



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2022 – 02:51 PM EDT

PDB ID : 7LU7  
Title : Human TDO (hTDO) in complex with NLG919 analog  
Authors : Yeh, S.-R.  
Deposited on : 2021-02-21  
Resolution : 2.30 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>.

---

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 : 2.29  
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) : 2.29

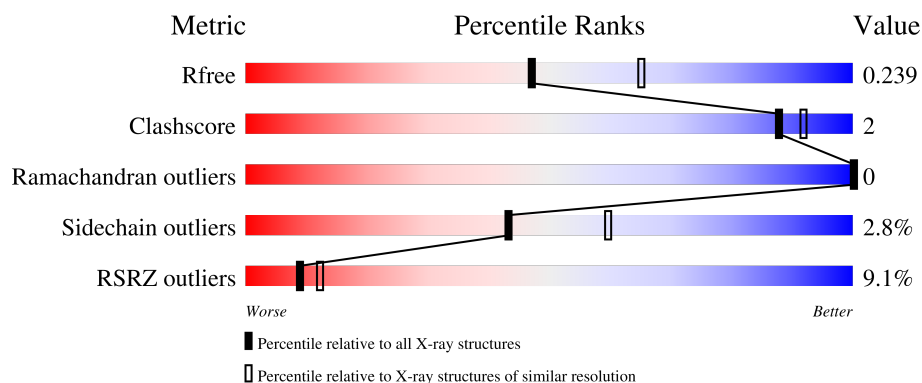
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AAA	380	<div> <div>7%</div> <div>86%</div> <div>10%</div> </div>
1	BBB	380	<div> <div>7%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
1	CCC	380	<div> <div>12%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
1	DDD	380	<div> <div>7%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23726 atoms, of which 11645 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	AAA	341	Total	C	H	N	O	S	77	0	0
			5791	1865	2895	503	517	11			
1	BBB	334	Total	C	H	N	O	S	69	0	0
			5655	1816	2834	488	506	11			
1	CCC	323	Total	C	H	N	O	S	71	0	0
			5480	1764	2742	475	488	11			
1	DDD	343	Total	C	H	N	O	S	76	0	0
			5819	1869	2910	510	519	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	17	MET	-	initiating methionine	UNP P48775
AAA	390	GLU	-	expression tag	UNP P48775
AAA	391	HIS	-	expression tag	UNP P48775
AAA	392	HIS	-	expression tag	UNP P48775
AAA	393	HIS	-	expression tag	UNP P48775
AAA	394	HIS	-	expression tag	UNP P48775
AAA	395	HIS	-	expression tag	UNP P48775
AAA	396	HIS	-	expression tag	UNP P48775
BBB	17	MET	-	initiating methionine	UNP P48775
BBB	390	GLU	-	expression tag	UNP P48775
BBB	391	HIS	-	expression tag	UNP P48775
BBB	392	HIS	-	expression tag	UNP P48775
BBB	393	HIS	-	expression tag	UNP P48775
BBB	394	HIS	-	expression tag	UNP P48775
BBB	395	HIS	-	expression tag	UNP P48775
BBB	396	HIS	-	expression tag	UNP P48775
CCC	17	MET	-	initiating methionine	UNP P48775
CCC	390	GLU	-	expression tag	UNP P48775
CCC	391	HIS	-	expression tag	UNP P48775
CCC	392	HIS	-	expression tag	UNP P48775
CCC	393	HIS	-	expression tag	UNP P48775

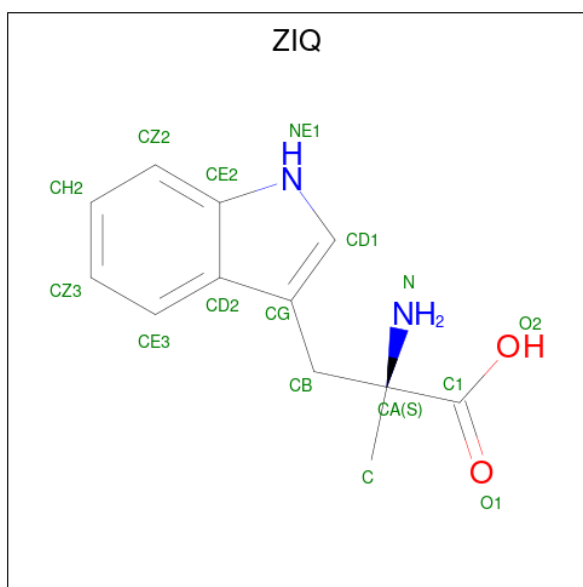
*Continued on next page...*

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	394	HIS	-	expression tag	UNP P48775
CCC	395	HIS	-	expression tag	UNP P48775
CCC	396	HIS	-	expression tag	UNP P48775
DDD	17	MET	-	initiating methionine	UNP P48775
DDD	390	GLU	-	expression tag	UNP P48775
DDD	391	HIS	-	expression tag	UNP P48775
DDD	392	HIS	-	expression tag	UNP P48775
DDD	393	HIS	-	expression tag	UNP P48775
DDD	394	HIS	-	expression tag	UNP P48775
DDD	395	HIS	-	expression tag	UNP P48775
DDD	396	HIS	-	expression tag	UNP P48775

- # HEM

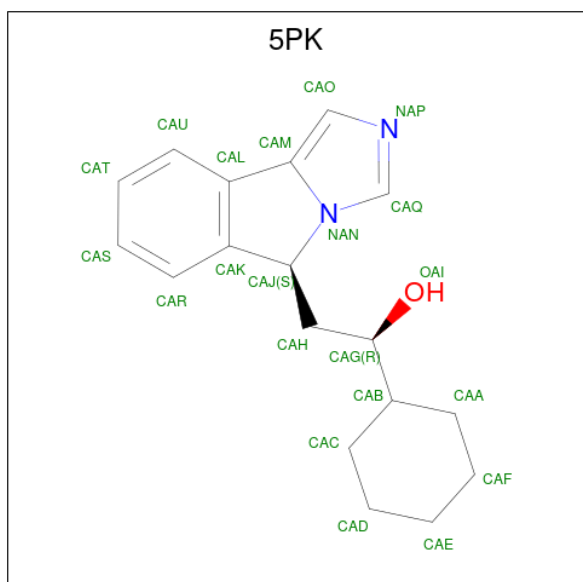
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	BBB	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	CCC	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	DDD	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
3	BBB	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
3	CCC	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
3	DDD	1	Total	C	H	N	O	0	0
			30	12	14	2	2		

- Molecule 4 is (1 {R})-1-cyclohexyl-2-[(5 {S})-5 {H}-imidazo[1,5-b]isoindol-5-yl]ethanol (three-letter code: 5PK) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	0	0
			43	18	22	2	1		
4	AAA	1	Total	C	H	N	O	0	0
			43	18	22	2	1		
4	CCC	1	Total	C	H	N	O	0	0
			43	18	22	2	1		
4	DDD	1	Total	C	H	N	O	0	0
			43	18	22	2	1		

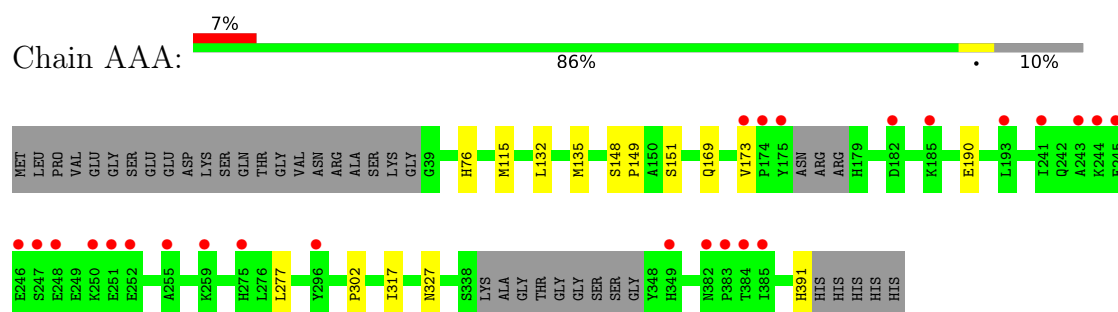
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	93	Total	O	0	0
			93	93		
5	BBB	123	Total	O	0	0
			123	123		
5	CCC	77	Total	O	0	0
			77	77		
5	DDD	104	Total	O	0	0
			104	104		

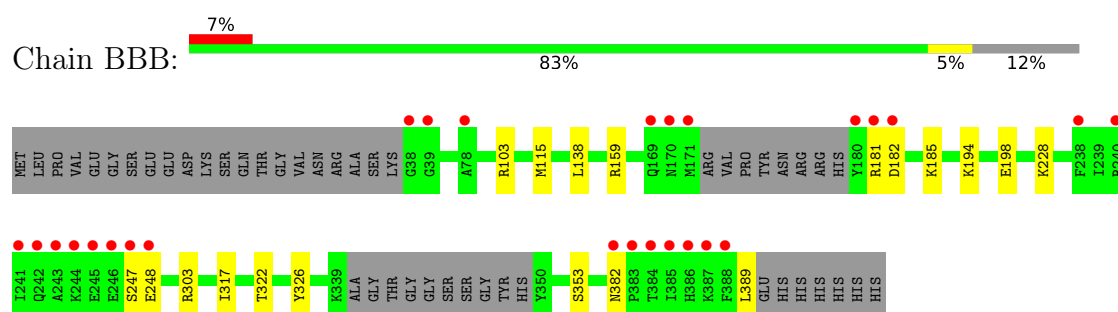
### 3 Residue-property plots [i](#)

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.

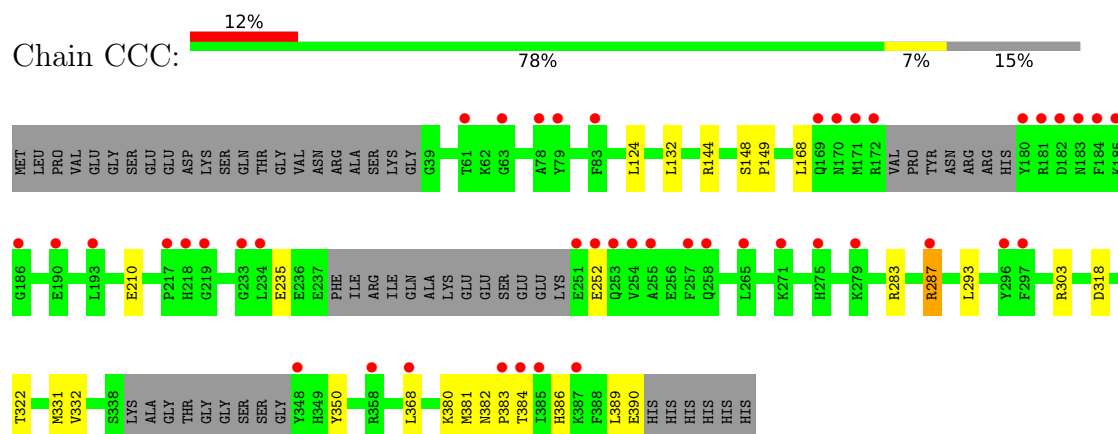
- Molecule 1: Tryptophan 2,3-dioxygenase



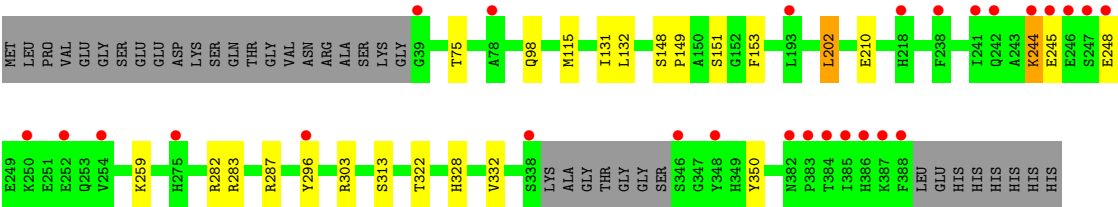
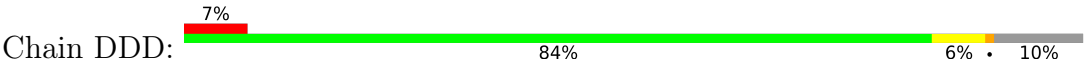
- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.26 Å   153.81 Å   87.97 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.95 – 2.30 29.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.95-2.30) 99.1 (29.95-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.189 , 0.236 0.194 , 0.239	Depositor DCC
$R_{free}$ test set	4277 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23726	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 3.25% 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: ZIQ, 5PK, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AAA	0.71	0/2964	0.77	0/3989
1	BBB	0.68	0/2883	0.78	0/3876
1	CCC	0.69	0/2800	0.79	0/3767
1	DDD	0.69	0/2977	0.78	0/4006
All	All	0.69	0/11624	0.78	0/15638

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 [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	AAA	2896	2895	2876	9	0
1	BBB	2821	2834	2818	6	0
1	CCC	2738	2742	2724	12	0
1	DDD	2909	2910	2893	11	0
2	AAA	43	30	30	5	0
2	BBB	43	30	30	2	0
2	CCC	43	30	30	3	0
2	DDD	43	30	30	3	0
3	AAA	16	14	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	16	14	0	1	0
3	CCC	16	14	0	0	0
3	DDD	16	14	0	0	0
4	AAA	42	44	44	6	0
4	CCC	21	22	22	1	0
4	DDD	21	22	22	2	0
5	AAA	93	0	0	0	0
5	BBB	123	0	0	0	0
5	CCC	77	0	0	0	0
5	DDD	104	0	0	0	0
All	All	12081	11645	11519	46	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 2.

All (46) 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)
2:AAA:401:HEM:C4A	4:AAA:403:5PK:H21	2.29	0.67
1:DDD:210:GLU:HG2	1:DDD:287:ARG:HB3	1.85	0.59
2:DDD:401:HEM:HBC2	2:DDD:401:HEM:HHD	1.84	0.57
4:AAA:404:5PK:H21	2:BBB:401:HEM:C4A	2.40	0.56
2:AAA:401:HEM:HBC2	2:AAA:401:HEM:HHD	1.89	0.55
2:CCC:401:HEM:HBC2	2:CCC:401:HEM:HHD	1.91	0.53
1:AAA:151:SER:HA	4:AAA:403:5PK:H16	1.91	0.52
1:CCC:303:ARG:HD3	1:CCC:389:LEU:HA	1.93	0.50
2:AAA:401:HEM:NA	4:AAA:403:5PK:H21	2.27	0.49
1:BBB:194:LYS:O	1:BBB:198:GLU:HG3	2.12	0.49
2:CCC:401:HEM:C4A	4:CCC:403:5PK:H21	2.47	0.49
1:BBB:159:ARG:HD2	1:BBB:181:ARG:HD3	1.95	0.48
1:BBB:115:MET:HE3	1:BBB:317:ILE:CD1	2.44	0.47
2:BBB:401:HEM:HBC2	2:BBB:401:HEM:HHD	1.96	0.47
1:CCC:382:ASN:HB2	1:CCC:383:PRO:HD2	1.96	0.47
1:CCC:168:LEU:HD23	1:CCC:168:LEU:HA	1.81	0.46
1:CCC:210:GLU:HG2	1:CCC:287:ARG:HB3	1.98	0.46
1:CCC:293:LEU:HD13	1:CCC:368:LEU:HD22	1.98	0.46
1:AAA:115:MET:HE3	1:AAA:317:ILE:HD12	1.98	0.45
1:DDD:244:LYS:O	1:DDD:245:GLU:HG2	2.16	0.45
1:AAA:76:HIS:NE2	4:AAA:403:5PK:H22	2.32	0.44
1:CCC:332:VAL:HG22	2:CCC:401:HEM:CHB	2.47	0.44
1:DDD:328:HIS:O	1:DDD:332:VAL:HG23	2.18	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:132:LEU:HD12	1:AAA:132:LEU:HA	1.83	0.44
1:AAA:391:HIS:HB2	1:DDD:303:ARG:HG3	2.00	0.44
1:AAA:277:LEU:HD23	1:AAA:277:LEU:HA	1.90	0.43
1:BBB:103:ARG:HA	3:BBB:402:ZIQ:O1	2.19	0.43
1:BBB:303:ARG:HD3	1:BBB:389:LEU:HA	2.01	0.43
2:DDD:401:HEM:C4A	4:DDD:403:5PK:H21	2.54	0.43
1:DDD:244:LYS:C	1:DDD:245:GLU:HG2	2.39	0.43
1:AAA:151:SER:HB2	2:AAA:401:HEM:O1A	2.19	0.43
2:DDD:401:HEM:O2A	4:DDD:403:5PK:OAI	2.33	0.42
1:CCC:148:SER:HA	1:CCC:149:PRO:HA	1.83	0.42
1:CCC:318:ASP:O	1:CCC:322:THR:HG22	2.20	0.42
1:DDD:202:LEU:HD22	1:DDD:283:ARG:NH1	2.34	0.42
1:CCC:168:LEU:HG	1:CCC:283:ARG:NH2	2.35	0.42
1:AAA:148:SER:HA	1:AAA:149:PRO:HA	1.81	0.42
2:AAA:401:HEM:C4A	4:AAA:403:5PK:CAQ	3.03	0.41
1:DDD:153:PHE:HZ	1:DDD:350:TYR:CE2	2.38	0.41
1:CCC:381:MET:HB3	1:CCC:386:HIS:CE1	2.56	0.41
1:CCC:132:LEU:HB3	1:CCC:331:MET:CE	2.51	0.40
1:BBB:326:TYR:OH	1:DDD:322:THR:HG22	2.20	0.40
1:CCC:124:LEU:HD22	1:DDD:131:ILE:CD1	2.52	0.40
1:DDD:75:THR:HG21	1:DDD:132:LEU:HD22	2.03	0.40
1:DDD:132:LEU:HD12	1:DDD:132:LEU:HA	1.93	0.40
1:AAA:115:MET:HE3	1:AAA:317:ILE:CD1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	335/380 (88%)	327 (98%)	8 (2%)	0	100	100
1	BBB	328/380 (86%)	319 (97%)	9 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	315/380 (83%)	303 (96%)	12 (4%)	0	100	100
1	DDD	339/380 (89%)	332 (98%)	7 (2%)	0	100	100
All	All	1317/1520 (87%)	1281 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	318/348 (91%)	312 (98%)	6 (2%)	57	73
1	BBB	310/348 (89%)	301 (97%)	9 (3%)	42	58
1	CCC	301/348 (86%)	293 (97%)	8 (3%)	44	61
1	DDD	319/348 (92%)	307 (96%)	12 (4%)	33	47
All	All	1248/1392 (90%)	1213 (97%)	35 (3%)	43	60

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	135	MET
1	AAA	169	GLN
1	AAA	173	VAL
1	AAA	190	GLU
1	AAA	302	PRO
1	AAA	327	ASN
1	BBB	138	LEU
1	BBB	182	ASP
1	BBB	185	LYS
1	BBB	228	LYS
1	BBB	247	SER
1	BBB	248	GLU
1	BBB	322	THR
1	BBB	353	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	BBB	382	ASN
1	CCC	144	ARG
1	CCC	235	GLU
1	CCC	252	GLU
1	CCC	287	ARG
1	CCC	350	TYR
1	CCC	380	LYS
1	CCC	384	THR
1	CCC	390	GLU
1	DDD	98	GLN
1	DDD	115	MET
1	DDD	148	SER
1	DDD	149	PRO
1	DDD	151	SER
1	DDD	202	LEU
1	DDD	244	LYS
1	DDD	248	GLU
1	DDD	259	LYS
1	DDD	282	ARG
1	DDD	296	TYR
1	DDD	313	SER

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 [i](#)

12 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
2	HEM	CCC	401	4,1	41,50,50	1.39	5 (12%)	45,82,82	2.10	13 (28%)
2	HEM	AAA	401	4,1	41,50,50	1.41	5 (12%)	45,82,82	2.03	16 (35%)
4	5PK	AAA	403	2	22,24,24	0.50	0	26,34,34	1.14	1 (3%)
3	ZIQ	AAA	402	-	13,17,17	0.76	0	14,25,25	0.98	1 (7%)
4	5PK	CCC	403	2	22,24,24	0.59	0	26,34,34	1.09	1 (3%)
4	5PK	AAA	404	2	22,24,24	0.43	0	26,34,34	1.14	1 (3%)
4	5PK	DDD	403	2	22,24,24	0.36	0	26,34,34	1.15	1 (3%)
2	HEM	BBB	401	4,1	41,50,50	1.48	7 (17%)	45,82,82	1.93	16 (35%)
3	ZIQ	CCC	402	-	13,17,17	0.72	0	14,25,25	0.90	1 (7%)
2	HEM	DDD	401	4,1	41,50,50	1.31	7 (17%)	45,82,82	2.12	16 (35%)
3	ZIQ	DDD	402	-	13,17,17	0.85	0	14,25,25	0.80	0
3	ZIQ	BBB	402	-	13,17,17	0.76	0	14,25,25	1.00	1 (7%)

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
2	HEM	CCC	401	4,1	-	2/12/54/54	-
2	HEM	AAA	401	4,1	-	3/12/54/54	-
4	5PK	AAA	403	2	-	4/8/28/28	0/4/4/4
3	ZIQ	AAA	402	-	-	4/9/11/11	0/2/2/2
4	5PK	CCC	403	2	-	2/8/28/28	0/4/4/4
4	5PK	AAA	404	2	-	4/8/28/28	0/4/4/4
4	5PK	DDD	403	2	-	5/8/28/28	0/4/4/4
2	HEM	BBB	401	4,1	-	2/12/54/54	-
3	ZIQ	CCC	402	-	-	2/9/11/11	0/2/2/2
2	HEM	DDD	401	4,1	-	3/12/54/54	-
3	ZIQ	DDD	402	-	-	4/9/11/11	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZIQ	BBB	402	-	-	1/9/11/11	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	401	HEM	C1B-NB	-3.91	1.33	1.40
2	BBB	401	HEM	C4D-ND	-3.48	1.34	1.40
2	BBB	401	HEM	C1B-NB	-3.21	1.34	1.40
2	AAA	401	HEM	C1B-NB	-3.19	1.34	1.40
2	AAA	401	HEM	C4D-ND	-3.06	1.35	1.40
2	BBB	401	HEM	C4B-NB	-3.06	1.32	1.38
2	CCC	401	HEM	C4B-NB	-2.98	1.32	1.38
2	BBB	401	HEM	CBD-CAD	2.96	1.61	1.52
2	CCC	401	HEM	C4D-ND	-2.94	1.35	1.40
2	DDD	401	HEM	C1B-NB	-2.73	1.35	1.40
2	BBB	401	HEM	CBD-CGD	2.46	1.56	1.50
2	BBB	401	HEM	C4D-C3D	2.38	1.49	1.45
2	BBB	401	HEM	FE-NB	2.38	2.08	1.96
2	CCC	401	HEM	FE-NB	2.36	2.08	1.96
2	AAA	401	HEM	CHB-C1B	2.33	1.40	1.35
2	DDD	401	HEM	C1D-ND	-2.30	1.34	1.38
2	DDD	401	HEM	C4B-NB	-2.30	1.34	1.38
2	AAA	401	HEM	FE-NB	2.29	2.08	1.96
2	DDD	401	HEM	FE-ND	-2.18	1.86	1.96
2	DDD	401	HEM	C4D-ND	-2.16	1.36	1.40
2	DDD	401	HEM	C1D-C2D	2.14	1.48	1.44
2	CCC	401	HEM	CHB-C1B	2.11	1.40	1.35
2	AAA	401	HEM	C3B-C4B	2.10	1.49	1.44
2	DDD	401	HEM	FE-NB	2.03	2.06	1.96

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	401	HEM	CHC-C4B-NB	5.41	130.31	124.43
2	CCC	401	HEM	CBD-CAD-C3D	-5.28	97.95	112.63
2	DDD	401	HEM	CHC-C4B-NB	4.74	129.59	124.43
2	DDD	401	HEM	CBD-CAD-C3D	-4.68	99.61	112.63
2	AAA	401	HEM	CBD-CAD-C3D	-4.68	99.63	112.63
2	AAA	401	HEM	CHC-C4B-NB	4.65	129.48	124.43
2	CCC	401	HEM	C1B-NB-C4B	4.46	109.68	105.07
2	DDD	401	HEM	C1B-NB-C4B	4.44	109.66	105.07
4	DDD	403	5PK	CAU-CAL-CAM	4.35	131.85	123.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	403	5PK	CAU-CAL-CAM	4.30	131.75	123.45
4	CCC	403	5PK	CAU-CAL-CAM	4.28	131.72	123.45
4	AAA	404	5PK	CAU-CAL-CAM	4.28	131.71	123.45
2	AAA	401	HEM	C1B-NB-C4B	4.15	109.36	105.07
2	CCC	401	HEM	CAD-CBD-CGD	4.10	122.43	113.60
2	DDD	401	HEM	CHA-C4D-ND	3.85	129.14	124.38
2	AAA	401	HEM	C4B-C3B-C2B	-3.80	104.09	107.11
2	AAA	401	HEM	CHD-C1D-ND	3.78	128.54	124.43
2	BBB	401	HEM	CAD-CBD-CGD	3.78	121.74	113.60
2	BBB	401	HEM	O2D-CGD-CBD	3.70	125.91	114.03
2	DDD	401	HEM	CHD-C1D-ND	3.68	128.43	124.43
2	CCC	401	HEM	CHD-C1D-ND	3.57	128.31	124.43
2	BBB	401	HEM	CHC-C4B-NB	3.46	128.19	124.43
2	DDD	401	HEM	CAD-CBD-CGD	3.46	121.04	113.60
2	BBB	401	HEM	CBD-CAD-C3D	-3.41	103.16	112.63
2	DDD	401	HEM	O2D-CGD-O1D	-3.26	115.18	123.30
2	DDD	401	HEM	CHB-C1B-NB	3.25	128.40	124.38
2	AAA	401	HEM	CMD-C2D-C1D	3.20	129.92	125.04
2	BBB	401	HEM	C1B-NB-C4B	3.14	108.32	105.07
2	DDD	401	HEM	CHA-C4D-C3D	-3.14	119.44	125.33
2	DDD	401	HEM	O2A-CGA-CBA	3.08	123.94	114.03
2	CCC	401	HEM	O2D-CGD-O1D	-2.96	115.93	123.30
2	CCC	401	HEM	CHD-C1D-C2D	-2.95	120.38	124.98
2	AAA	401	HEM	CHD-C1D-C2D	-2.88	120.48	124.98
2	DDD	401	HEM	C4A-C3A-C2A	2.86	108.99	107.00
2	BBB	401	HEM	O2D-CGD-O1D	-2.85	116.19	123.30
2	CCC	401	HEM	CBA-CAA-C2A	-2.85	107.75	112.62
2	BBB	401	HEM	C4B-CHC-C1C	2.78	126.22	122.56
2	BBB	401	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
2	BBB	401	HEM	CHD-C1D-ND	2.77	127.44	124.43
2	AAA	401	HEM	CHA-C4D-ND	2.73	127.75	124.38
2	CCC	401	HEM	CMD-C2D-C1D	2.64	129.05	125.04
2	AAA	401	HEM	CHB-C1B-NB	2.63	127.63	124.38
2	CCC	401	HEM	CHA-C4D-ND	2.62	127.61	124.38
2	BBB	401	HEM	O2A-CGA-CBA	2.58	122.31	114.03
2	CCC	401	HEM	CHB-C1B-NB	2.56	127.55	124.38
2	BBB	401	HEM	C4B-C3B-C2B	-2.51	105.12	107.11
2	AAA	401	HEM	CAD-C3D-C4D	2.46	128.96	124.66
2	AAA	401	HEM	O2D-CGD-O1D	-2.42	117.27	123.30
2	AAA	401	HEM	O2D-CGD-CBD	2.42	121.79	114.03
2	BBB	401	HEM	C3C-C4C-NC	-2.34	106.53	110.94
2	BBB	401	HEM	CHA-C4D-C3D	-2.29	121.03	125.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	402	ZIQ	CH2-CZ2-CE2	-2.27	116.81	120.08
3	BBB	402	ZIQ	CH2-CZ2-CE2	-2.26	116.82	120.08
2	DDD	401	HEM	CMD-C2D-C1D	2.21	128.41	125.04
2	BBB	401	HEM	O2A-CGA-O1A	-2.19	117.83	123.30
2	DDD	401	HEM	O2A-CGA-O1A	-2.19	117.84	123.30
2	BBB	401	HEM	CHA-C4D-ND	2.15	127.04	124.38
2	AAA	401	HEM	C3B-C2B-C1B	2.12	108.06	106.49
2	DDD	401	HEM	O2D-CGD-CBD	2.12	120.83	114.03
2	AAA	401	HEM	CAD-C3D-C2D	-2.10	123.96	127.88
2	CCC	401	HEM	O2A-CGA-CBA	2.08	120.71	114.03
2	AAA	401	HEM	CHC-C4B-C3B	-2.08	121.39	124.57
2	CCC	401	HEM	C4B-C3B-C2B	-2.08	105.47	107.11
2	BBB	401	HEM	CBA-CAA-C2A	-2.05	109.11	112.62
2	AAA	401	HEM	CBA-CAA-C2A	-2.05	109.12	112.62
2	DDD	401	HEM	CAD-C3D-C4D	2.04	128.22	124.66
2	DDD	401	HEM	CHD-C1D-C2D	-2.02	121.82	124.98
3	CCC	402	ZIQ	CH2-CZ2-CE2	-2.01	117.20	120.08

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DDD	402	ZIQ	O1-C1-CA-C
3	DDD	402	ZIQ	O2-C1-CA-C
4	AAA	403	5PK	CAC-CAB-CAG-OAI
4	AAA	403	5PK	CAC-CAB-CAG-CAH
4	AAA	404	5PK	CAC-CAB-CAG-OAI
4	AAA	404	5PK	CAC-CAB-CAG-CAH
4	DDD	403	5PK	CAC-CAB-CAG-OAI
4	DDD	403	5PK	CAC-CAB-CAG-CAH
2	DDD	401	HEM	C2A-CAA-CBA-CGA
3	AAA	402	ZIQ	O2-C1-CA-C
3	AAA	402	ZIQ	O1-C1-CA-C
4	AAA	403	5PK	CAG-CAH-CAJ-CAK
4	AAA	404	5PK	CAG-CAH-CAJ-CAK
4	DDD	403	5PK	CAG-CAH-CAJ-CAK
3	DDD	402	ZIQ	O1-C1-CA-CB
3	DDD	402	ZIQ	O2-C1-CA-CB
4	DDD	403	5PK	CAG-CAH-CAJ-NAN
4	CCC	403	5PK	CAG-CAH-CAJ-CAK
3	AAA	402	ZIQ	O2-C1-CA-CB
2	CCC	401	HEM	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	BBB	401	HEM	CAA-CBA-CGA-O1A
2	AAA	401	HEM	CAA-CBA-CGA-O1A
2	AAA	401	HEM	CAA-CBA-CGA-O2A
2	CCC	401	HEM	CAA-CBA-CGA-O2A
2	DDD	401	HEM	CAA-CBA-CGA-O2A
2	BBB	401	HEM	CAA-CBA-CGA-O2A
2	DDD	401	HEM	CAA-CBA-CGA-O1A
3	BBB	402	ZIQ	O1-C1-CA-C
3	CCC	402	ZIQ	O1-C1-CA-C
3	CCC	402	ZIQ	O2-C1-CA-C
2	AAA	401	HEM	C2A-CAA-CBA-CGA
3	AAA	402	ZIQ	O1-C1-CA-CB
4	AAA	403	5PK	CAG-CAH-CAJ-NAN
4	AAA	404	5PK	CAG-CAH-CAJ-NAN
4	CCC	403	5PK	CAG-CAH-CAJ-NAN
4	DDD	403	5PK	CAA-CAB-CAG-OAI

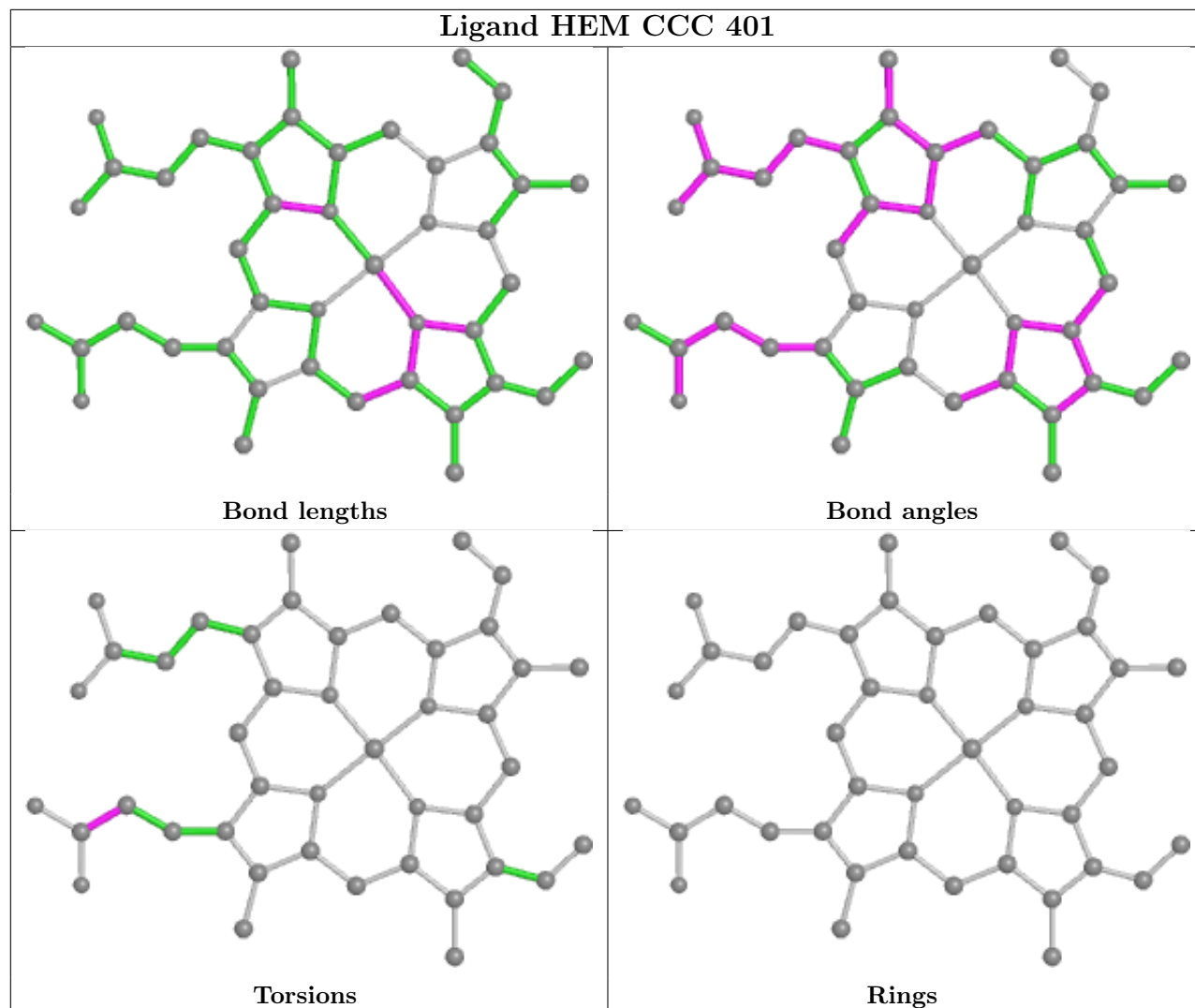
There are no ring outliers.

9 monomers are involved in 16 short contacts:

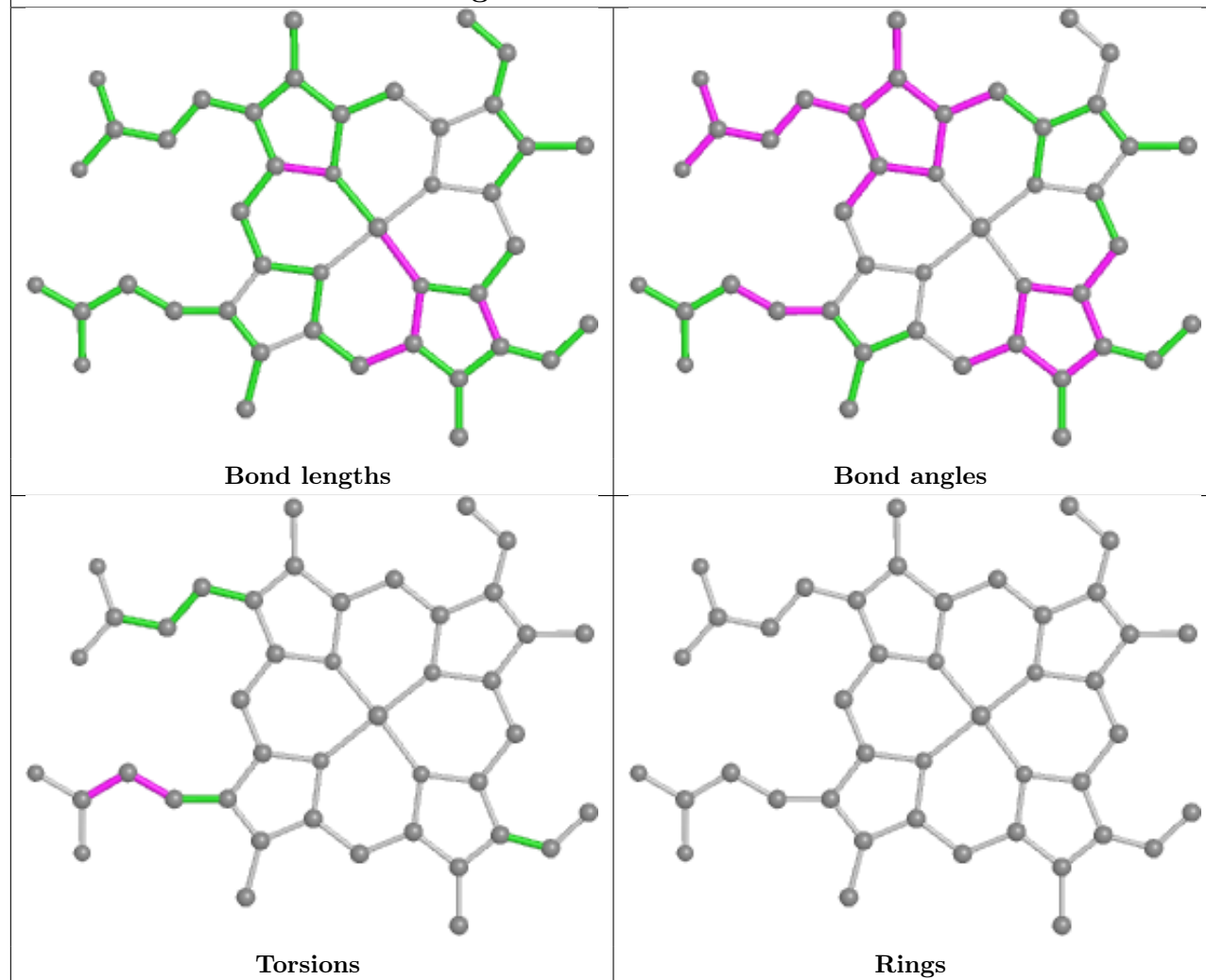
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	401	HEM	3	0
2	AAA	401	HEM	5	0
4	AAA	403	5PK	5	0
4	CCC	403	5PK	1	0
4	AAA	404	5PK	1	0
4	DDD	403	5PK	2	0
2	BBB	401	HEM	2	0
2	DDD	401	HEM	3	0
3	BBB	402	ZIQ	1	0

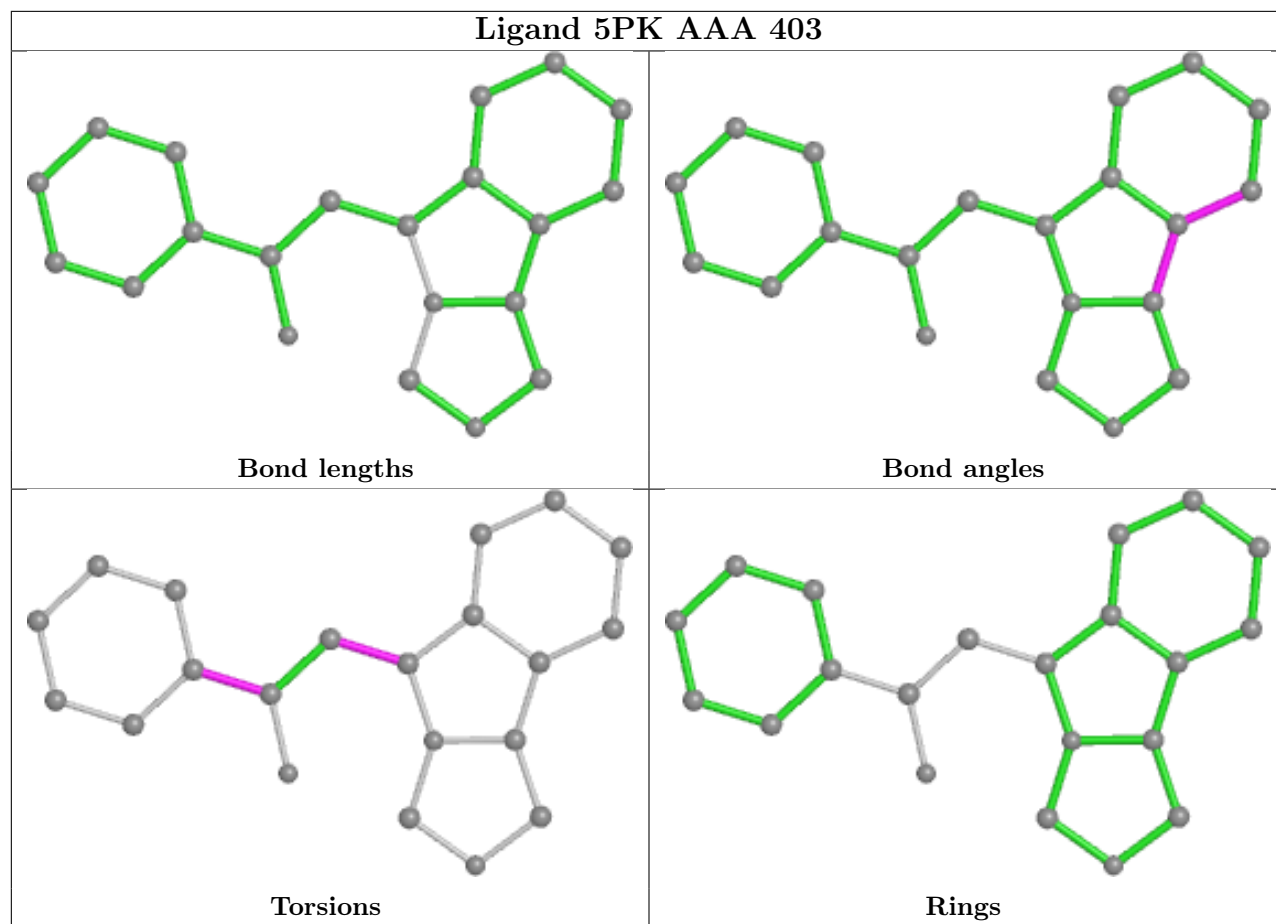
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

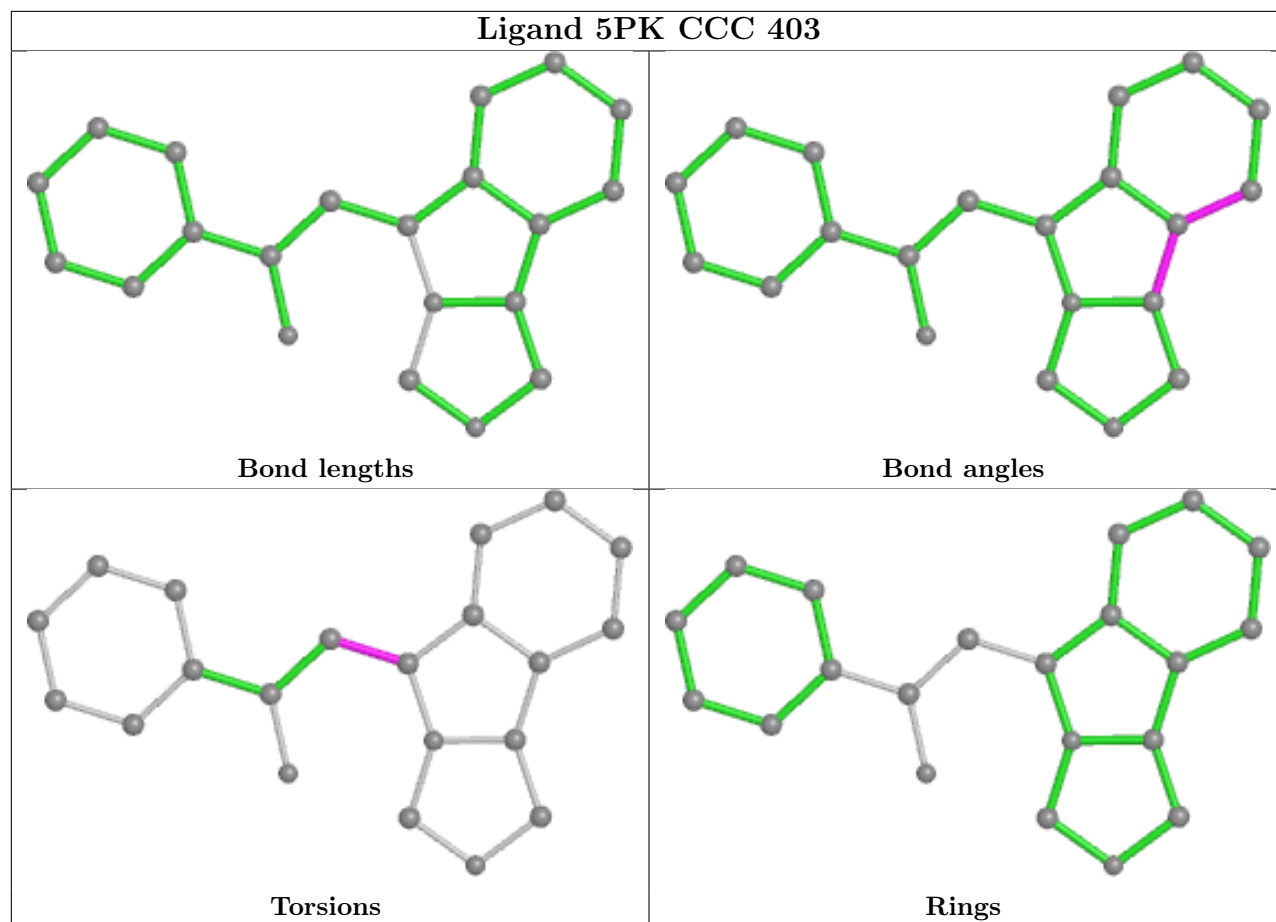
equivalents in the CSD to analyse the geometry.

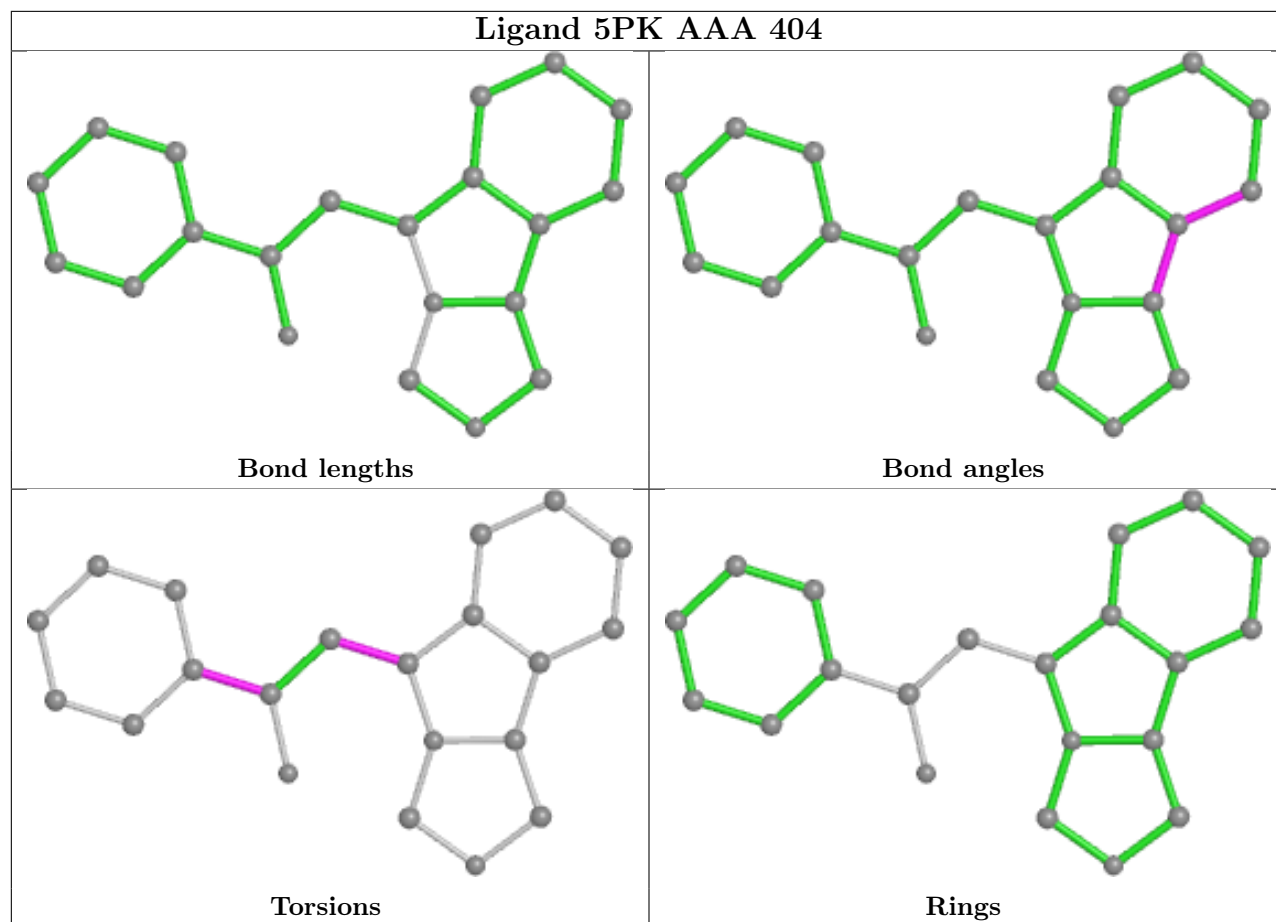


## Ligand HEM AAA 401

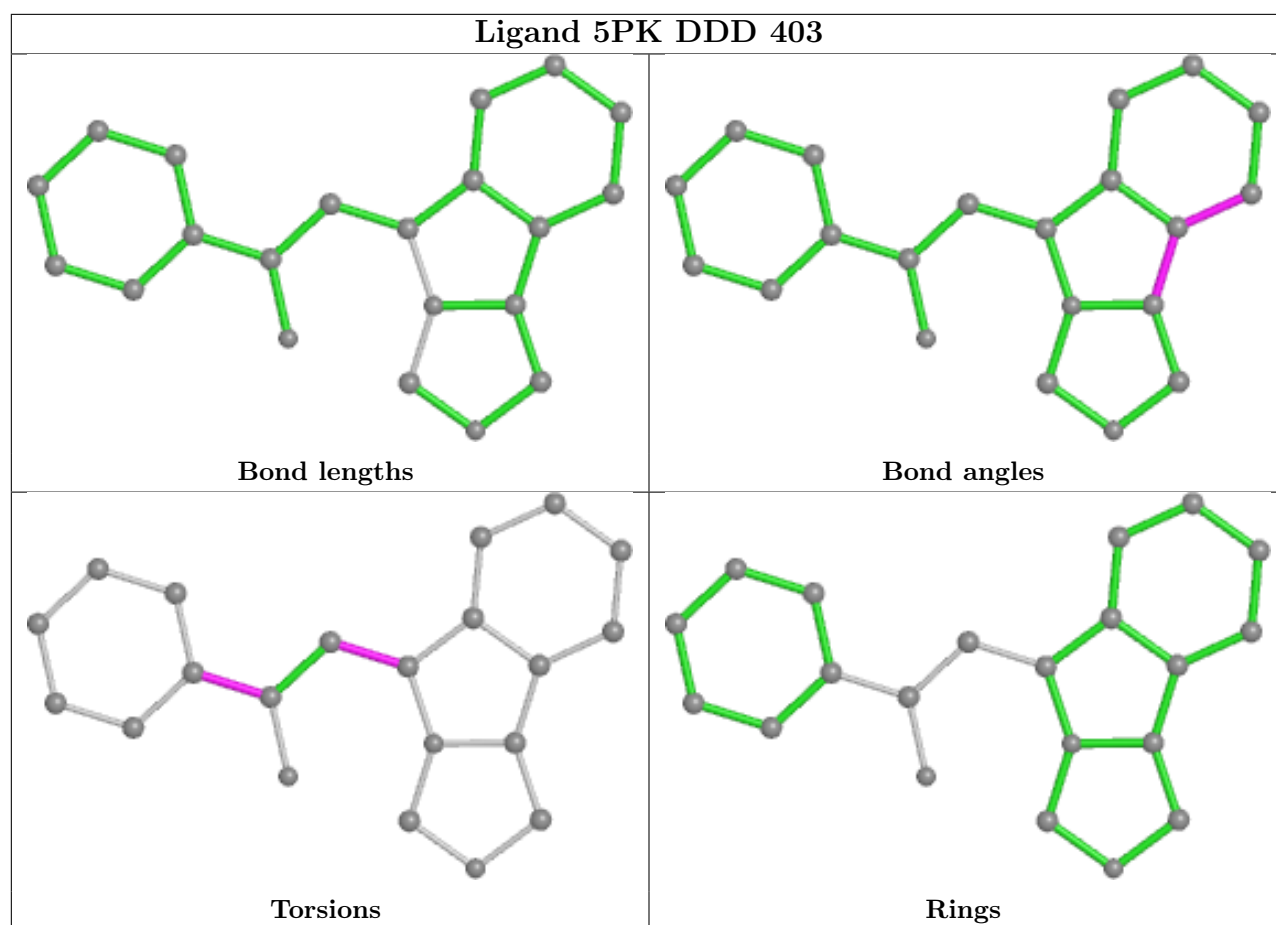




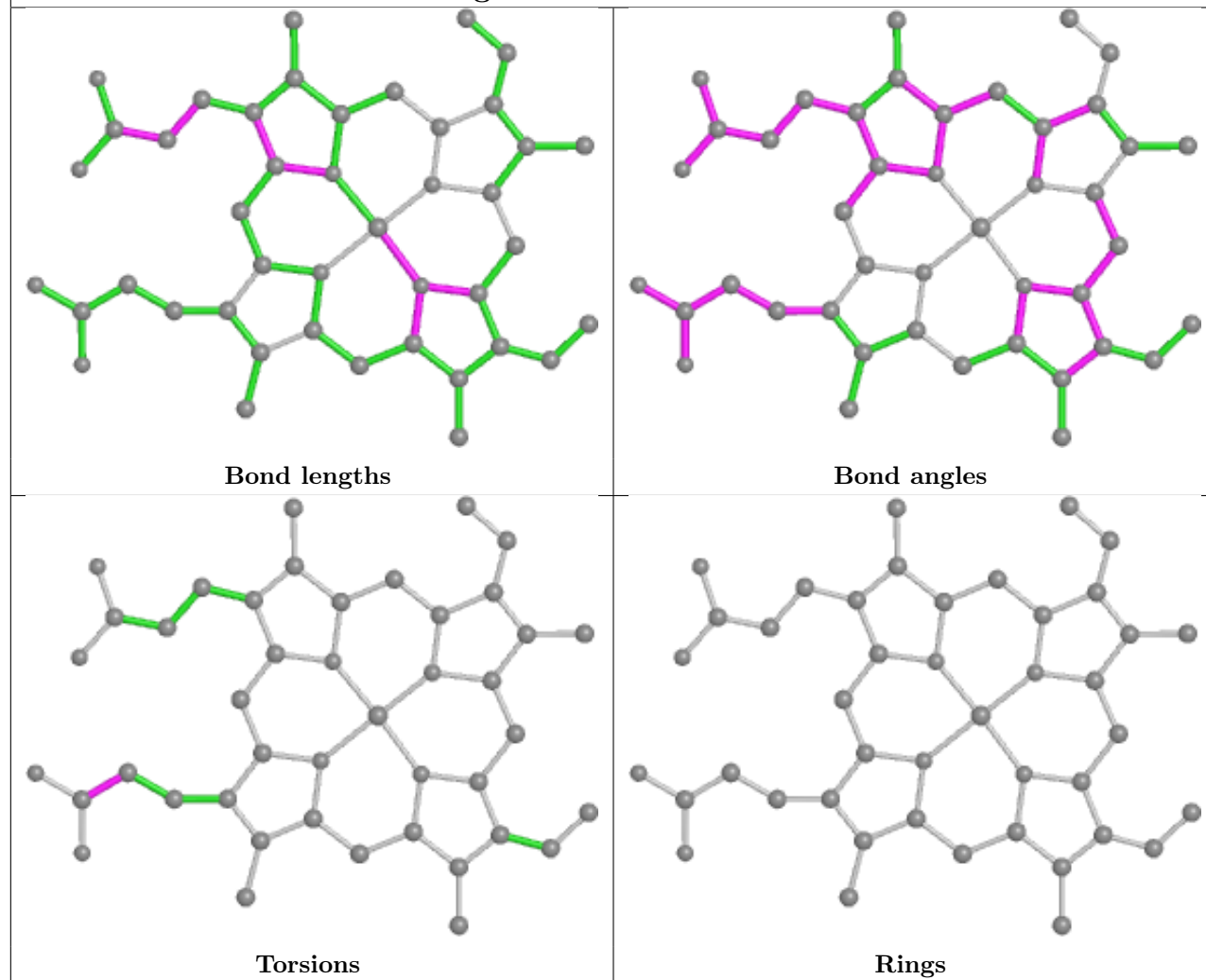


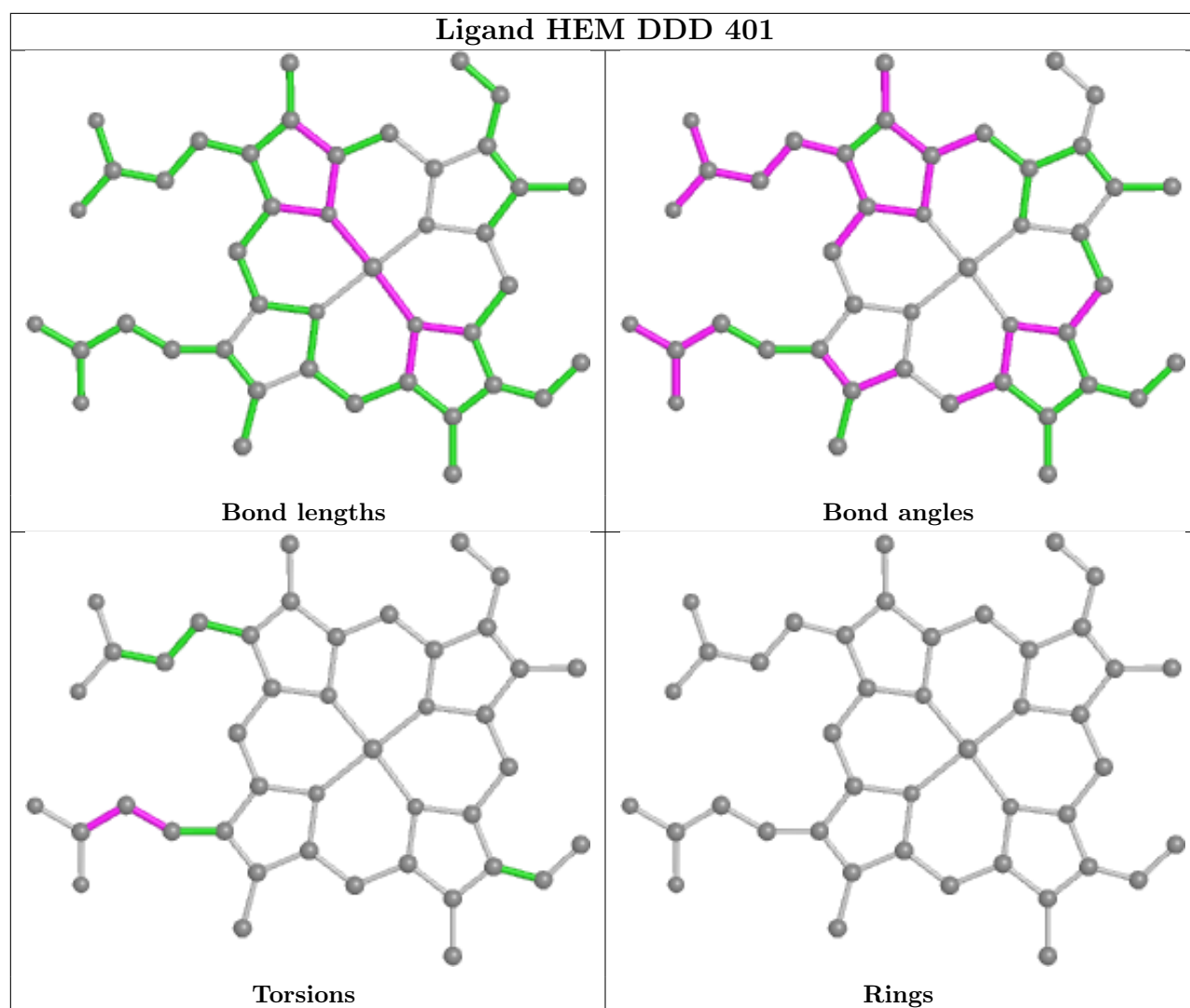






## Ligand HEM BBB 401





## 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	AAA	341/380 (89%)	0.27	25 (7%)	15 20	26, 45, 93, 122	0
1	BBB	334/380 (87%)	0.21	26 (7%)	13 17	25, 40, 98, 131	0
1	CCC	323/380 (85%)	0.60	44 (13%)	3 4	30, 57, 118, 152	0
1	DDD	343/380 (90%)	0.21	27 (7%)	12 17	29, 49, 99, 143	0
All	All	1341/1520 (88%)	0.32	122 (9%)	9 12	25, 47, 103, 152	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	193	LEU	6.0
1	BBB	180	TYR	6.0
1	BBB	384	THR	5.9
1	BBB	38	GLY	5.8
1	BBB	245	GLU	5.5
1	BBB	387	LYS	5.4
1	CCC	218	HIS	5.3
1	CCC	182	ASP	5.3
1	AAA	247	SER	5.0
1	CCC	252	GLU	4.9
1	CCC	180	TYR	4.9
1	BBB	182	ASP	4.8
1	AAA	245	GLU	4.8
1	CCC	171	MET	4.7
1	DDD	385	ILE	4.7
1	CCC	255	ALA	4.6
1	BBB	241	ILE	4.5
1	AAA	248	GLU	4.4
1	BBB	386	HIS	4.4
1	BBB	242	GLN	4.3
1	AAA	175	TYR	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	BBB	382	ASN	4.1
1	AAA	246	GLU	4.1
1	BBB	385	ILE	4.1
1	CCC	169	GLN	4.0
1	CCC	383	PRO	4.0
1	CCC	254	VAL	4.0
1	AAA	383	PRO	3.9
1	CCC	190	GLU	3.8
1	BBB	170	ASN	3.8
1	BBB	243	ALA	3.8
1	CCC	253	GLN	3.8
1	BBB	383	PRO	3.8
1	CCC	170	ASN	3.8
1	AAA	241	ILE	3.7
1	DDD	348	TYR	3.6
1	CCC	384	THR	3.6
1	BBB	171	MET	3.6
1	DDD	250	LYS	3.6
1	CCC	172	ARG	3.6
1	CCC	265	LEU	3.6
1	CCC	186	GLY	3.5
1	CCC	358	ARG	3.5
1	CCC	258	GLN	3.5
1	CCC	348	TYR	3.2
1	DDD	386	HIS	3.2
1	DDD	383	PRO	3.2
1	CCC	387	LYS	3.1
1	BBB	240	ARG	3.1
1	DDD	384	THR	3.0
1	CCC	234	LEU	3.0
1	AAA	250	LYS	3.0
1	AAA	349	HIS	3.0
1	DDD	296	TYR	3.0
1	CCC	217	PRO	3.0
1	CCC	385	ILE	2.9
1	DDD	346	SER	2.9
1	DDD	246	GLU	2.9
1	AAA	384	THR	2.8
1	DDD	254	VAL	2.8
1	DDD	248	GLU	2.8
1	CCC	63	GLY	2.8
1	CCC	219	GLY	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	BBB	244	LYS	2.8
1	AAA	382	ASN	2.8
1	DDD	39	GLY	2.8
1	CCC	184	PHE	2.8
1	AAA	252	GLU	2.8
1	DDD	241	ILE	2.7
1	CCC	257	PHE	2.7
1	CCC	251	GLU	2.6
1	DDD	382	ASN	2.6
1	CCC	296	TYR	2.6
1	CCC	185	LYS	2.6
1	BBB	248	GLU	2.6
1	DDD	218	HIS	2.6
1	BBB	246	GLU	2.6
1	AAA	255	ALA	2.5
1	BBB	247	SER	2.5
1	DDD	388	PHE	2.5
1	AAA	296	TYR	2.5
1	DDD	252	GLU	2.5
1	DDD	193	LEU	2.5
1	CCC	183	ASN	2.4
1	DDD	244	LYS	2.4
1	AAA	275	HIS	2.4
1	DDD	245	GLU	2.4
1	AAA	244	LYS	2.4
1	CCC	79	TYR	2.4
1	CCC	275	HIS	2.4
1	AAA	173	VAL	2.4
1	CCC	61	THR	2.4
1	AAA	193	LEU	2.3
1	CCC	368	LEU	2.3
1	DDD	387	LYS	2.3
1	BBB	238	PHE	2.3
1	BBB	388	PHE	2.3
1	AAA	243	ALA	2.3
1	AAA	251	GLU	2.2
1	AAA	259	LYS	2.2
1	DDD	238	PHE	2.2
1	CCC	78	ALA	2.2
1	DDD	78	ALA	2.2
1	DDD	275	HIS	2.2
1	DDD	242	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	DDD	247	SER	2.2
1	CCC	287	ARG	2.2
1	BBB	78	ALA	2.2
1	AAA	185	LYS	2.1
1	CCC	271	LYS	2.1
1	AAA	174	PRO	2.1
1	DDD	338	SER	2.1
1	AAA	182	ASP	2.1
1	CCC	83	PHE	2.1
1	CCC	181	ARG	2.1
1	CCC	297	PHE	2.1
1	AAA	385	ILE	2.1
1	BBB	39	GLY	2.0
1	BBB	169	GLN	2.0
1	BBB	181	ARG	2.0
1	CCC	233	GLY	2.0
1	CCC	279	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZIQ	CCC	402	16/16	0.94	0.12	39,45,55,63	0
4	5PK	CCC	403	21/21	0.95	0.18	38,50,74,75	0
4	5PK	AAA	403	21/21	0.96	0.15	45,57,73,74	0
3	ZIQ	BBB	402	16/16	0.96	0.12	33,35,38,42	0
4	5PK	DDD	403	21/21	0.96	0.13	45,50,59,60	0
2	HEM	CCC	401	43/43	0.97	0.15	45,51,67,81	0

*Continued on next page...*

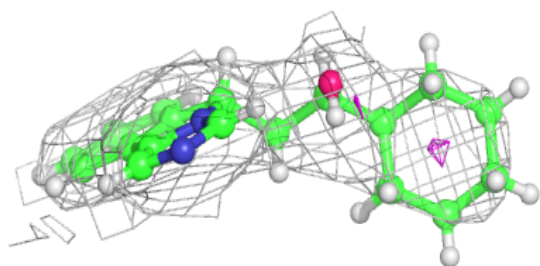
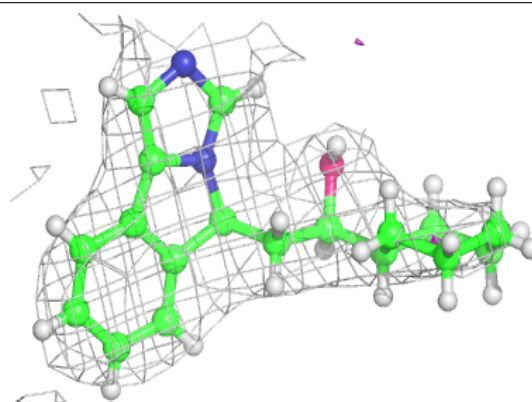
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZIQ	AAA	402	16/16	0.97	0.13	29,35,42,46	0
3	ZIQ	DDD	402	16/16	0.97	0.09	37,41,48,50	0
2	HEM	AAA	401	43/43	0.98	0.14	37,43,58,70	0
4	5PK	AAA	404	21/21	0.98	0.13	33,45,62,65	0
2	HEM	DDD	401	43/43	0.98	0.12	33,40,52,68	0
2	HEM	BBB	401	43/43	0.98	0.12	32,39,56,68	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 5PK CCC 403:**

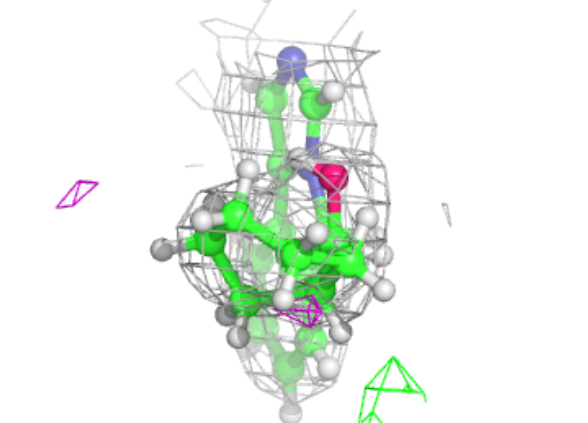
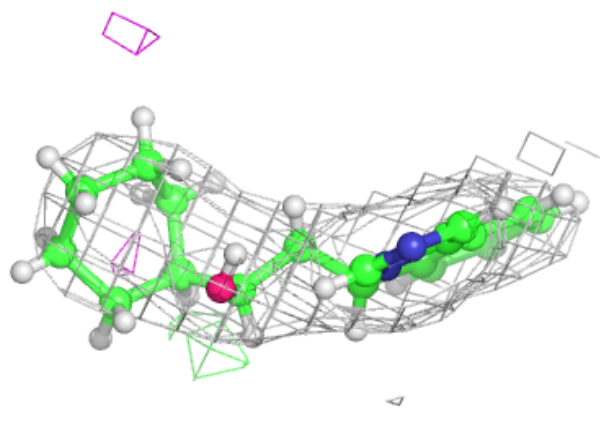
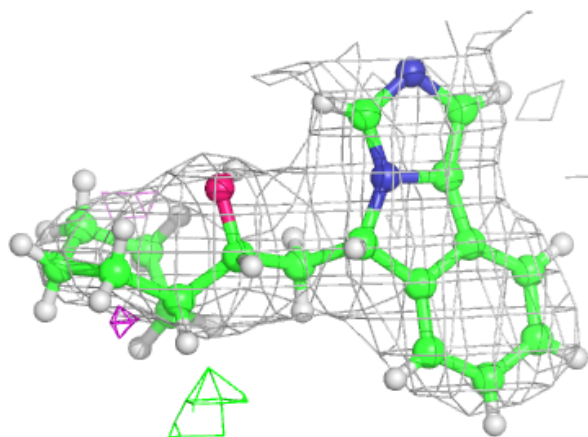
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





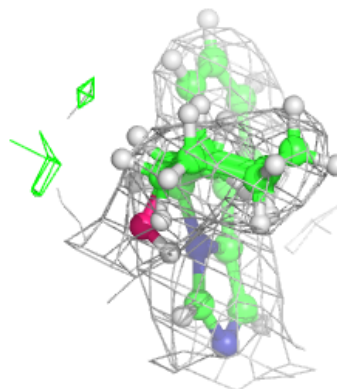
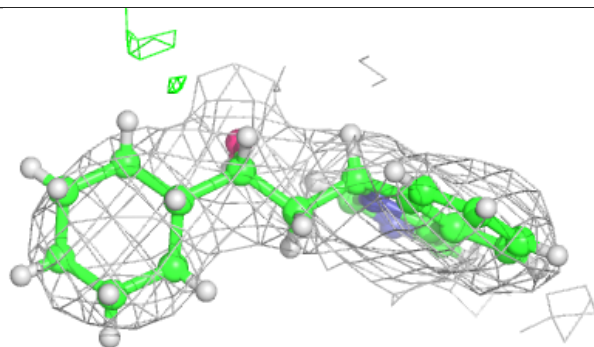
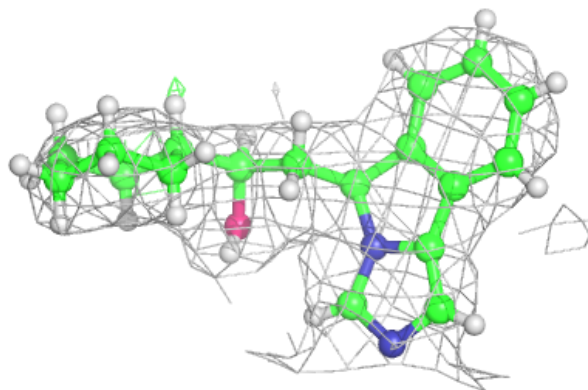
**Electron density around 5PK AAA 403:**

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



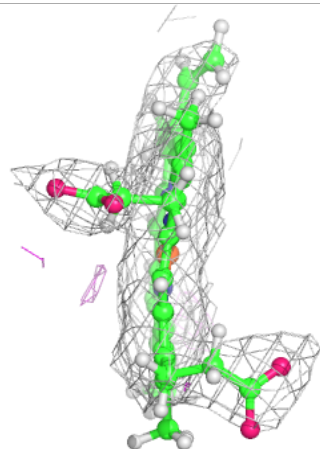
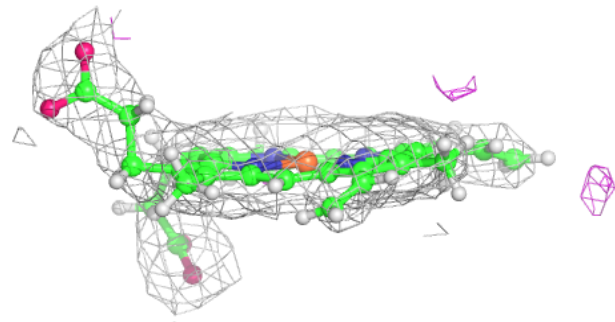
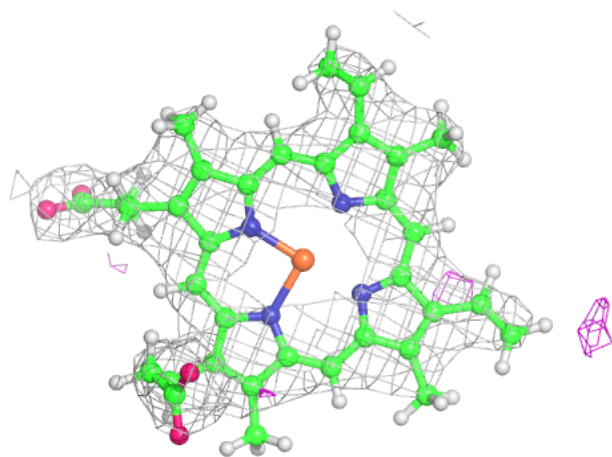
**Electron density around 5PK DDD 403:**

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



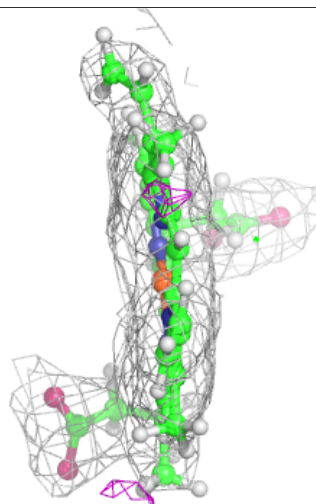
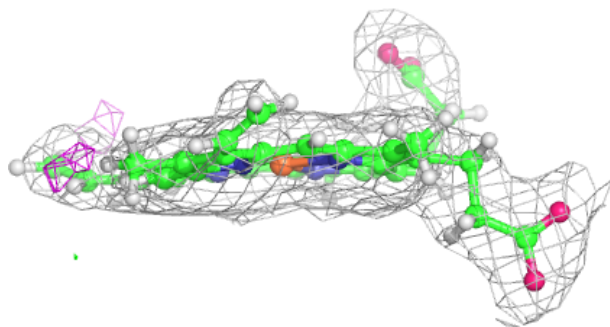
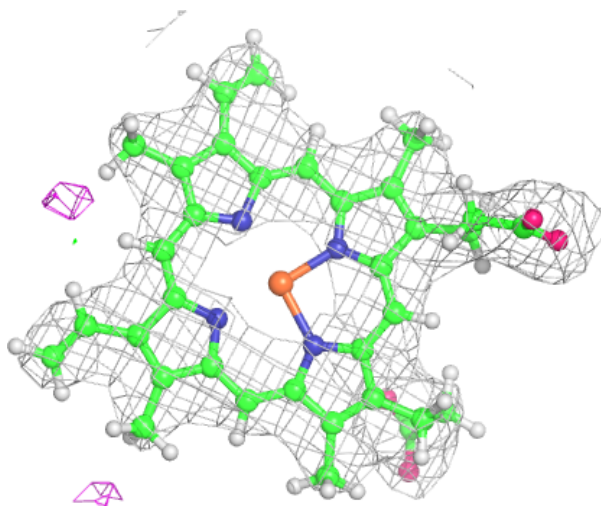
**Electron density around HEM CCC 401:**

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



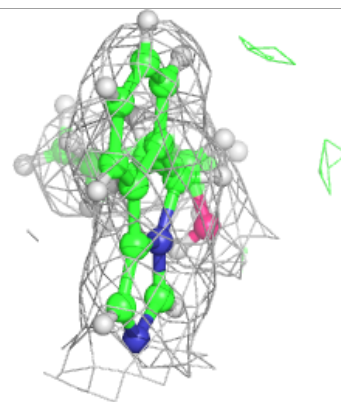
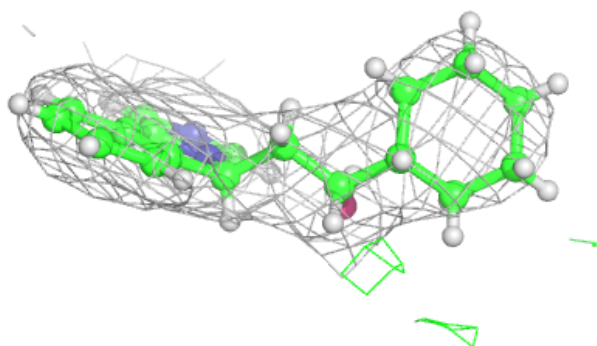
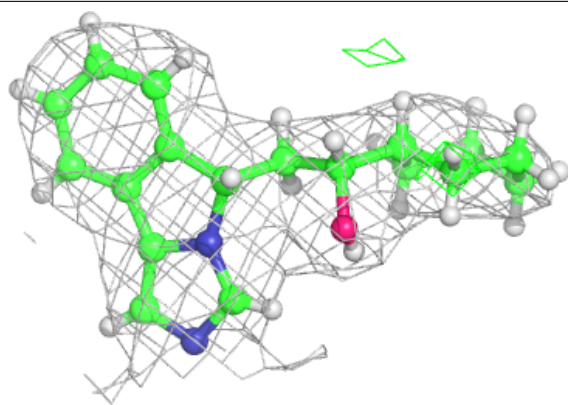
**Electron density around HEM AAA 401:**

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



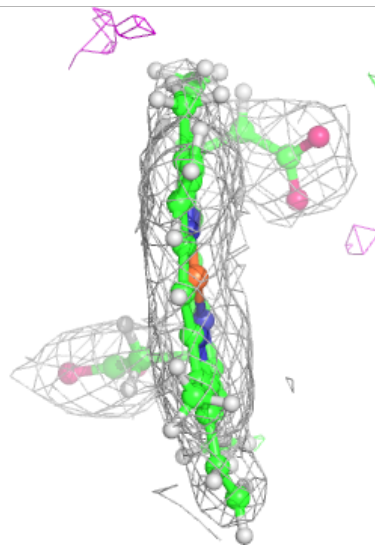
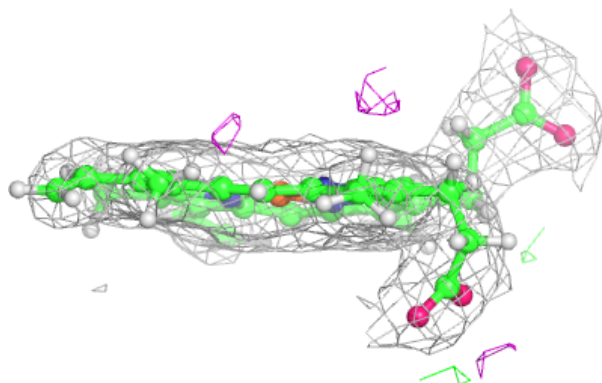
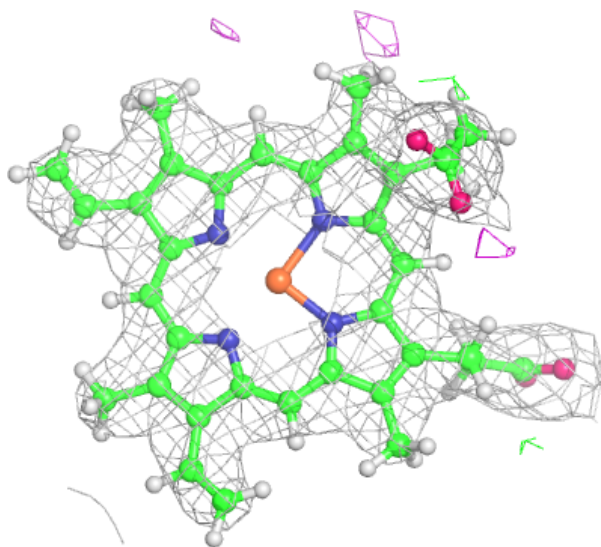
**Electron density around 5PK AAA 404:**

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



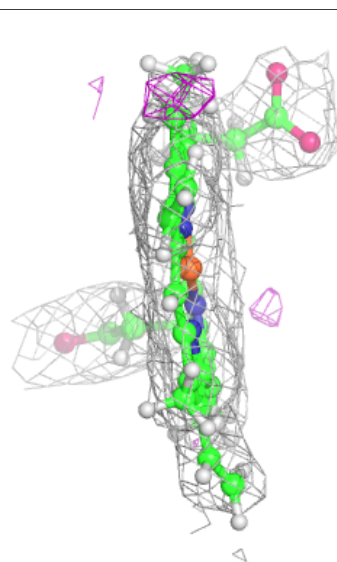
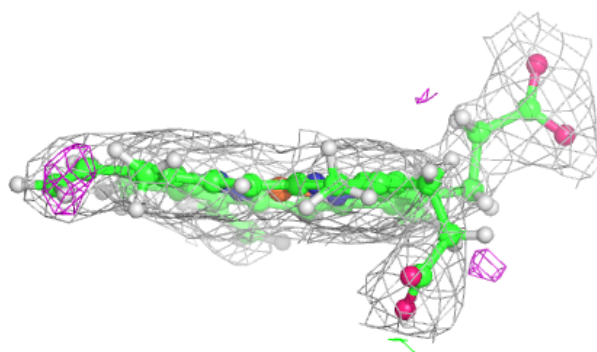
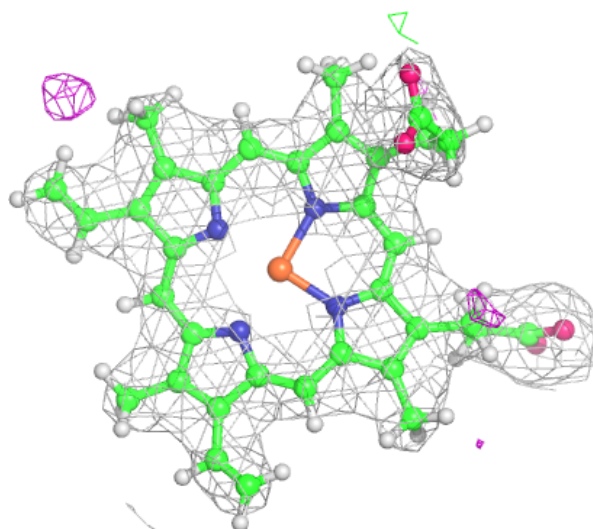
**Electron density around HEM DDD 401:**

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



**Electron density around HEM BBB 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.