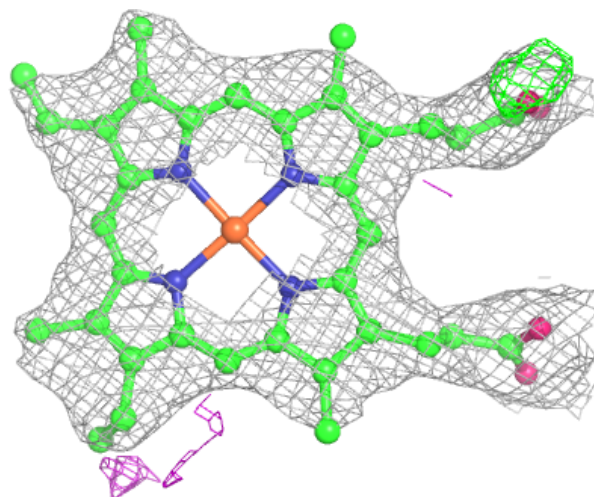
**Electron density around HEM C 601:**

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



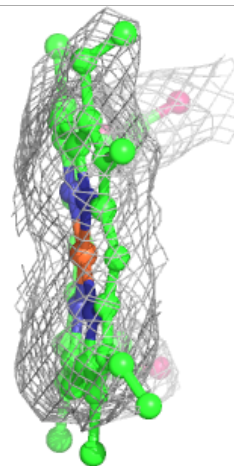
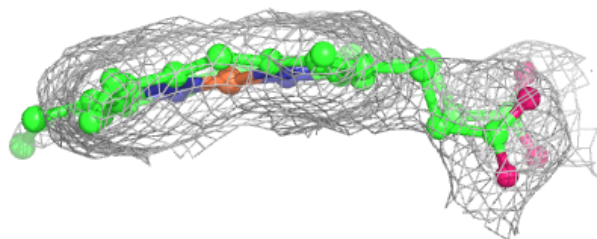
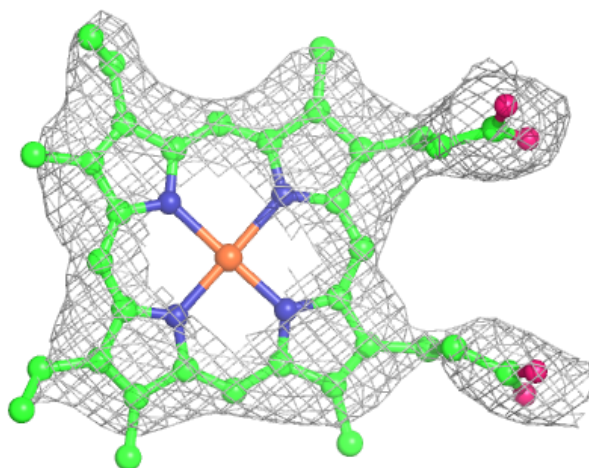
**Electron density around HEM D 601:**

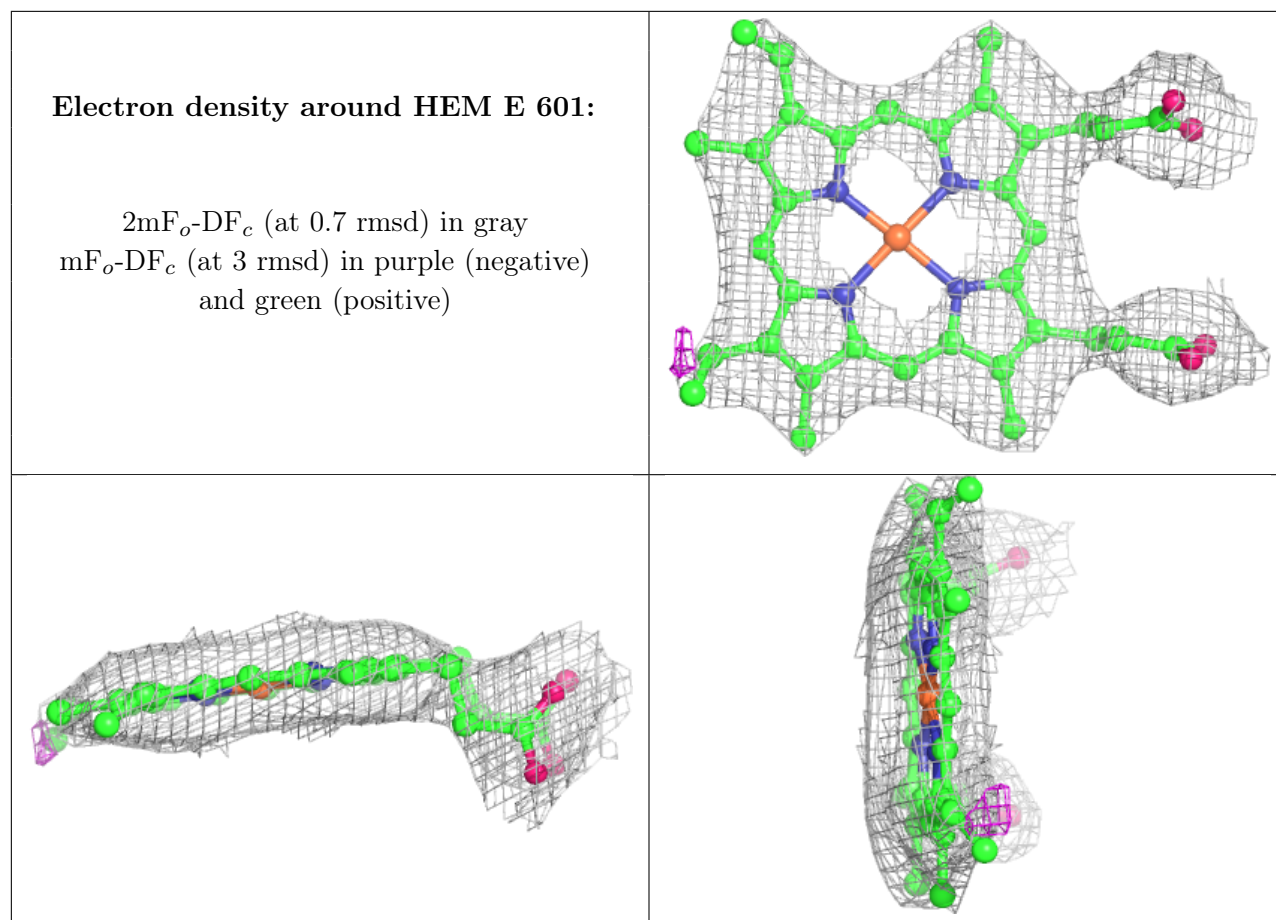
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

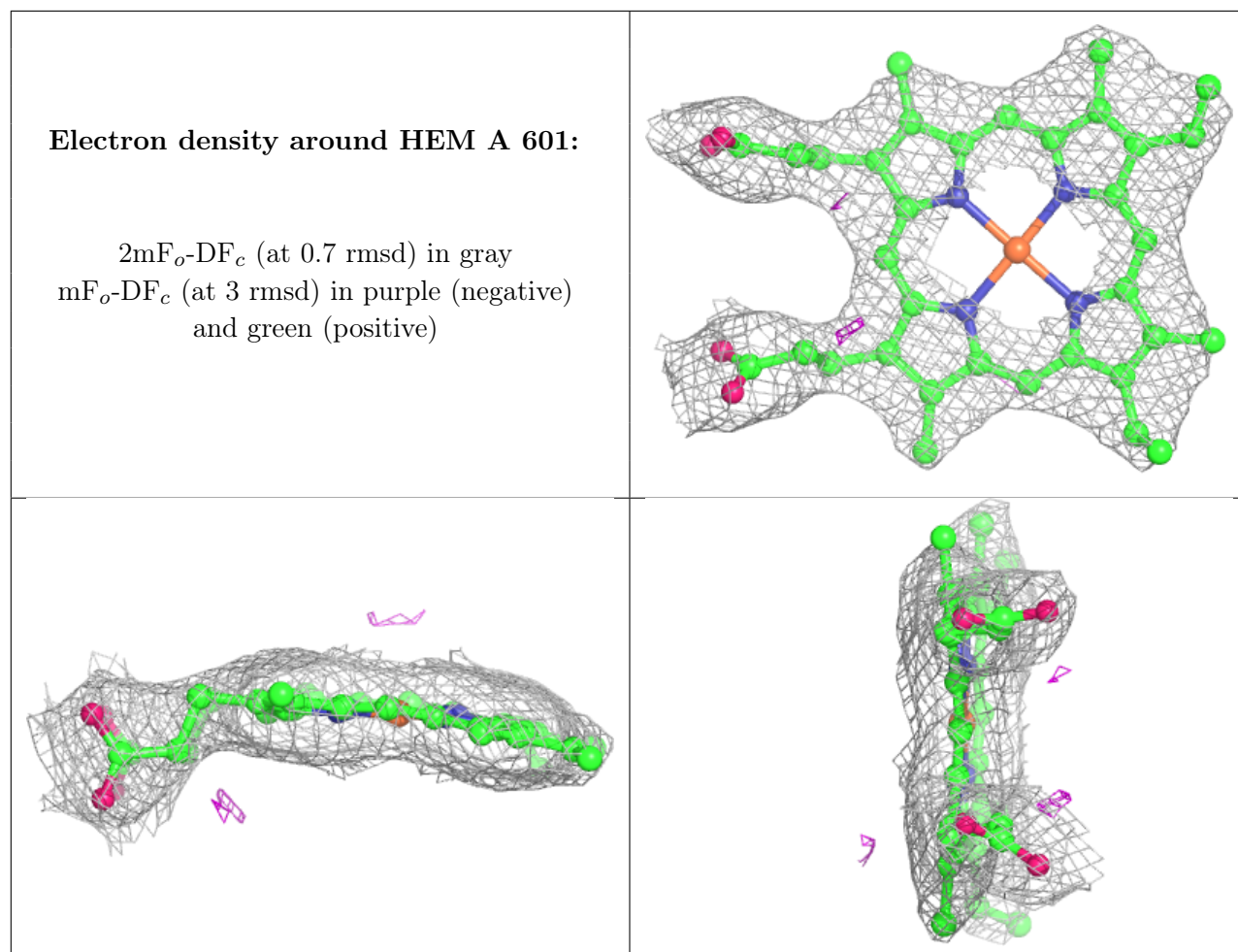


**Electron density around HEM L 601:**

$2mF_o-DF_c$  (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.