



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:18 pm BST

PDB ID : 6CIR  
Title : Human Cytochrome P450 17A1 in complex with inhibitor: abiraterone C6 oxime  
Authors : Scott, E.E.; Fehl, C.  
Deposited on : 2018-02-25  
Resolution : 2.65 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.

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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 : 2.11  
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) : 2.11

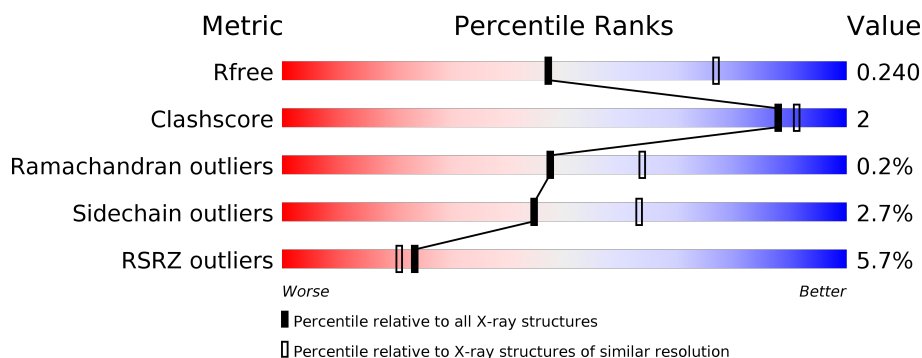
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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	494	<div> <div>7%</div> <div>87% 7% 6%</div> </div>
1	B	494	<div> <div>5%</div> <div>87% 7% 6%</div> </div>
1	C	494	<div> <div>5%</div> <div>90% 5% .</div> </div>
1	D	494	<div> <div>4%</div> <div>88% 7% 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30516 atoms, of which 15168 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	466	Total	C	H	N	O	S	0	0	0
			7453	2383	3740	642	673	15			
1	B	466	Total	C	H	N	O	S	0	0	0
			7455	2384	3739	643	674	15			
1	C	472	Total	C	H	N	O	S	0	0	0
			7537	2405	3784	650	683	15			
1	D	471	Total	C	H	N	O	S	0	0	0
			7534	2402	3785	649	683	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	initiating methionine	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	initiating methionine	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	initiating methionine	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

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



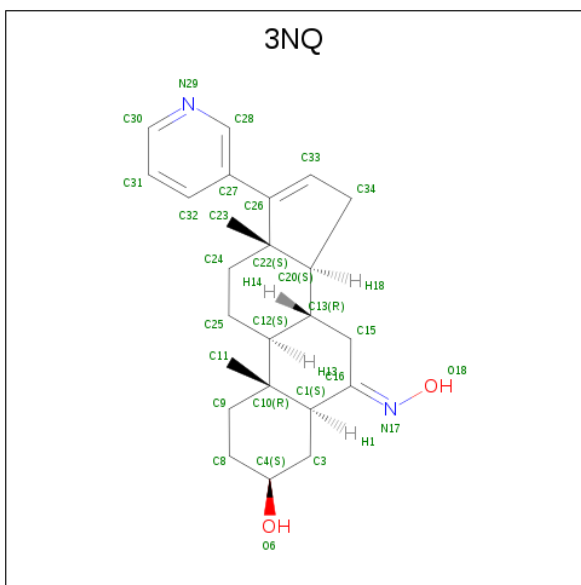
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

- Molecule 3 is 6-oxime-17-(3-pyridyl)-androster-16-en-3-ol (three-letter code: 3NQ) (formula:  $C_{24}H_{32}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	24	2	2		
3	B	1	Total	C	N	O	0	0
			28	24	2	2		
3	C	1	Total	C	N	O	0	0
			28	24	2	2		
3	D	1	Total	C	N	O	0	0
			28	24	2	2		

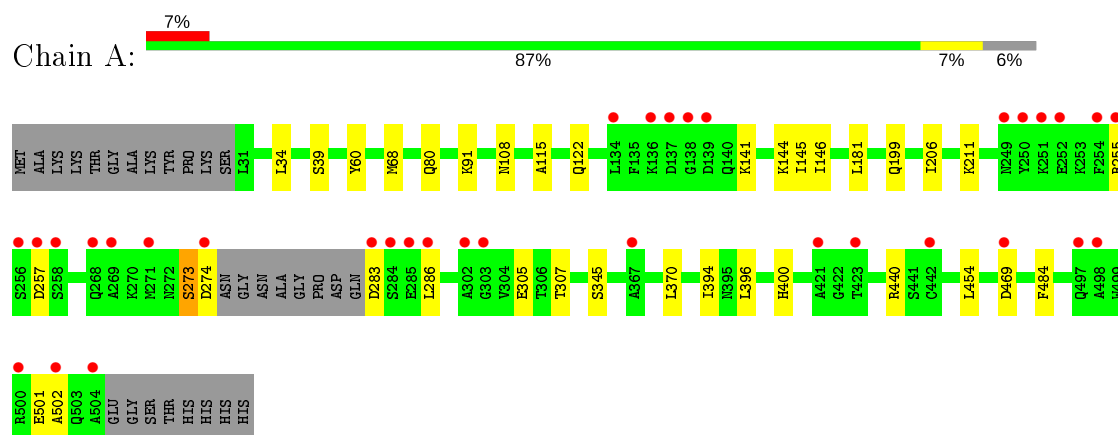
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	38	Total	O	0	0
			38	38		
4	C	40	Total	O	0	0
			40	40		
4	D	28	Total	O	0	0
			28	28		

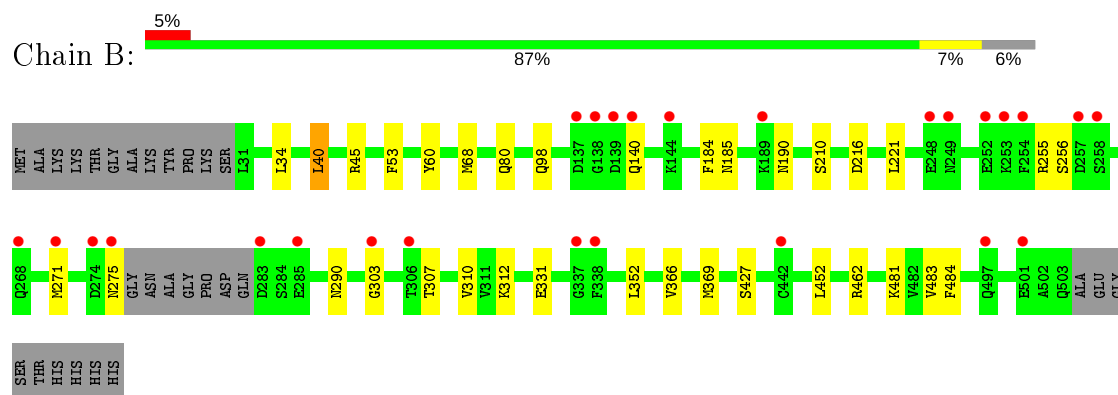
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

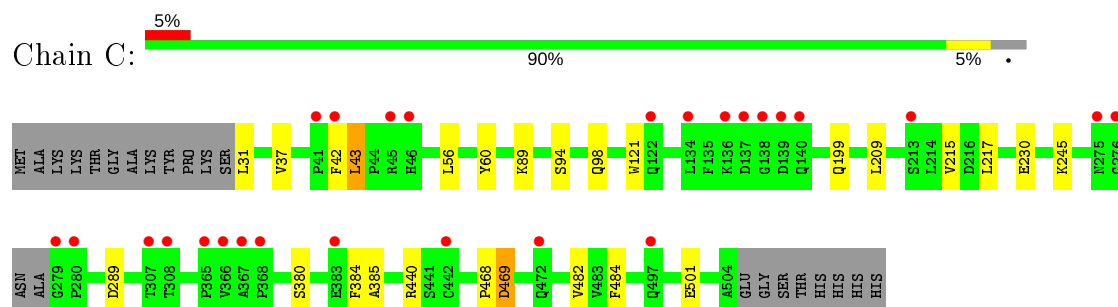
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



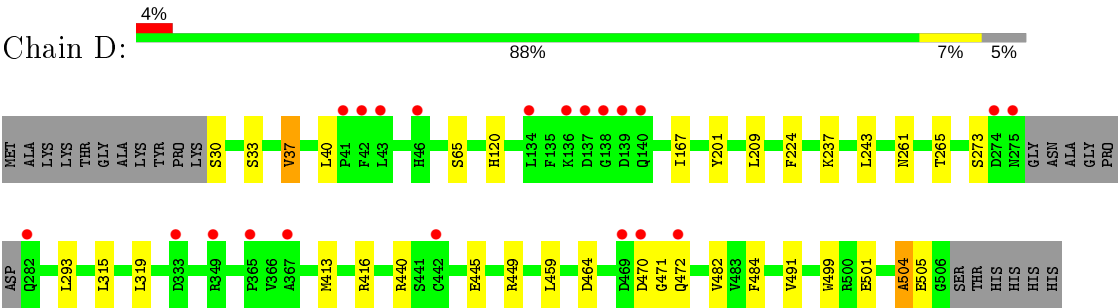
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



● Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.90Å 151.87Å 168.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.31 – 2.65 39.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.31-2.65) 90.1 (39.31-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.187 , 0.240 0.187 , 0.240	Depositor DCC
$R_{free}$ test set	3465 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 3NQ

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	0.32	0/3793	0.43	0/5135
1	B	0.24	0/3796	0.42	0/5139
1	C	0.24	0/3834	0.42	0/5191
1	D	0.25	0/3829	0.43	0/5183
All	All	0.26	0/15252	0.43	0/20648

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	A	3713	3740	3785	16	0
1	B	3716	3739	3785	15	0
1	C	3753	3784	3815	15	0
1	D	3749	3785	3813	16	0
2	A	43	30	30	3	0
2	B	43	30	30	2	0
2	C	43	30	30	2	0
2	D	43	30	30	2	0
3	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
4	A	27	0	0	0	0
4	B	38	0	0	0	0
4	C	40	0	0	0	0
4	D	28	0	0	1	0
All	All	15348	15168	15318	60	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 (60) 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:34:LEU:HD11	1:C:385:ALA:O	1.80	0.81
2:D:600:HEM:HBB2	2:D:600:HEM:HHC	1.78	0.65
2:A:600:HEM:HHH	2:A:600:HEM:HBC2	1.80	0.63
2:C:600:HEM:HBB2	2:C:600:HEM:HHC	1.81	0.62
1:C:42:PHE:HE2	1:C:60:TYR:HE2	1.47	0.62
2:D:600:HEM:HBC2	2:D:600:HEM:HHH	1.80	0.62
1:C:42:PHE:O	1:C:43:LEU:HB2	2.00	0.60
1:D:201:TYR:HB3	4:D:705:HOH:O	1.99	0.60
1:C:209:LEU:HD23	1:C:482:VAL:HG11	1.85	0.58
2:C:600:HEM:HBC2	2:C:600:HEM:HHH	1.87	0.56
1:D:209:LEU:HD23	1:D:482:VAL:HG11	1.87	0.56
1:B:60:TYR:CD2	1:C:37:VAL:HG21	2.41	0.55
1:B:271:MET:O	1:B:275:ASN:HB2	2.07	0.54
1:B:366:VAL:HG13	1:B:483:VAL:HG13	1.92	0.51
1:B:331:GLU:OE2	1:B:352:LEU:N	2.42	0.51
1:A:370:LEU:HD22	2:A:600:HEM:HMA1	1.91	0.51
1:B:45:ARG:NH1	1:B:216:ASP:OD1	2.44	0.50
1:A:141:LYS:O	1:A:144:LYS:N	2.41	0.49
1:A:370:LEU:HD12	1:A:394:ILE:HB	1.95	0.49
1:B:140:GLN:OE1	1:B:185:ASN:ND2	2.45	0.49
1:A:273:SER:O	1:A:274:ASP:HB3	2.14	0.48
1:C:469:ASP:N	1:C:469:ASP:OD1	2.44	0.48
1:B:310:VAL:HG11	1:B:452:LEU:HD13	1.96	0.48
2:B:600:HEM:HMC1	2:B:600:HEM:HBC2	1.95	0.48
1:C:94:SER:O	1:C:440:ARG:NH1	2.46	0.48
1:D:470:ASP:O	1:D:472:GLN:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:GLU:OE2	1:D:449:ARG:NH2	2.48	0.46
1:C:98:GLN:N	1:C:98:GLN:OE1	2.48	0.46
1:D:499:TRP:CH2	1:D:504:ALA:HB1	2.51	0.46
1:C:230:GLU:OE1	1:C:230:GLU:N	2.45	0.45
2:A:600:HEM:HMA1	2:A:600:HEM:HBA1	1.97	0.45
1:B:34:LEU:CD1	1:C:385:ALA:O	2.59	0.45
1:A:211:LYS:HD3	1:D:224:PHE:C	2.38	0.45
1:A:501:GLU:O	1:A:502:ALA:HB3	2.17	0.44
1:C:89:LYS:NZ	1:C:380:SER:OG	2.51	0.44
1:C:42:PHE:CE2	1:C:60:TYR:HE2	2.33	0.44
1:D:261:ASN:O	1:D:265:THR:HG23	2.17	0.44
1:A:396:LEU:HD11	1:A:400:HIS:NE2	2.34	0.43
1:B:34:LEU:HD12	1:C:384:PHE:HB3	2.01	0.43
1:A:115:ALA:O	1:A:440:ARG:NH2	2.43	0.43
1:D:413:MET:O	1:D:416:ARG:HB2	2.19	0.43
1:A:255:ARG:NH1	1:A:257:ASP:OD2	2.52	0.43
1:B:303:GLY:HA2	2:B:600:HEM:HMC3	2.01	0.42
1:A:60:TYR:CD2	1:D:37:VAL:HG21	2.54	0.42
1:A:34:LEU:HD23	1:D:65:SER:HB3	2.00	0.42
1:A:146:ILE:HG21	1:A:454:LEU:HD12	2.01	0.42
1:A:68:MET:HE1	1:D:40:LEU:HD12	2.01	0.42
1:B:210:SER:O	1:B:481:LYS:NZ	2.44	0.42
1:C:215:VAL:HG12	1:C:217:LEU:H	1.84	0.42
1:B:221:LEU:HD12	1:B:221:LEU:C	2.40	0.41
1:B:40:LEU:HD11	1:B:68:MET:HE1	2.02	0.41
1:B:53:PHE:HD2	1:B:369:MET:HE3	1.84	0.41
1:A:145:ILE:HG23	1:A:181:LEU:HD12	2.02	0.41
1:D:319:LEU:HD21	1:D:491:VAL:HG12	2.03	0.41
1:C:121:TRP:CZ2	1:C:440:ARG:HD2	2.55	0.41
1:D:243:LEU:HB3	1:D:293:LEU:HG	2.03	0.41
1:A:68:MET:CE	1:D:40:LEU:HD12	2.51	0.40
1:A:206:ILE:HD11	1:A:305:GLU:HG3	2.03	0.40
1:D:167:ILE:HD13	1:D:315:LEU:HD12	2.04	0.40
1:D:120:HIS:H	1:D:120:HIS:CD2	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	462/494 (94%)	441 (96%)	21 (4%)	0	100	100
1	B	462/494 (94%)	441 (96%)	21 (4%)	0	100	100
1	C	468/494 (95%)	449 (96%)	17 (4%)	2 (0%)	34	48
1	D	467/494 (94%)	443 (95%)	22 (5%)	2 (0%)	34	48
All	All	1859/1976 (94%)	1774 (95%)	81 (4%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	LEU
1	D	504	ALA
1	C	468	PRO
1	D	471	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/436 (95%)	402 (97%)	13 (3%)	40	58
1	B	416/436 (95%)	403 (97%)	13 (3%)	40	58
1	C	419/436 (96%)	411 (98%)	8 (2%)	57	74
1	D	419/436 (96%)	408 (97%)	11 (3%)	46	65
All	All	1669/1744 (96%)	1624 (97%)	45 (3%)	44	63

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	80	GLN
1	A	91	LYS
1	A	108	ASN
1	A	122	GLN
1	A	199	GLN
1	A	273	SER
1	A	283	ASP
1	A	286	LEU
1	A	307	THR
1	A	345	SER
1	A	469	ASP
1	A	484	PHE
1	B	40	LEU
1	B	80	GLN
1	B	98	GLN
1	B	184	PHE
1	B	190	ASN
1	B	255	ARG
1	B	256	SER
1	B	290	ASN
1	B	307	THR
1	B	312	LYS
1	B	427	SER
1	B	462	ARG
1	B	484	PHE
1	C	31	LEU
1	C	56	LEU
1	C	199	GLN
1	C	245	LYS
1	C	289	ASP
1	C	469	ASP
1	C	484	PHE
1	C	501	GLU
1	D	30	SER
1	D	33	SER
1	D	37	VAL
1	D	237	LYS
1	D	273	SER
1	D	440	ARG
1	D	459	LEU
1	D	464	ASP

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Mol	Chain	Res	Type
1	D	484	PHE
1	D	501	GLU
1	D	505	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	HIS
1	B	120	HIS
1	C	401	HIS
1	D	120	HIS
1	D	200	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	3NQ	C	601	2	32,32,32	1.11	2 (6%)	43,50,50	2.37	16 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	D	600	1,3	27,50,50	1.95	5 (18%)	17,82,82	1.38	3 (17%)
2	HEM	A	600	1,3	27,50,50	1.88	5 (18%)	17,82,82	1.81	3 (17%)
2	HEM	C	600	1,3	27,50,50	1.97	5 (18%)	17,82,82	1.41	2 (11%)
3	3NQ	B	601	2	32,32,32	1.09	2 (6%)	43,50,50	2.48	13 (30%)
3	3NQ	A	601	2	32,32,32	1.12	2 (6%)	43,50,50	2.37	14 (32%)
3	3NQ	D	601	2	32,32,32	1.10	2 (6%)	43,50,50	2.55	16 (37%)
2	HEM	B	600	1,3	27,50,50	1.83	5 (18%)	17,82,82	1.76	5 (29%)

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	3NQ	C	601	2	-	4/6/67/67	0/5/5/5
2	HEM	D	600	1,3	-	2/6/54/54	-
2	HEM	A	600	1,3	-	2/6/54/54	-
2	HEM	C	600	1,3	-	2/6/54/54	-
3	3NQ	B	601	2	-	2/6/67/67	0/5/5/5
3	3NQ	A	601	2	-	4/6/67/67	0/5/5/5
3	3NQ	D	601	2	-	2/6/67/67	0/5/5/5
2	HEM	B	600	1,3	-	2/6/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	C3C-C2C	-4.69	1.33	1.40
3	A	601	3NQ	C22-C26	-4.66	1.49	1.53
2	D	600	HEM	C3C-C2C	-4.64	1.33	1.40
3	C	601	3NQ	C22-C26	-4.59	1.49	1.53
2	C	600	HEM	C3B-C2B	-4.53	1.34	1.40
2	A	600	HEM	C3C-C2C	-4.50	1.34	1.40
3	B	601	3NQ	C22-C26	-4.30	1.49	1.53
2	D	600	HEM	C3B-C2B	-4.22	1.34	1.40
3	D	601	3NQ	C22-C26	-4.19	1.49	1.53
2	D	600	HEM	C3B-CAB	3.97	1.56	1.47
2	B	600	HEM	C3C-CAC	3.87	1.55	1.47
2	A	600	HEM	C3B-C2B	-3.87	1.35	1.40
2	C	600	HEM	C3B-CAB	3.85	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3B-C2B	-3.82	1.35	1.40
2	B	600	HEM	C3B-CAB	3.81	1.55	1.47
2	A	600	HEM	C3C-CAC	3.81	1.55	1.47
2	D	600	HEM	C3C-CAC	3.77	1.55	1.47
2	B	600	HEM	C3C-C2C	-3.68	1.35	1.40
2	A	600	HEM	C3B-CAB	3.65	1.55	1.47
2	C	600	HEM	C3C-CAC	3.63	1.55	1.47
2	C	600	HEM	CAA-C2A	2.40	1.55	1.52
2	D	600	HEM	CAA-C2A	2.30	1.55	1.52
2	A	600	HEM	CAA-C2A	2.24	1.55	1.52
3	A	601	3NQ	C34-C33	2.18	1.53	1.50
3	B	601	3NQ	C34-C33	2.14	1.53	1.50
3	C	601	3NQ	C34-C33	2.13	1.53	1.50
3	D	601	3NQ	C34-C33	2.09	1.53	1.50
2	B	600	HEM	CAA-C2A	2.05	1.55	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	3NQ	C34-C20-C22	-8.52	97.66	104.05
3	D	601	3NQ	C34-C20-C22	-7.91	98.12	104.05
3	C	601	3NQ	C34-C20-C22	-7.55	98.39	104.05
3	A	601	3NQ	C34-C20-C22	-7.53	98.40	104.05
3	D	601	3NQ	C22-C20-C13	-6.48	106.19	113.12
3	B	601	3NQ	O18-N17-C16	6.33	120.75	112.15
3	B	601	3NQ	C22-C20-C13	-5.94	106.76	113.12
3	D	601	3NQ	O18-N17-C16	5.72	119.91	112.15
3	A	601	3NQ	C22-C20-C13	-5.58	107.15	113.12
3	C	601	3NQ	C22-C20-C13	-5.54	107.19	113.12
3	A	601	3NQ	O18-N17-C16	5.27	119.31	112.15
3	C	601	3NQ	O18-N17-C16	5.26	119.29	112.15
3	B	601	3NQ	C34-C33-C26	-4.76	108.96	112.87
3	D	601	3NQ	C20-C13-C12	-4.31	103.32	109.09
3	D	601	3NQ	C34-C33-C26	-4.27	109.36	112.87
3	C	601	3NQ	C20-C13-C12	-4.14	103.54	109.09
3	A	601	3NQ	C20-C13-C12	-4.12	103.57	109.09
2	B	600	HEM	CAA-CBA-CGA	-3.80	106.30	112.67
2	A	600	HEM	CAA-CBA-CGA	-3.77	106.35	112.67
3	B	601	3NQ	C20-C13-C12	-3.50	104.40	109.09
3	A	601	3NQ	C34-C20-C13	-3.40	117.48	121.57
3	A	601	3NQ	C34-C33-C26	-3.40	110.07	112.87
3	C	601	3NQ	C34-C20-C13	-3.39	117.50	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	3NQ	C30-N29-C28	3.38	122.70	116.85
3	C	601	3NQ	C34-C33-C26	-3.38	110.09	112.87
3	C	601	3NQ	C30-N29-C28	3.37	122.69	116.85
3	D	601	3NQ	C25-C12-C10	-3.24	110.18	113.91
2	A	600	HEM	CMA-C3A-C4A	-3.17	123.58	128.46
3	D	601	3NQ	C9-C10-C1	3.14	111.43	107.46
3	B	601	3NQ	C30-N29-C28	3.12	122.24	116.85
3	D	601	3NQ	C30-N29-C28	3.05	122.12	116.85
2	B	600	HEM	CMC-C2C-C3C	3.02	130.33	124.68
3	D	601	3NQ	C20-C22-C26	3.02	102.27	99.70
3	B	601	3NQ	C34-C20-C13	-2.83	118.17	121.57
3	A	601	3NQ	C15-C16-N17	-2.66	120.69	125.35
3	C	601	3NQ	C15-C16-N17	-2.66	120.70	125.35
3	D	601	3NQ	C34-C20-C13	-2.62	118.42	121.57
3	A	601	3NQ	C3-C1-C10	-2.53	109.32	112.80
3	C	601	3NQ	C3-C1-C10	-2.53	109.33	112.80
2	C	600	HEM	CMA-C3A-C4A	-2.48	124.65	128.46
3	D	601	3NQ	C23-C22-C24	-2.47	108.23	111.13
2	B	600	HEM	CMA-C3A-C4A	-2.41	124.76	128.46
3	A	601	3NQ	C27-C28-N29	-2.40	119.94	123.49
2	D	600	HEM	CAA-CBA-CGA	-2.40	108.64	112.67
3	C	601	3NQ	C25-C12-C10	-2.40	111.15	113.91
3	A	601	3NQ	C25-C12-C13	-2.39	108.31	111.75
3	C	601	3NQ	C27-C28-N29	-2.39	119.96	123.49
3	A	601	3NQ	C25-C12-C10	-2.38	111.17	113.91
3	C	601	3NQ	C25-C12-C13	-2.35	108.36	111.75
2	A	600	HEM	CMB-C2B-C3B	2.35	129.07	124.68
3	D	601	3NQ	C27-C28-N29	-2.34	120.03	123.49
3	B	601	3NQ	C25-C12-C10	-2.34	111.22	113.91
3	B	601	3NQ	C27-C28-N29	-2.33	120.04	123.49
3	D	601	3NQ	C15-C16-N17	-2.32	121.29	125.35
3	D	601	3NQ	C10-C1-C16	-2.31	106.54	109.75
3	D	601	3NQ	C23-C22-C20	-2.25	109.65	112.98
3	B	601	3NQ	C23-C22-C20	-2.25	109.66	112.98
2	B	600	HEM	CBD-CAD-C3D	-2.25	108.34	112.48
3	B	601	3NQ	C3-C1-C10	-2.23	109.74	112.80
2	D	600	HEM	C1D-C2D-C3D	2.23	108.54	107.00
3	B	601	3NQ	C9-C10-C1	2.12	110.14	107.46
2	C	600	HEM	CAA-CBA-CGA	-2.11	109.13	112.67
3	A	601	3NQ	C20-C22-C26	2.09	101.48	99.70
3	C	601	3NQ	C20-C22-C26	2.08	101.47	99.70
2	D	600	HEM	CMA-C3A-C4A	-2.08	125.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	3NQ	C1-C3-C4	-2.07	105.43	110.53
3	A	601	3NQ	C1-C3-C4	-2.06	105.44	110.53
3	B	601	3NQ	C15-C16-N17	-2.05	121.75	125.35
3	D	601	3NQ	C25-C24-C22	-2.01	108.38	112.74
2	B	600	HEM	CMB-C2B-C3B	2.01	128.43	124.68
3	C	601	3NQ	C25-C24-C22	-2.00	108.40	112.74
3	C	601	3NQ	C3-C4-C8	-2.00	108.16	110.55

There are no chirality outliers.

All (20) torsion outliers are listed below:

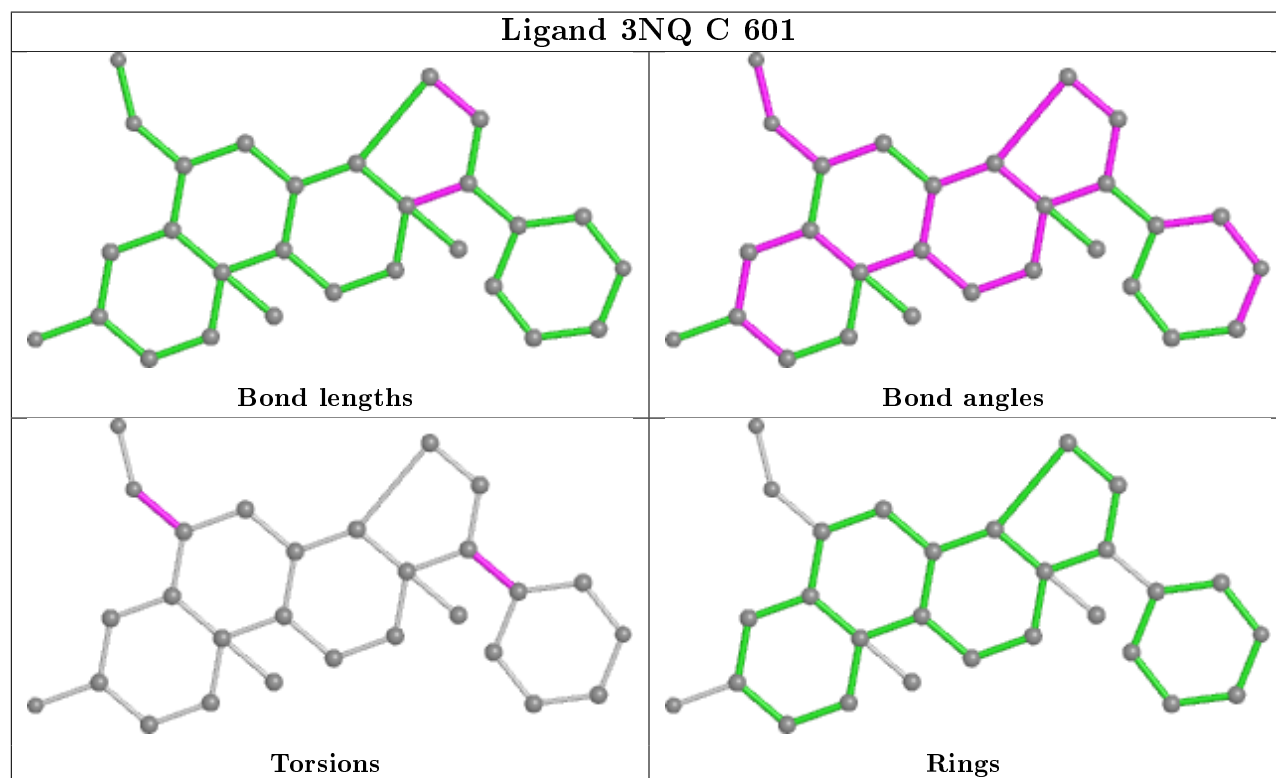
Mol	Chain	Res	Type	Atoms
3	C	601	3NQ	C1-C16-N17-O18
3	C	601	3NQ	C15-C16-N17-O18
2	D	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C3A-C2A-CAA-CBA
2	A	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	C3A-C2A-CAA-CBA
2	C	600	HEM	C1A-C2A-CAA-CBA
2	C	600	HEM	C3A-C2A-CAA-CBA
3	A	601	3NQ	C1-C16-N17-O18
3	A	601	3NQ	C15-C16-N17-O18
2	B	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C3A-C2A-CAA-CBA
3	C	601	3NQ	C33-C26-C27-C32
3	B	601	3NQ	C33-C26-C27-C32
3	A	601	3NQ	C33-C26-C27-C32
3	B	601	3NQ	C33-C26-C27-C28
3	C	601	3NQ	C33-C26-C27-C28
3	D	601	3NQ	C33-C26-C27-C32
3	A	601	3NQ	C33-C26-C27-C28
3	D	601	3NQ	C33-C26-C27-C28

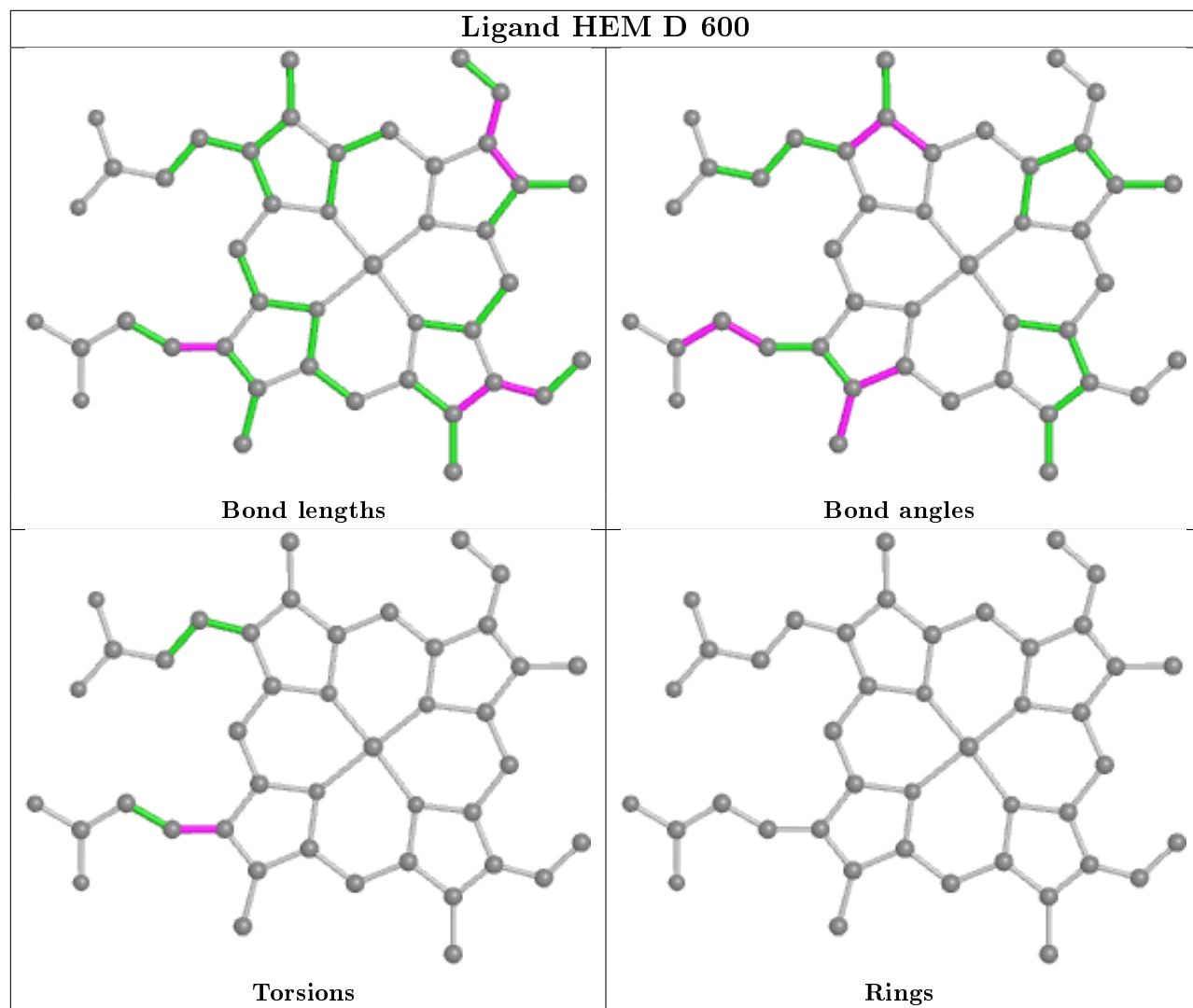
There are no ring outliers.

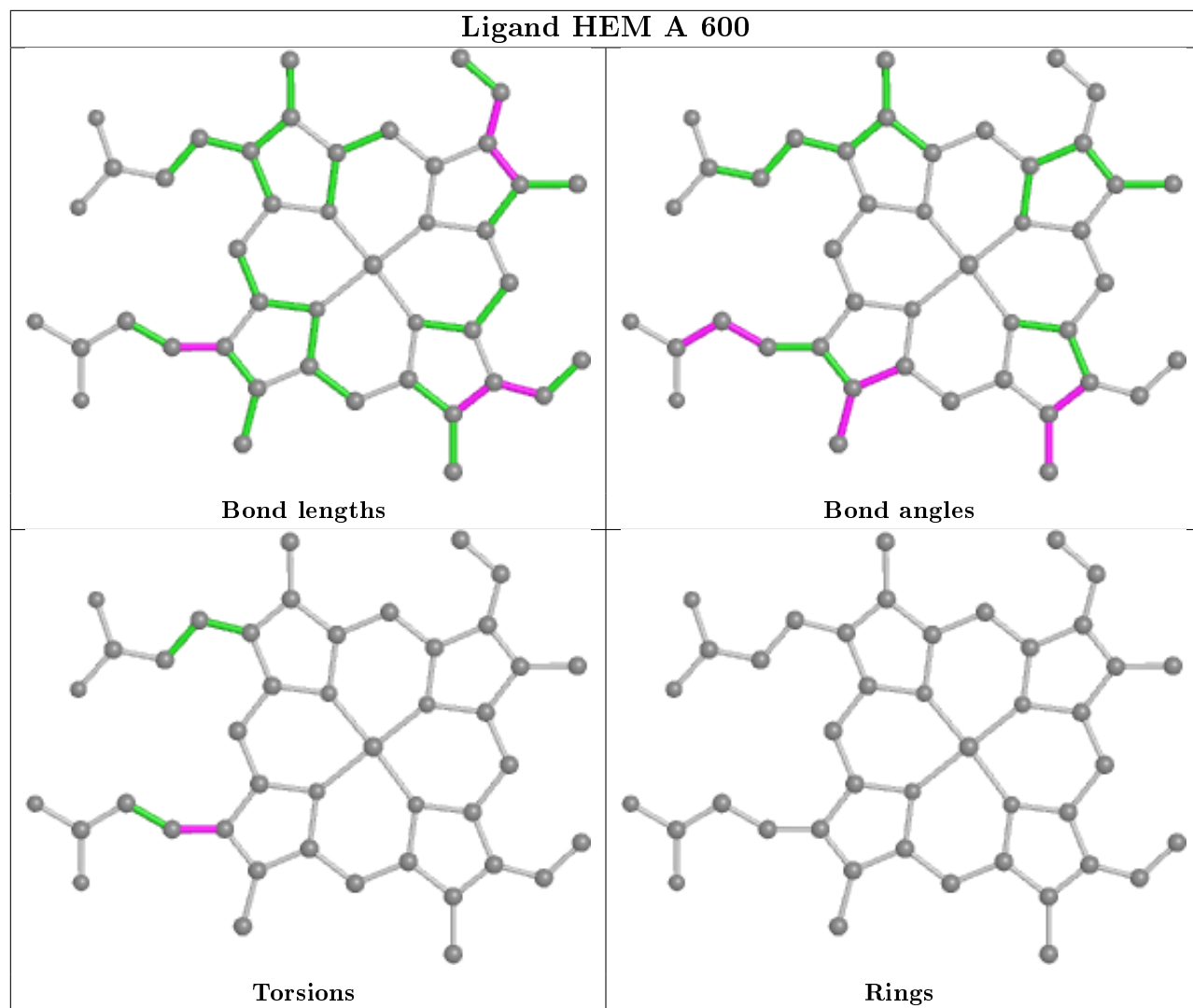
4 monomers are involved in 9 short contacts:

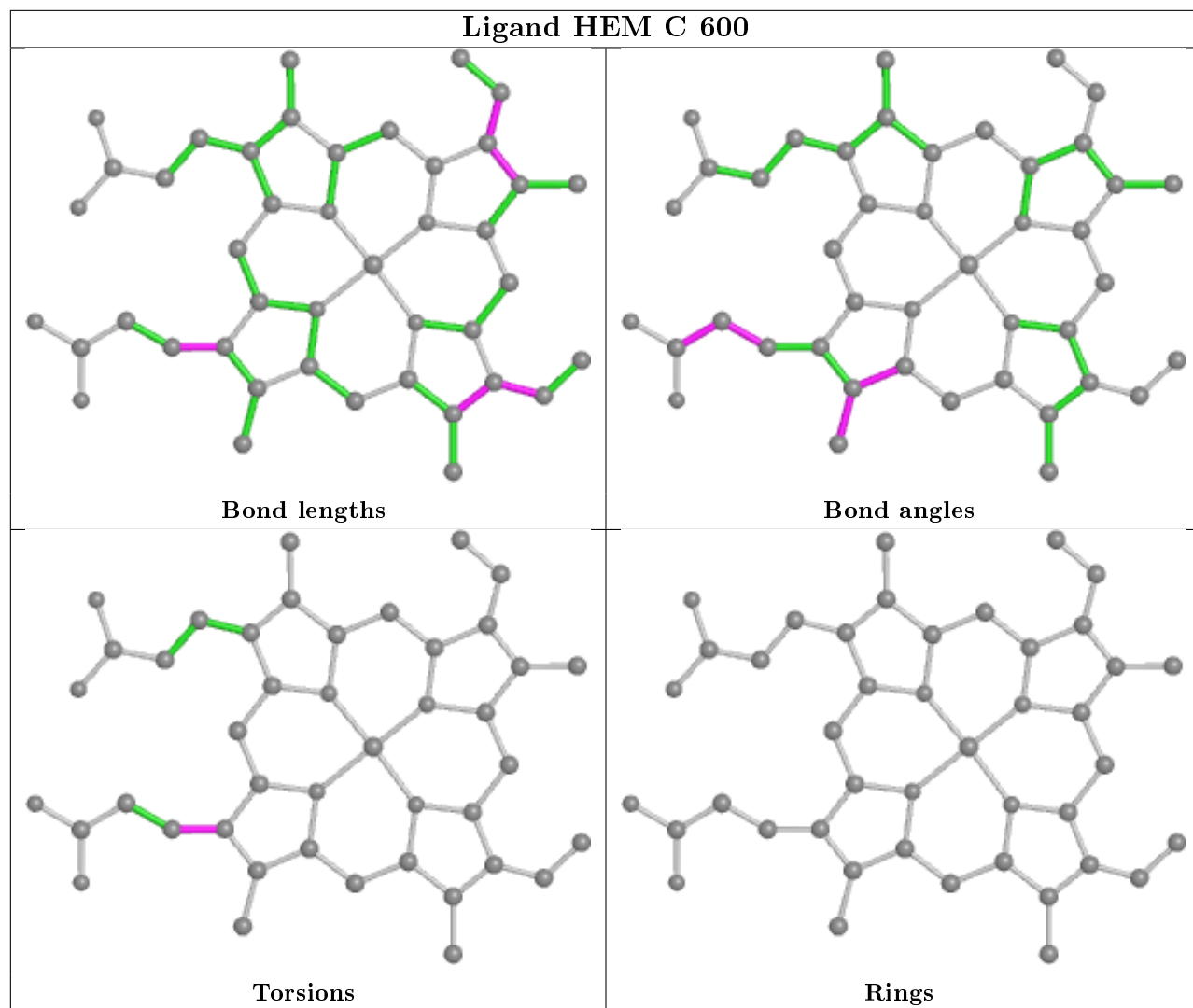
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	HEM	2	0
2	A	600	HEM	3	0
2	C	600	HEM	2	0
2	B	600	HEM	2	0

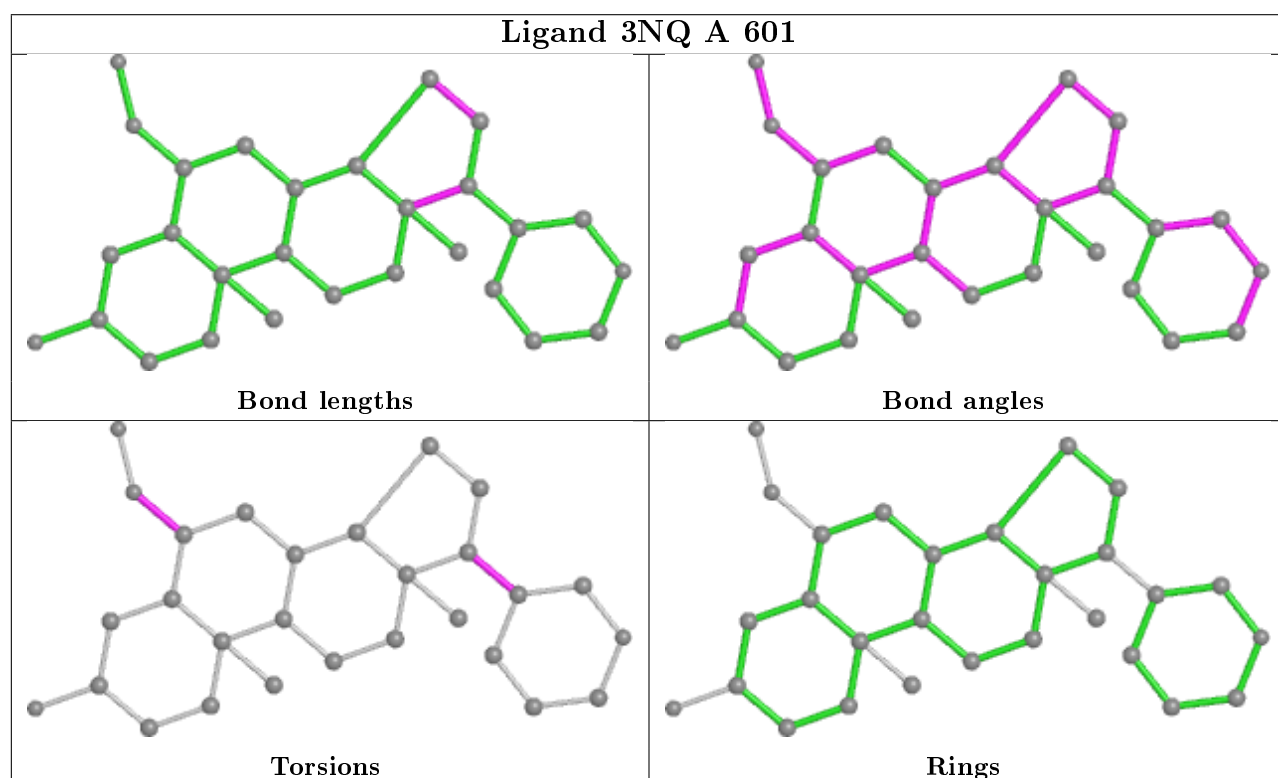
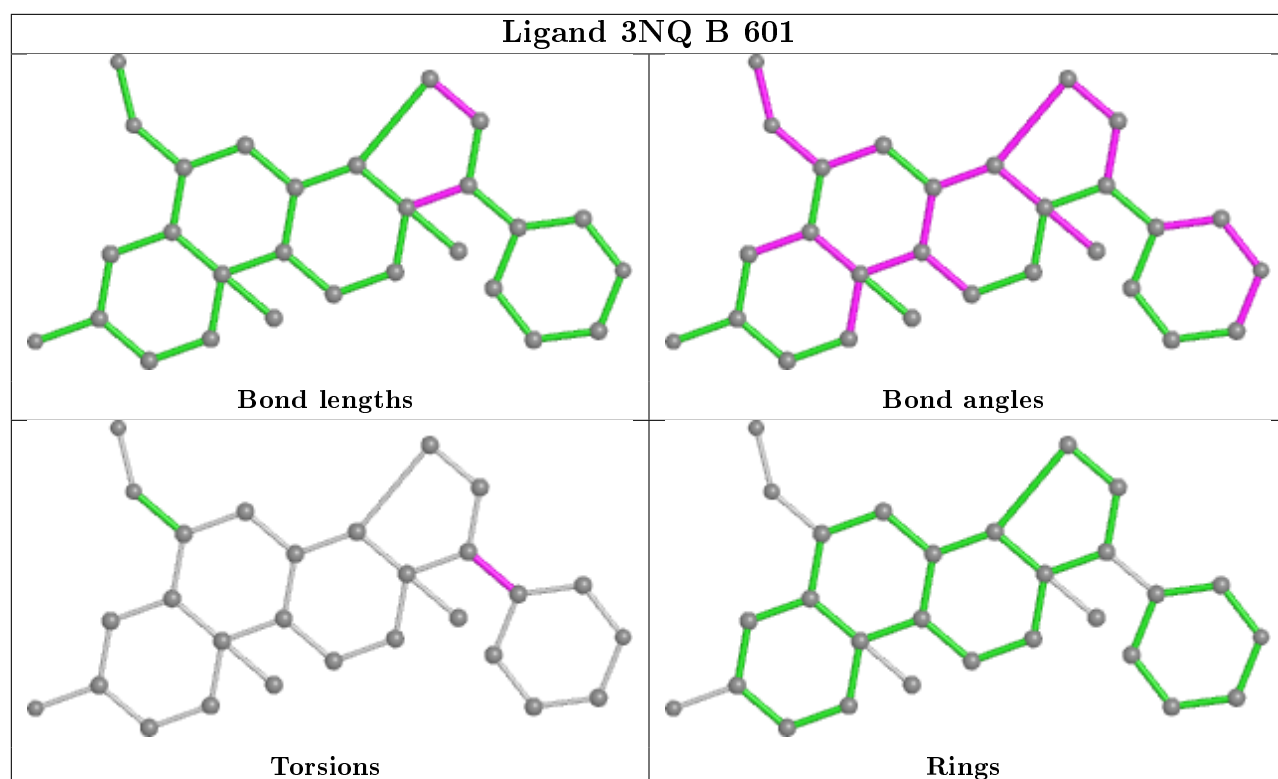
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

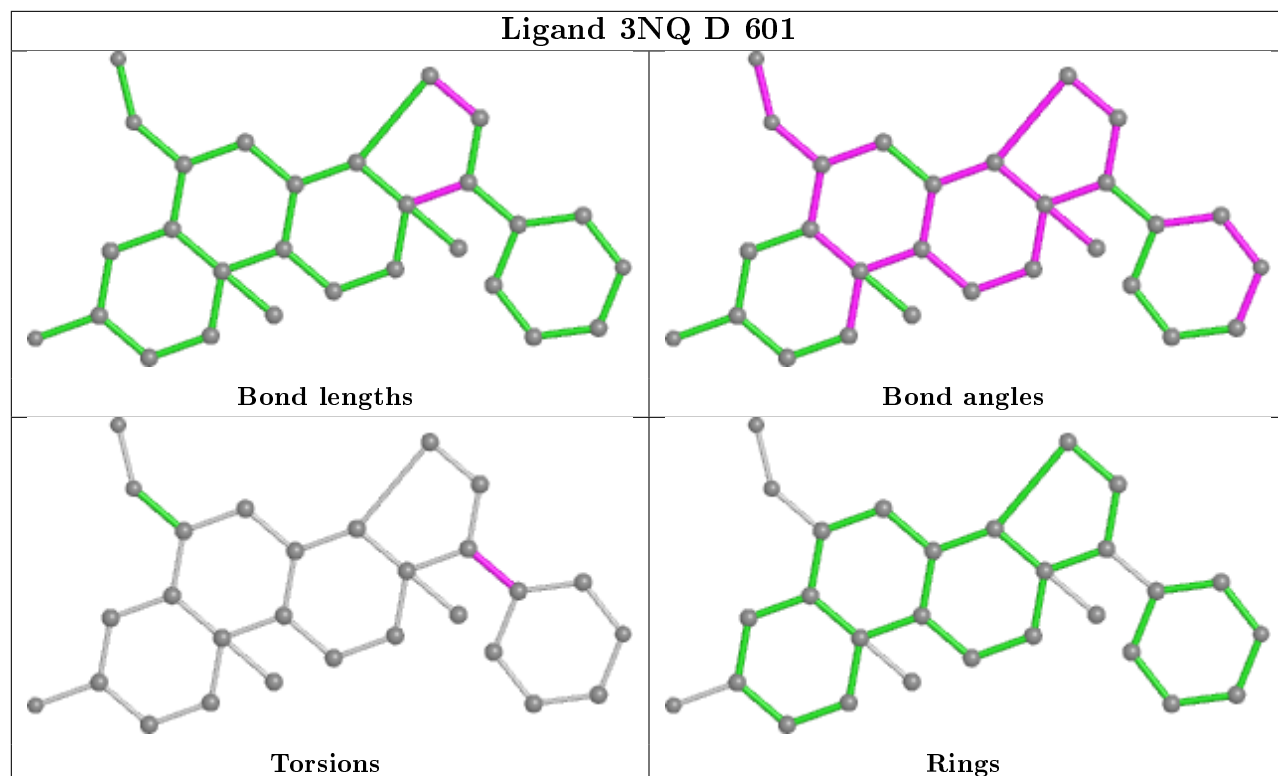




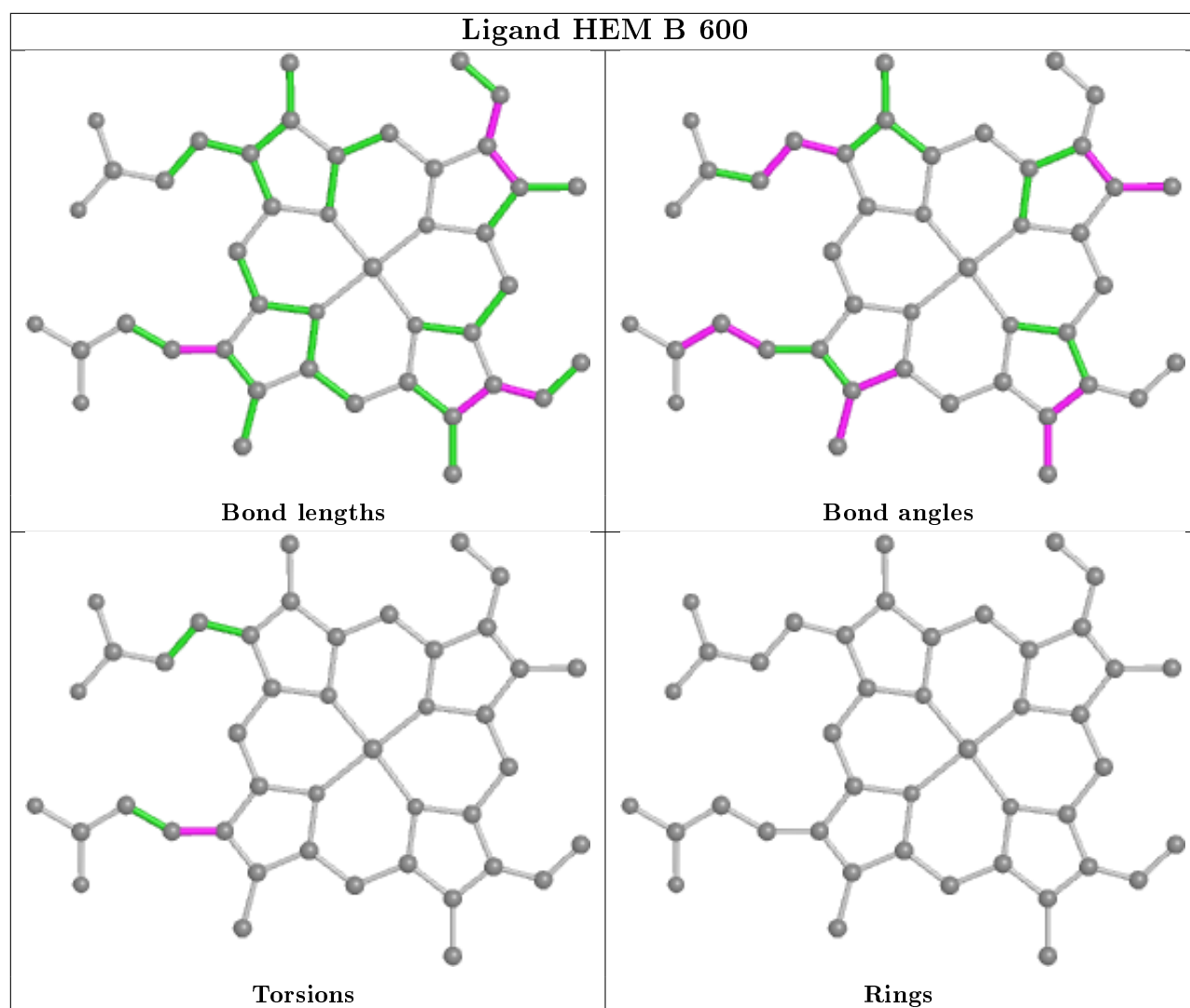












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	466/494 (94%)	0.38	34 (7%) 15 12	34, 52, 85, 120	0
1	B	466/494 (94%)	0.26	26 (5%) 24 21	35, 51, 79, 125	0
1	C	472/494 (95%)	0.26	26 (5%) 25 22	33, 47, 80, 120	0
1	D	471/494 (95%)	0.25	21 (4%) 33 30	34, 50, 78, 107	0
All	All	1875/1976 (94%)	0.29	107 (5%) 23 21	33, 50, 81, 125	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	7.3
1	B	139	ASP	6.2
1	B	140	GLN	5.3
1	C	279	GLY	5.1
1	C	46	HIS	5.0
1	C	42	PHE	4.8
1	A	283	ASP	4.6
1	D	139	ASP	4.5
1	A	138	GLY	4.5
1	C	139	ASP	4.5
1	A	137	ASP	4.3
1	D	282	GLN	4.2
1	D	469	ASP	4.1
1	A	257	ASP	4.1
1	A	504	ALA	4.0
1	A	271	MET	3.9
1	C	136	LYS	3.7
1	A	251	LYS	3.7
1	C	45	ARG	3.5
1	B	275	ASN	3.5
1	A	502	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	284	SER	3.4
1	A	254	PHE	3.4
1	D	349	ARG	3.4
1	D	46	HIS	3.4
1	A	498	ALA	3.3
1	D	470	ASP	3.3
1	B	252	GLU	3.2
1	A	286	LEU	3.2
1	B	138	GLY	3.1
1	D	136	LYS	3.1
1	C	367	ALA	3.1
1	C	138	GLY	3.1
1	A	285	GLU	3.0
1	C	140	GLN	3.0
1	D	274	ASP	3.0
1	B	258	SER	2.8
1	A	256	SER	2.8
1	A	255	ARG	2.8
1	B	274	ASP	2.8
1	B	283	ASP	2.8
1	B	497	GLN	2.8
1	D	140	GLN	2.8
1	C	276	GLY	2.8
1	C	41	PRO	2.7
1	B	137	ASP	2.7
1	C	497	GLN	2.7
1	A	268	GLN	2.7
1	B	338	PHE	2.7
1	A	250	TYR	2.7
1	B	337	GLY	2.6
1	C	368	PRO	2.6
1	A	423	THR	2.6
1	C	280	PRO	2.6
1	A	442	CYS	2.6
1	C	472	GLN	2.6
1	A	136	LYS	2.6
1	B	253	LYS	2.6
1	B	303	GLY	2.6
1	B	144	LYS	2.5
1	C	366	VAL	2.5
1	A	258	SER	2.5
1	B	501	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	302	ALA	2.5
1	C	134	LEU	2.4
1	C	442	CYS	2.4
1	A	134	LEU	2.4
1	A	249	ASN	2.4
1	D	137	ASP	2.4
1	A	497	GLN	2.4
1	D	367	ALA	2.3
1	A	252	GLU	2.3
1	B	248	GLU	2.3
1	B	285	GLU	2.3
1	A	421	ALA	2.3
1	D	138	GLY	2.3
1	C	307	THR	2.3
1	A	469	ASP	2.3
1	D	442	CYS	2.3
1	A	500	ARG	2.3
1	D	43	LEU	2.3
1	B	254	PHE	2.3
1	D	365	PRO	2.3
1	D	275	ASN	2.3
1	B	306	THR	2.3
1	A	274	ASP	2.3
1	A	303	GLY	2.2
1	D	41	PRO	2.2
1	D	134	LEU	2.2
1	D	333	ASP	2.2
1	C	275	ASN	2.2
1	B	257	ASP	2.2
1	B	189	LYS	2.2
1	A	367	ALA	2.1
1	C	383	GLU	2.1
1	A	269	ALA	2.1
1	D	472	GLN	2.1
1	B	442	CYS	2.1
1	C	365	PRO	2.1
1	B	268	GLN	2.1
1	C	122	GLN	2.1
1	B	249	ASN	2.1
1	B	271	MET	2.1
1	C	137	ASP	2.1
1	D	42	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	213	SER	2.0
1	C	308	THR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

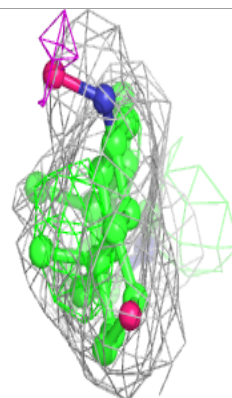
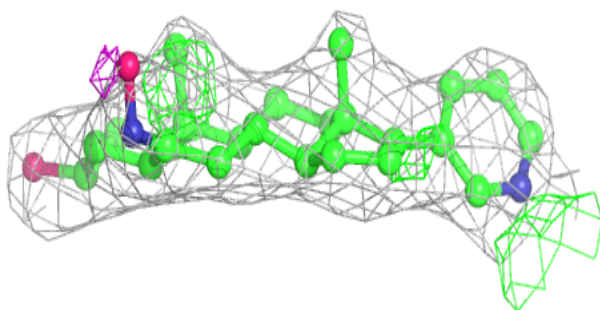
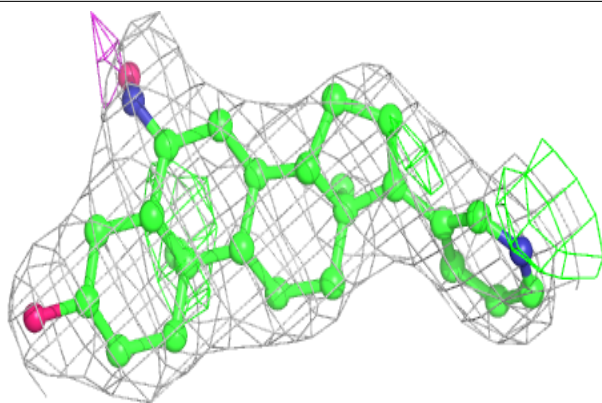
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	3NQ	C	601	28/28	0.91	0.41	38,49,56,60	0
2	HEM	C	600	43/43	0.92	0.34	30,45,65,77	0
3	3NQ	D	601	28/28	0.94	0.30	32,42,49,61	0
3	3NQ	A	601	28/28	0.95	0.36	38,49,56,60	0
3	3NQ	B	601	28/28	0.95	0.34	34,47,52,71	0
2	HEM	B	600	43/43	0.95	0.31	33,46,59,67	0
2	HEM	A	600	43/43	0.96	0.37	36,51,72,73	0
2	HEM	D	600	43/43	0.96	0.32	33,43,54,58	0

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

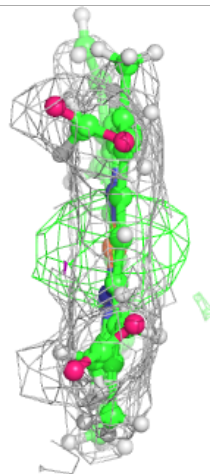
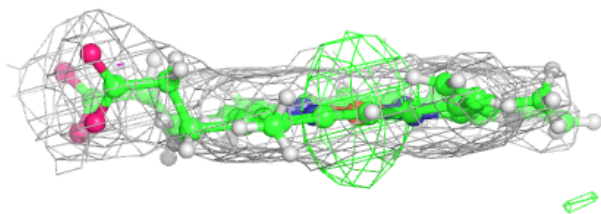
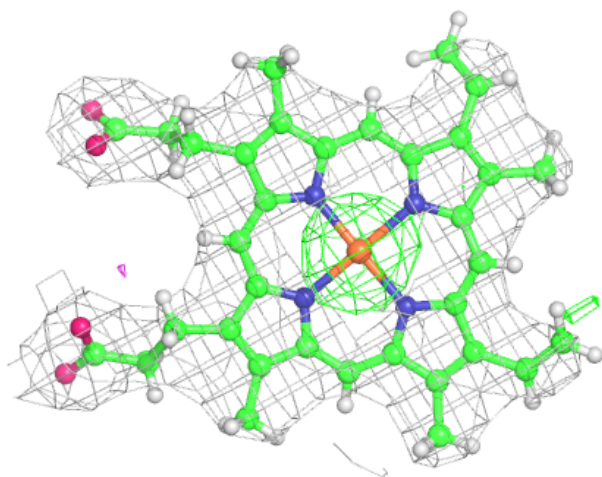
**Electron density around 3NQ C 601:**

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



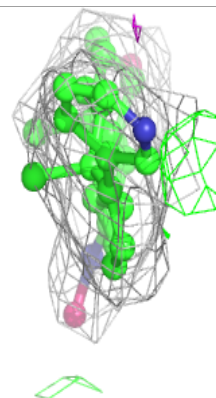
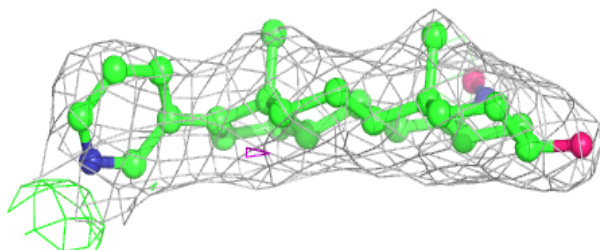
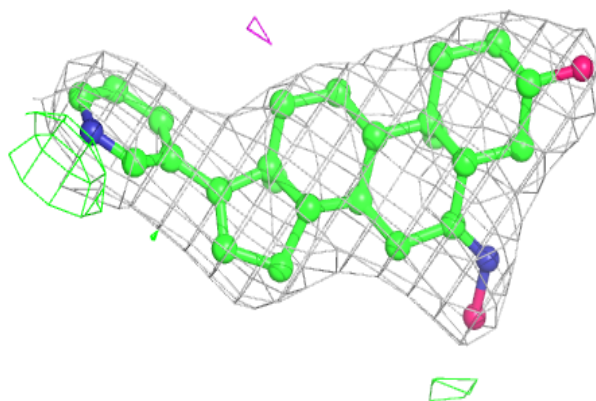
**Electron density around HEM C 600:**

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

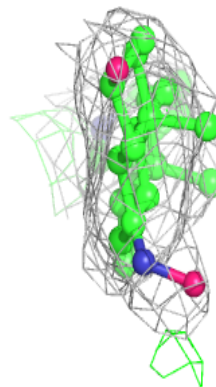
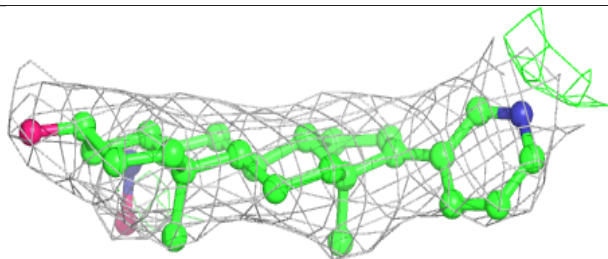
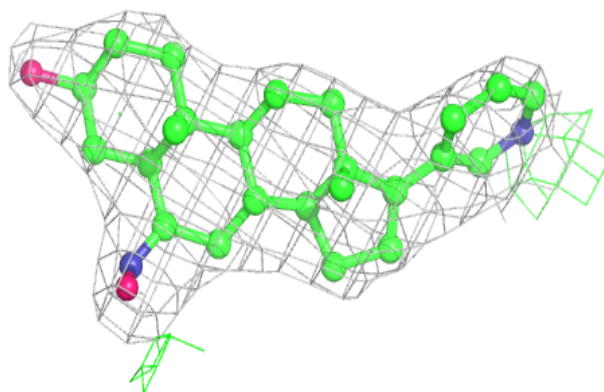


**Electron density around 3NQ D 601:**

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

**Electron density around 3NQ A 601:**

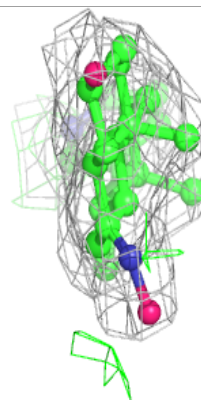
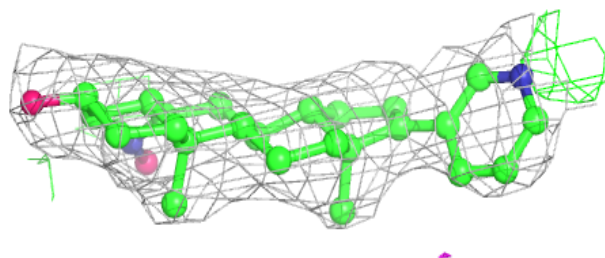
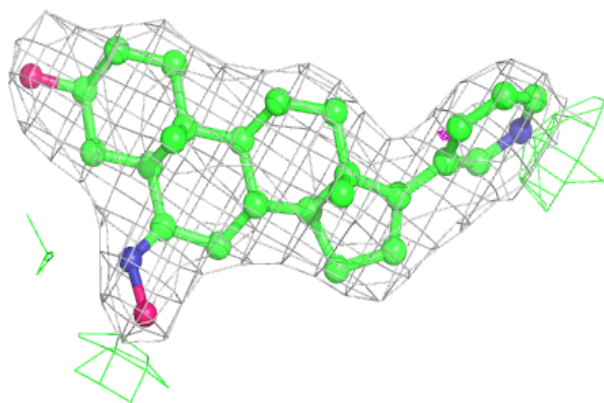
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





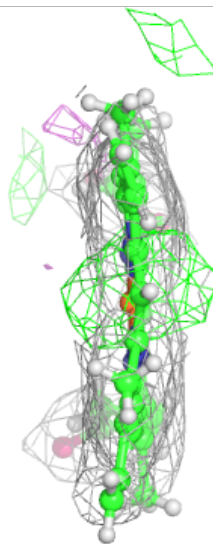
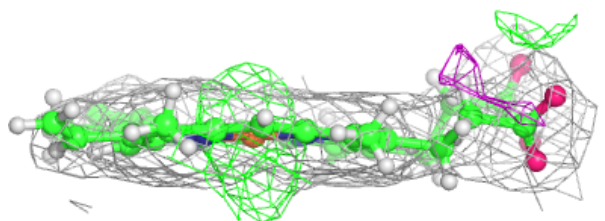
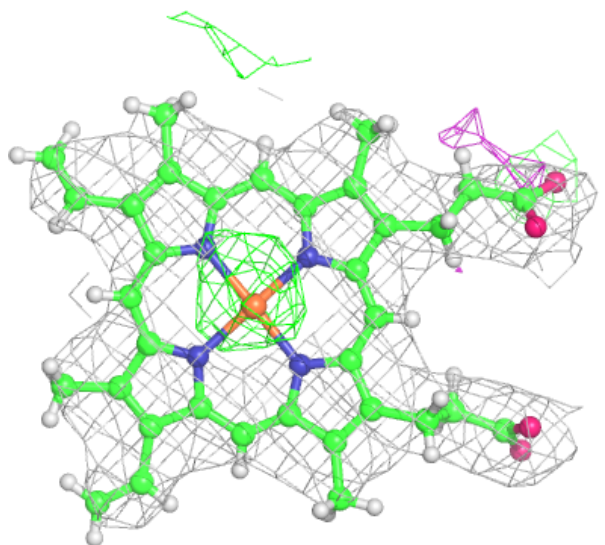
**Electron density around 3NQ B 601:**

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



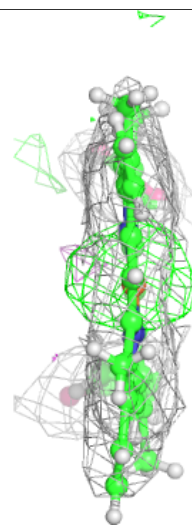
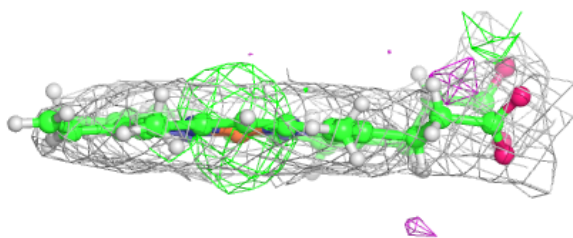
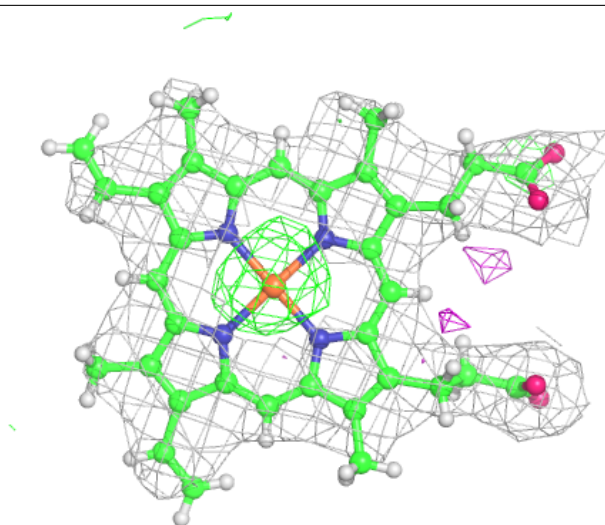
**Electron density around HEM B 600:**

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



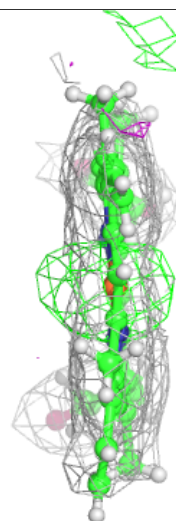
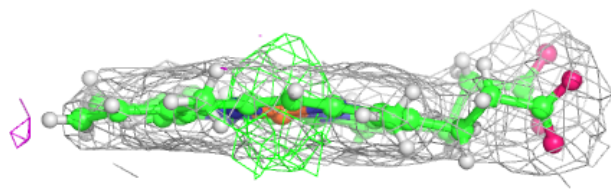
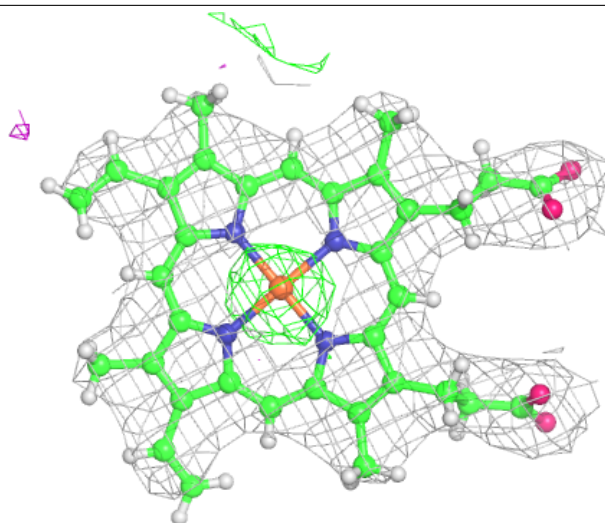
**Electron density around HEM A 600:**

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



**Electron density around HEM D 600:**

$2mF_o-DF_c$  (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.