



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:12 pm BST

PDB ID : 4NKV  
Title : Human steroidogenic cytochrome P450 17A1 mutant A105L with inhibitor abiraterone  
Authors : Scott, E.E.; Petrunak, E.M.  
Deposited on : 2013-11-13  
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

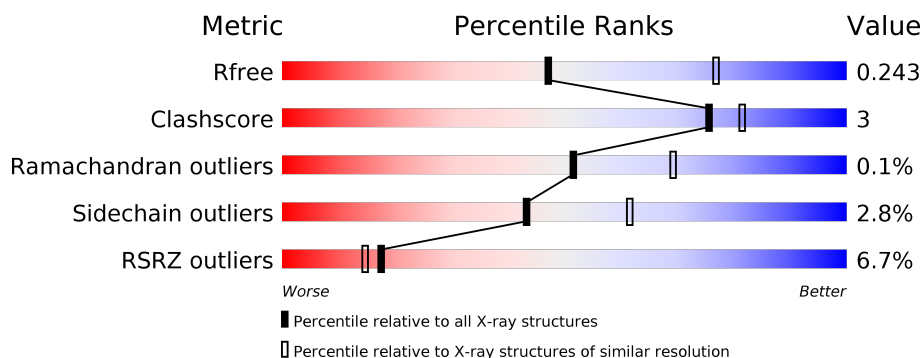
# 1 Overall quality at a glance

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>6%</div> <div>87%</div> <div>6% • 6%</div> </div>
1	B	494	<div> <div>3%</div> <div>88%</div> <div>6% • 5%</div> </div>
1	C	494	<div> <div>7%</div> <div>88%</div> <div>7% 5%</div> </div>
1	D	494	<div> <div>10%</div> <div>83%</div> <div>10% • 6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30823 atoms, of which 15495 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
			7528	2388	3808	643	674	15			
1	B	467	Total	C	H	N	O	S	0	0	0
			7533	2390	3808	644	676	15			
1	C	471	Total	C	H	N	O	S	0	0	0
			7583	2405	3832	649	682	15			
1	D	466	Total	C	H	N	O	S	0	0	0
			7520	2386	3803	642	674	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	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	105	LEU	ALA	ENGINEERED MUTATION	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	-	EXPRESSION TAG	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	105	LEU	ALA	ENGINEERED MUTATION	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	-	EXPRESSION TAG	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	EXPRESSION TAG	UNP P05093
C	21	LYS	-	EXPRESSION TAG	UNP P05093
C	22	LYS	-	EXPRESSION TAG	UNP P05093
C	23	THR	-	EXPRESSION TAG	UNP P05093
C	105	LEU	ALA	ENGINEERED MUTATION	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	-	EXPRESSION TAG	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	105	LEU	ALA	ENGINEERED MUTATION	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

- # HEM

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

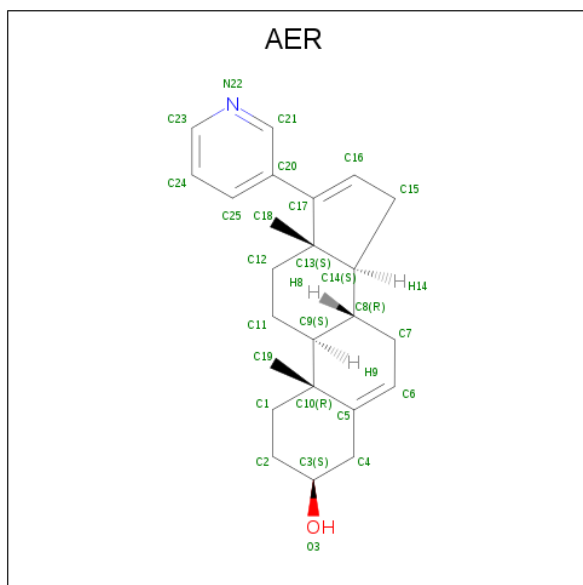


WORLD WIDE  
PDB  
PROTEIN DATA BANK

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

- Molecule 3 is Abiraterone (three-letter code: AER) (formula:  $C_{24}H_{31}NO$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	B	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	C	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	D	1	Total	C	H	N	O	0	0
			57	24	31	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O	0	0
			37 37		
4	B	38	Total O	0	0
			38 38		

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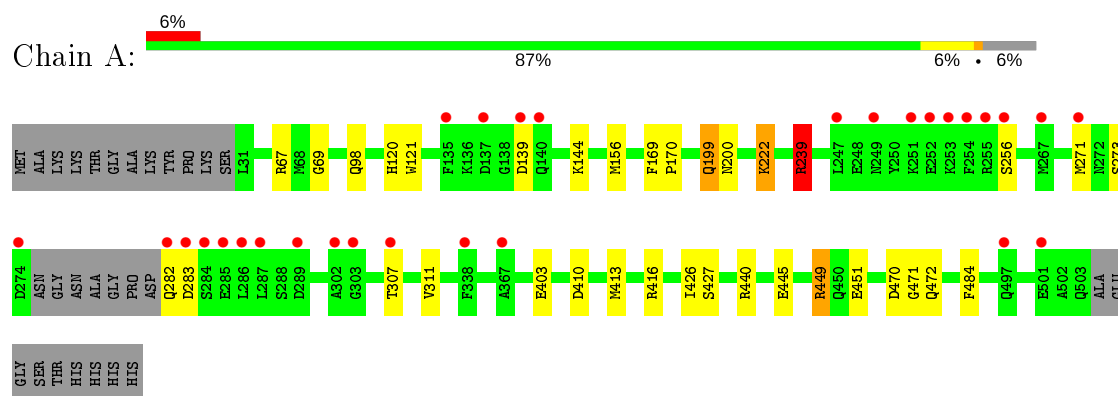
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total	O	0	0
			37	37		
4	D	27	Total	O	0	0
			27	27		

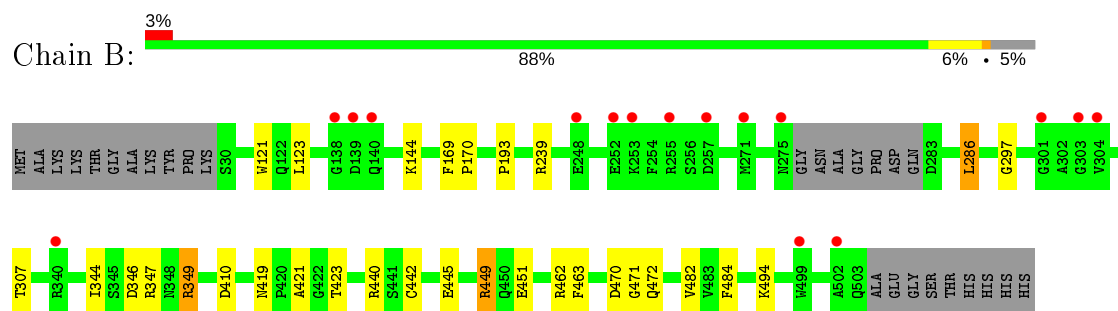
### 3 Residue-property plots [i](#)

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.

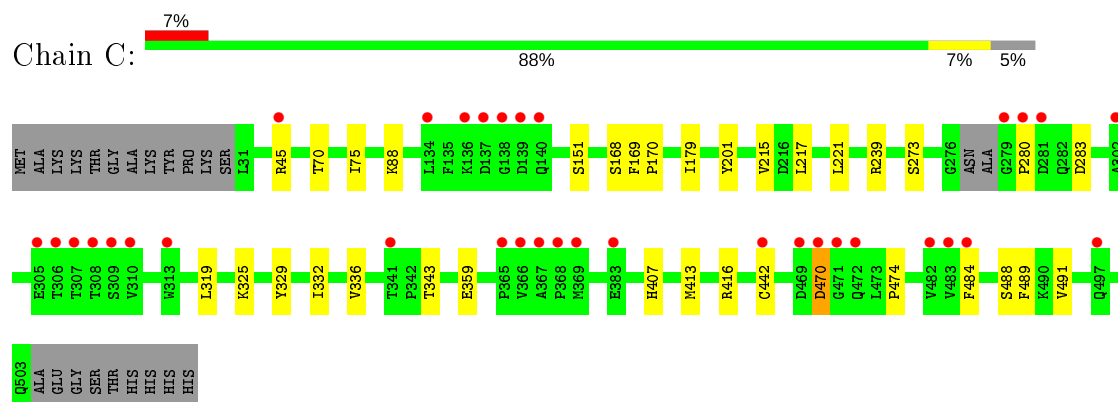
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



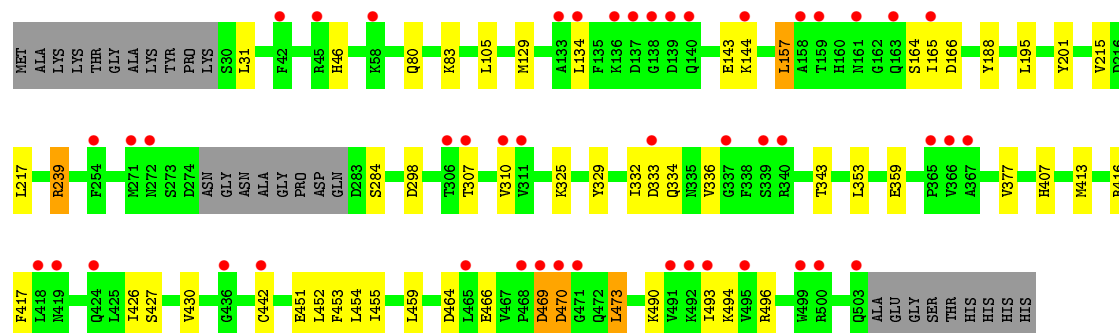
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



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



Chain D:  10% 83% 10% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.67Å 153.25Å 167.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 2.65 38.59 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.59-2.65) 99.1 (38.59-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.191 , 0.242 0.192 , 0.243	Depositor DCC
$R_{free}$ test set	3463 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.2	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	30823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, AER

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	0.43	0/3800	0.53	1/5144 (0.0%)
1	B	0.45	0/3805	0.52	0/5151
1	C	0.46	1/3832 (0.0%)	0.54	0/5188
1	D	0.43	1/3797 (0.0%)	0.54	0/5140
All	All	0.44	2/15234 (0.0%)	0.53	1/20623 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	442	CYS	CB-SG	-5.19	1.73	1.81
1	C	442	CYS	CB-SG	-5.04	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH1	5.84	123.22	120.30

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	3720	3808	3793	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3725	3808	3796	18	0
1	C	3751	3832	3816	16	0
1	D	3717	3803	3790	33	0
2	A	43	30	30	2	0
2	B	43	30	30	4	0
2	C	43	30	30	2	0
2	D	43	30	30	2	0
3	A	26	31	31	2	0
3	B	26	31	31	4	0
3	C	26	31	31	0	0
3	D	26	31	31	3	0
4	A	37	0	0	1	0
4	B	38	0	0	1	0
4	C	37	0	0	0	0
4	D	27	0	0	1	0
All	All	15328	15495	15439	95	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 3.

All (95) 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:C:600:HEM:HBB2	2:C:600:HEM:HHC	1.65	0.77
2:A:600:HEM:HHB	2:A:600:HEM:HBC2	1.77	0.66
2:C:600:HEM:HBC2	2:C:600:HEM:HHB	1.78	0.64
1:A:239:ARG:HG2	1:A:239:ARG:HH11	1.63	0.62
1:D:188:TYR:CG	1:D:195:LEU:HD11	2.34	0.62
1:C:470:ASP:OD1	1:C:470:ASP:N	2.33	0.62
2:D:600:HEM:HBC2	2:D:600:HEM:HHB	1.81	0.62
1:D:359:GLU:OE2	1:D:416:ARG:NH2	2.33	0.61
1:D:470:ASP:OD1	1:D:470:ASP:N	2.32	0.61
2:B:600:HEM:C1B	3:B:601:AER:H23	2.31	0.61
1:D:310:VAL:HG23	1:D:452:LEU:HD21	1.81	0.61
2:B:600:HEM:HMC1	2:B:600:HEM:HBC2	1.82	0.60
1:D:105:LEU:HD21	3:D:601:AER:H19	1.83	0.60
3:A:601:AER:H12	3:A:601:AER:H25	1.85	0.57
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.37	0.57
2:A:600:HEM:HMB2	2:A:600:HEM:HBB2	1.87	0.56
1:D:473:LEU:H	1:D:473:LEU:HD12	1.69	0.56
1:B:445:GLU:OE2	1:B:449:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:MET:O	1:C:416:ARG:HG2	2.06	0.56
1:D:310:VAL:CG2	1:D:452:LEU:HD21	2.37	0.54
1:D:165:ILE:HG13	1:D:166:ASP:N	2.22	0.54
1:A:121:TRP:CZ2	1:A:440:ARG:HD2	2.43	0.53
1:C:359:GLU:OE2	1:C:416:ARG:NH1	2.42	0.53
1:A:470:ASP:O	1:A:472:GLN:N	2.39	0.51
1:D:407:HIS:O	1:D:416:ARG:NH1	2.44	0.51
1:C:332:ILE:O	1:C:336:VAL:HG12	2.11	0.51
1:A:199:GLN:HG3	1:A:200:ASN:N	2.25	0.50
1:B:421:ALA:HB3	1:B:423:THR:HG22	1.93	0.50
1:A:67:ARG:NH1	1:A:69:GLY:O	2.44	0.49
1:D:298:ASP:HA	3:D:601:AER:H7A	1.94	0.49
1:D:453:PHE:HD2	1:D:454:LEU:HD12	1.78	0.49
1:A:139:ASP:O	1:A:144:LYS:HE2	2.12	0.49
1:B:462:ARG:HD2	1:B:463:PHE:CZ	2.48	0.48
1:C:407:HIS:O	1:C:416:ARG:NH2	2.46	0.48
1:B:470:ASP:O	1:B:472:GLN:N	2.38	0.48
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.73	0.48
1:A:156:MET:SD	1:B:193:PRO:HB3	2.54	0.48
1:B:346:ASP:HA	1:B:349:ARG:HD2	1.95	0.48
1:D:310:VAL:HG23	1:D:452:LEU:CD2	2.43	0.48
1:A:239:ARG:HG2	1:A:239:ARG:NH1	2.29	0.48
2:D:600:HEM:HBB2	2:D:600:HEM:HMB2	1.94	0.47
1:B:419:ASN:HD21	1:B:423:THR:HG23	1.80	0.47
1:D:332:ILE:O	1:D:336:VAL:HG12	2.14	0.46
1:D:46:HIS:O	1:D:46:HIS:ND1	2.49	0.46
1:B:410:ASP:N	1:B:410:ASP:OD1	2.45	0.46
1:C:273:SER:O	1:C:280:PRO:HA	2.16	0.46
1:A:307:THR:HG21	1:A:451:GLU:OE1	2.16	0.46
1:B:239:ARG:HH21	1:B:297:GLY:HA3	1.81	0.46
1:B:442:CYS:HB2	2:B:600:HEM:NA	2.30	0.45
2:B:600:HEM:C4A	3:B:601:AER:H23	2.51	0.45
1:C:325:LYS:HE2	1:C:329:TYR:HE2	1.81	0.45
1:D:413:MET:O	1:D:416:ARG:HG2	2.16	0.45
1:A:222:LYS:O	1:A:222:LYS:HG2	2.16	0.45
1:D:157:LEU:HG	1:D:493:ILE:CD1	2.47	0.45
1:B:470:ASP:O	4:B:701:HOH:O	2.21	0.44
1:A:169:PHE:HB3	1:A:170:PRO:HD3	1.99	0.44
1:C:215:VAL:HG12	1:C:217:LEU:H	1.83	0.44
1:C:319:LEU:HD21	1:C:491:VAL:HG12	2.00	0.44
1:A:426:ILE:HG13	1:A:427:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LYS:HE2	1:C:329:TYR:CE2	2.52	0.44
1:D:455:ILE:O	1:D:459:LEU:HB2	2.17	0.44
3:D:601:AER:H25	3:D:601:AER:H12	1.99	0.44
1:D:239:ARG:NH2	4:D:715:HOH:O	2.50	0.44
1:D:353:LEU:HD23	1:D:453:PHE:CE1	2.53	0.44
1:B:123:LEU:HD23	1:B:286:LEU:HD13	2.00	0.43
1:C:75:ILE:HD12	1:C:75:ILE:N	2.33	0.43
1:D:310:VAL:HG21	1:D:452:LEU:HD11	2.00	0.43
1:D:143:GLU:OE2	1:D:343:THR:HG23	2.18	0.43
1:D:426:ILE:HG13	1:D:427:SER:N	2.34	0.43
1:D:157:LEU:HG	1:D:493:ILE:HD13	1.99	0.43
1:D:325:LYS:HE2	1:D:329:TYR:CE2	2.53	0.43
1:C:169:PHE:HB3	1:C:170:PRO:HD3	2.01	0.43
1:A:307:THR:O	1:A:311:VAL:HG23	2.18	0.43
1:B:307:THR:HG21	1:B:451:GLU:OE1	2.18	0.43
1:A:410:ASP:OD1	1:A:410:ASP:N	2.49	0.43
1:D:188:TYR:CB	1:D:195:LEU:HD11	2.47	0.43
1:B:123:LEU:CD2	1:B:286:LEU:HD13	2.48	0.42
1:D:333:ASP:OD1	1:D:334:GLN:N	2.52	0.42
1:A:413:MET:O	1:A:416:ARG:HG2	2.20	0.42
3:B:601:AER:H21	3:B:601:AER:H16	1.72	0.42
1:A:239:ARG:NE	4:A:732:HOH:O	2.44	0.42
1:D:464:ASP:OD1	1:D:496:ARG:NH1	2.53	0.42
1:B:121:TRP:CZ2	1:B:440:ARG:HD2	2.55	0.42
1:C:280:PRO:CD	1:D:377:VAL:HG12	2.50	0.41
1:B:344:ILE:O	1:B:347:ARG:HG2	2.20	0.41
1:D:416:ARG:HG3	1:D:417:PHE:CD1	2.56	0.41
1:D:469:ASP:N	1:D:469:ASP:OD1	2.53	0.41
1:C:474:PRO:HB3	1:C:489:PHE:CG	2.56	0.41
1:D:83:LYS:NZ	1:D:430:VAL:HG22	2.36	0.41
1:D:307:THR:HG21	1:D:451:GLU:OE1	2.21	0.41
1:C:179:ILE:HD12	1:C:179:ILE:HA	1.96	0.40
1:B:482:VAL:HG22	3:B:601:AER:C18	2.52	0.40
3:A:601:AER:C12	3:A:601:AER:H25	2.51	0.40
1:D:215:VAL:HG12	1:D:217:LEU:H	1.85	0.40
1:B:169:PHE:HB3	1:B:170:PRO:HD3	2.03	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	A	462/494 (94%)	446 (96%)	15 (3%)	1 (0%)	47	64
1	B	463/494 (94%)	447 (96%)	15 (3%)	1 (0%)	47	64
1	C	467/494 (94%)	449 (96%)	18 (4%)	0	100	100
1	D	462/494 (94%)	446 (96%)	16 (4%)	0	100	100
All	All	1854/1976 (94%)	1788 (96%)	64 (4%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	GLY
1	B	471	GLY

### 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	417/437 (95%)	404 (97%)	13 (3%)	40	58
1	B	418/437 (96%)	412 (99%)	6 (1%)	67	80
1	C	420/437 (96%)	408 (97%)	12 (3%)	42	60
1	D	417/437 (95%)	401 (96%)	16 (4%)	33	50
All	All	1672/1748 (96%)	1625 (97%)	47 (3%)	43	61

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	120	HIS
1	A	199	GLN
1	A	222	LYS
1	A	239	ARG
1	A	256	SER
1	A	271	MET
1	A	273	SER
1	A	282	GLN
1	A	283	ASP
1	A	403	GLU
1	A	449	ARG
1	A	484	PHE
1	B	144	LYS
1	B	286	LEU
1	B	349	ARG
1	B	449	ARG
1	B	484	PHE
1	B	494	LYS
1	C	70	THR
1	C	88	LYS
1	C	151	SER
1	C	168	SER
1	C	201	TYR
1	C	221	LEU
1	C	239	ARG
1	C	283	ASP
1	C	343	THR
1	C	470	ASP
1	C	484	PHE
1	C	488	SER
1	D	31	LEU
1	D	80	GLN
1	D	129	MET
1	D	134	LEU
1	D	144	LYS
1	D	157	LEU
1	D	164	SER
1	D	201	TYR
1	D	239	ARG
1	D	284	SER
1	D	466	GLU
1	D	469	ASP

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Mol	Chain	Res	Type
1	D	470	ASP
1	D	473	LEU
1	D	490	LYS
1	D	494	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	B	50	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	AER	B	601	2	30,30,30	3.45	14 (46%)	44,47,47	4.55	30 (68%)
2	HEM	B	600	1,3	27,50,50	2.04	5 (18%)	17,82,82	1.73	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	600	1,3	27,50,50	2.29	6 (22%)	17,82,82	1.53	3 (17%)
2	HEM	D	600	1,3	27,50,50	2.10	6 (22%)	17,82,82	1.36	2 (11%)
3	AER	D	601	2	30,30,30	3.89	17 (56%)	44,47,47	4.33	26 (59%)
3	AER	C	601	2	30,30,30	3.62	13 (43%)	44,47,47	4.29	23 (52%)
3	AER	A	601	2	30,30,30	3.83	16 (53%)	44,47,47	4.04	24 (54%)
2	HEM	A	600	1,3	27,50,50	2.21	6 (22%)	17,82,82	1.49	3 (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	AER	B	601	2	-	0/4/62/62	0/5/5/5
2	HEM	B	600	1,3	-	0/6/54/54	-
2	HEM	C	600	1,3	-	0/6/54/54	-
2	HEM	D	600	1,3	-	2/6/54/54	-
3	AER	D	601	2	-	0/4/62/62	0/5/5/5
3	AER	C	601	2	-	0/4/62/62	0/5/5/5
3	AER	A	601	2	-	0/4/62/62	0/5/5/5
2	HEM	A	600	1,3	-	0/6/54/54	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	AER	C15-C14	-8.51	1.41	1.54
3	D	601	AER	C20-C17	-8.49	1.34	1.48
3	B	601	AER	C8-C9	-8.33	1.37	1.53
3	B	601	AER	C15-C14	-8.32	1.42	1.54
3	C	601	AER	C20-C17	-8.19	1.34	1.48
3	A	601	AER	C20-C17	-8.14	1.34	1.48
3	D	601	AER	C15-C14	-7.98	1.42	1.54
3	A	601	AER	C13-C17	-7.96	1.45	1.53
3	A	601	AER	C15-C14	-7.77	1.43	1.54
3	B	601	AER	C20-C17	-7.63	1.35	1.48
3	D	601	AER	C13-C17	-7.62	1.46	1.53
3	C	601	AER	C13-C17	-6.94	1.46	1.53
3	A	601	AER	C8-C9	-6.83	1.40	1.53
3	D	601	AER	C8-C9	-6.73	1.40	1.53
3	C	601	AER	C8-C9	-6.63	1.40	1.53
3	D	601	AER	C10-C5	-6.47	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	AER	C10-C5	-6.36	1.40	1.52
2	C	600	HEM	C3C-C2C	-6.12	1.31	1.40
2	C	600	HEM	C3B-C2B	-5.96	1.32	1.40
2	A	600	HEM	C3C-C2C	-5.76	1.32	1.40
2	B	600	HEM	C3C-C2C	-5.43	1.32	1.40
3	A	601	AER	C15-C16	-5.42	1.42	1.50
3	C	601	AER	C4-C5	-5.26	1.40	1.51
3	B	601	AER	C10-C5	-5.19	1.42	1.52
2	D	600	HEM	C3C-C2C	-5.03	1.33	1.40
3	D	601	AER	C4-C5	-5.01	1.40	1.51
3	B	601	AER	C15-C16	-5.00	1.43	1.50
3	C	601	AER	C10-C5	-4.99	1.43	1.52
2	A	600	HEM	C3D-C2D	4.98	1.52	1.37
3	D	601	AER	C15-C16	-4.97	1.43	1.50
2	D	600	HEM	C3D-C2D	4.93	1.52	1.37
3	C	601	AER	C15-C16	-4.87	1.43	1.50
2	B	600	HEM	C3D-C2D	4.83	1.52	1.37
3	A	601	AER	C4-C5	-4.82	1.41	1.51
2	A	600	HEM	C3B-C2B	-4.75	1.33	1.40
2	C	600	HEM	C3D-C2D	4.46	1.50	1.37
3	D	601	AER	C21-N22	4.32	1.43	1.34
3	D	601	AER	C7-C6	-4.31	1.40	1.50
2	D	600	HEM	C3B-C2B	-4.24	1.34	1.40
2	B	600	HEM	C3B-C2B	-4.14	1.34	1.40
3	B	601	AER	C4-C5	-4.12	1.42	1.51
3	A	601	AER	C7-C6	-4.09	1.41	1.50
3	A	601	AER	C13-C14	-4.09	1.47	1.54
3	A	601	AER	C12-C13	3.98	1.61	1.54
3	B	601	AER	C6-C5	3.86	1.41	1.33
3	C	601	AER	C7-C6	-3.86	1.41	1.50
3	D	601	AER	C12-C13	3.78	1.61	1.54
3	B	601	AER	C12-C11	3.76	1.61	1.53
2	D	600	HEM	C3B-CAB	3.56	1.55	1.47
3	B	601	AER	C10-C9	3.48	1.61	1.56
3	C	601	AER	C16-C17	3.44	1.39	1.33
3	D	601	AER	C8-C14	3.42	1.60	1.53
3	C	601	AER	C8-C14	3.36	1.60	1.53
3	B	601	AER	C16-C17	3.34	1.39	1.33
2	D	600	HEM	C3C-CAC	3.33	1.54	1.47
3	A	601	AER	C6-C5	3.32	1.40	1.33
3	C	601	AER	C6-C5	3.28	1.40	1.33
2	A	600	HEM	C3C-CAC	3.26	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	C3C-CAC	3.21	1.54	1.47
3	A	601	AER	C16-C17	3.19	1.39	1.33
3	A	601	AER	C8-C14	3.13	1.59	1.53
3	D	601	AER	C16-C17	2.93	1.39	1.33
3	B	601	AER	C8-C14	2.92	1.59	1.53
3	C	601	AER	C21-N22	2.87	1.40	1.34
3	C	601	AER	C12-C13	2.82	1.59	1.54
2	B	600	HEM	C3C-CAC	2.81	1.53	1.47
3	D	601	AER	C4-C3	2.77	1.57	1.52
2	C	600	HEM	C3B-CAB	2.77	1.53	1.47
2	B	600	HEM	C3B-CAB	2.75	1.53	1.47
2	A	600	HEM	C3B-CAB	2.73	1.53	1.47
3	D	601	AER	C6-C5	2.68	1.38	1.33
3	D	601	AER	C13-C14	-2.68	1.49	1.54
3	D	601	AER	C7-C8	-2.64	1.48	1.53
3	B	601	AER	C19-C10	-2.64	1.50	1.54
3	A	601	AER	C21-N22	2.54	1.39	1.34
3	B	601	AER	C7-C6	-2.45	1.44	1.50
3	D	601	AER	C23-N22	2.41	1.40	1.33
3	A	601	AER	C11-C9	-2.21	1.50	1.53
2	C	600	HEM	CAA-C2A	2.16	1.55	1.52
3	A	601	AER	C10-C9	2.15	1.59	1.56
2	D	600	HEM	CAD-C3D	2.08	1.55	1.52
2	A	600	HEM	C4B-CHC	-2.07	1.35	1.41
3	B	601	AER	C12-C13	2.02	1.58	1.54

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AER	C14-C13-C17	-14.19	87.58	99.70
3	C	601	AER	C14-C13-C17	-13.90	87.83	99.70
3	D	601	AER	C14-C13-C17	-12.06	89.40	99.70
3	B	601	AER	C7-C8-C9	-11.60	95.65	109.71
3	D	601	AER	C15-C16-C17	-10.78	104.01	112.87
3	A	601	AER	C15-C16-C17	-10.50	104.23	112.87
3	A	601	AER	C7-C8-C9	-10.47	97.03	109.71
3	D	601	AER	C7-C8-C9	-10.20	97.35	109.71
3	C	601	AER	C15-C16-C17	-9.91	104.72	112.87
3	A	601	AER	C14-C13-C17	-9.45	91.63	99.70
3	C	601	AER	C7-C8-C9	-9.42	98.30	109.71
3	B	601	AER	C15-C16-C17	-8.54	105.85	112.87
3	B	601	AER	C15-C14-C8	-7.95	112.03	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	AER	C1-C2-C3	-7.22	101.20	110.47
3	B	601	AER	C7-C8-C14	-6.89	100.91	110.91
3	C	601	AER	C13-C14-C8	-6.80	105.84	113.12
3	D	601	AER	C18-C13-C12	6.43	118.69	111.13
3	B	601	AER	C20-C17-C16	-6.14	116.77	125.19
3	A	601	AER	C13-C14-C8	-6.11	106.58	113.12
3	A	601	AER	C1-C2-C3	-5.99	102.78	110.47
3	D	601	AER	C13-C14-C8	-5.94	106.77	113.12
3	A	601	AER	C18-C13-C12	5.93	118.11	111.13
3	C	601	AER	C18-C13-C12	5.87	118.03	111.13
3	B	601	AER	C18-C13-C12	5.75	117.89	111.13
3	C	601	AER	C8-C7-C6	5.69	120.90	112.73
3	C	601	AER	C1-C2-C3	-5.61	103.27	110.47
3	D	601	AER	C9-C10-C5	5.59	118.42	109.65
3	B	601	AER	C1-C10-C9	-5.55	100.97	108.73
3	C	601	AER	C7-C6-C5	-5.53	114.86	125.06
3	D	601	AER	C8-C7-C6	5.48	120.61	112.73
3	D	601	AER	C10-C9-C8	-5.44	104.58	112.73
3	A	601	AER	C10-C9-C8	-5.29	104.81	112.73
3	A	601	AER	C15-C14-C8	-5.27	115.24	121.57
3	A	601	AER	C7-C6-C5	-5.16	115.54	125.06
3	A	601	AER	C7-C8-C14	-5.16	103.43	110.91
3	C	601	AER	C10-C9-C8	-5.13	105.05	112.73
3	B	601	AER	C9-C10-C5	5.08	117.62	109.65
3	D	601	AER	C15-C14-C8	-5.07	115.48	121.57
3	C	601	AER	C15-C14-C8	-5.04	115.52	121.57
3	D	601	AER	C7-C6-C5	-5.01	115.82	125.06
3	B	601	AER	C7-C6-C5	-4.94	115.94	125.06
3	C	601	AER	C9-C10-C5	4.91	117.34	109.65
3	C	601	AER	C7-C8-C14	-4.90	103.81	110.91
3	B	601	AER	C8-C7-C6	4.89	119.75	112.73
3	A	601	AER	C8-C7-C6	4.87	119.72	112.73
3	D	601	AER	C1-C10-C9	-4.84	101.96	108.73
3	D	601	AER	C7-C8-C14	-4.76	104.01	110.91
3	B	601	AER	C12-C13-C14	-4.73	101.53	108.99
3	C	601	AER	C14-C15-C16	-4.66	93.89	101.39
3	B	601	AER	C1-C2-C3	-4.50	104.69	110.47
3	A	601	AER	C9-C10-C5	4.50	116.70	109.65
2	C	600	HEM	CAA-CBA-CGA	-4.48	105.16	112.67
3	C	601	AER	C12-C11-C9	-4.44	105.43	113.11
3	A	601	AER	C12-C11-C9	-4.42	105.45	113.11
3	A	601	AER	C12-C13-C14	-4.40	102.05	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AER	C12-C11-C9	-4.36	105.56	113.11
3	B	601	AER	C10-C5-C6	-4.25	116.40	122.90
3	D	601	AER	C10-C5-C6	-4.17	116.52	122.90
3	C	601	AER	C1-C10-C9	-3.93	103.24	108.73
3	D	601	AER	C12-C11-C9	-3.87	106.42	113.11
3	D	601	AER	C14-C15-C16	-3.85	95.20	101.39
3	A	601	AER	C14-C15-C16	-3.79	95.29	101.39
3	D	601	AER	C12-C13-C14	-3.78	103.03	108.99
3	B	601	AER	C10-C9-C8	-3.76	107.09	112.73
3	A	601	AER	C1-C10-C9	-3.74	103.50	108.73
3	B	601	AER	C13-C14-C8	-3.73	109.12	113.12
3	B	601	AER	C14-C15-C16	-3.53	95.71	101.39
3	C	601	AER	C12-C13-C14	-3.52	103.43	108.99
3	C	601	AER	C11-C9-C8	3.49	116.79	111.75
2	B	600	HEM	CAA-CBA-CGA	-3.45	106.89	112.67
3	A	601	AER	C10-C5-C6	-3.37	117.75	122.90
3	B	601	AER	C25-C20-C17	3.35	126.34	120.99
3	C	601	AER	C10-C5-C6	-3.27	117.90	122.90
3	D	601	AER	C11-C9-C8	3.24	116.42	111.75
3	B	601	AER	C1-C10-C5	-3.18	102.92	108.75
2	D	600	HEM	CAA-CBA-CGA	-3.10	107.46	112.67
2	A	600	HEM	CAA-CBA-CGA	-3.09	107.48	112.67
3	A	601	AER	C23-N22-C21	3.07	122.16	116.85
3	B	601	AER	C23-N22-C21	3.03	122.09	116.85
2	B	600	HEM	CMB-C2B-C3B	2.99	130.28	124.68
3	A	601	AER	C11-C9-C8	2.96	116.01	111.75
3	C	601	AER	C23-N22-C21	2.93	121.92	116.85
3	D	601	AER	C15-C14-C13	-2.93	101.86	104.05
2	A	600	HEM	CMB-C2B-C3B	2.90	130.10	124.68
3	C	601	AER	C18-C13-C14	2.82	117.14	112.98
3	A	601	AER	C18-C13-C14	2.80	117.12	112.98
2	B	600	HEM	CAD-CBD-CGD	-2.76	108.04	112.67
3	B	601	AER	C4-C5-C6	2.72	124.53	120.61
2	B	600	HEM	CMC-C2C-C3C	2.71	129.74	124.68
3	D	601	AER	C4-C5-C10	2.65	119.94	116.42
2	C	600	HEM	CBA-CAA-C2A	2.57	117.23	112.49
3	B	601	AER	C3-C4-C5	-2.55	107.69	112.03
2	A	600	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
3	A	601	AER	C15-C14-C13	-2.49	102.18	104.05
3	D	601	AER	C3-C4-C5	-2.47	107.83	112.03
3	B	601	AER	C24-C25-C20	2.38	123.16	120.34
2	D	600	HEM	CMB-C2B-C3B	2.35	129.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	HEM	C1D-C2D-C3D	-2.29	105.40	107.00
3	C	601	AER	C3-C4-C5	-2.20	108.29	112.03
3	D	601	AER	C18-C13-C14	2.19	116.22	112.98
3	B	601	AER	C25-C20-C21	-2.17	115.17	117.63
3	D	601	AER	C1-C10-C5	-2.16	104.80	108.75
3	C	601	AER	C4-C5-C10	2.14	119.26	116.42
3	C	601	AER	C18-C13-C17	2.12	112.47	108.00
3	A	601	AER	C20-C21-N22	-2.11	120.37	123.49
3	A	601	AER	C3-C4-C5	-2.09	108.47	112.03
3	B	601	AER	C11-C12-C13	-2.08	108.23	112.74
3	D	601	AER	C11-C12-C13	-2.06	108.28	112.74
3	B	601	AER	C18-C13-C17	2.04	112.30	108.00
3	B	601	AER	C19-C10-C5	2.03	111.63	108.34
3	D	601	AER	C4-C5-C6	2.03	123.53	120.61
3	B	601	AER	C15-C14-C13	-2.02	102.53	104.05
2	C	600	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
3	B	601	AER	C20-C21-N22	-2.01	120.51	123.49
3	D	601	AER	C24-C25-C20	2.00	122.71	120.34
3	A	601	AER	C4-C5-C6	2.00	123.50	120.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C3A-C2A-CAA-CBA

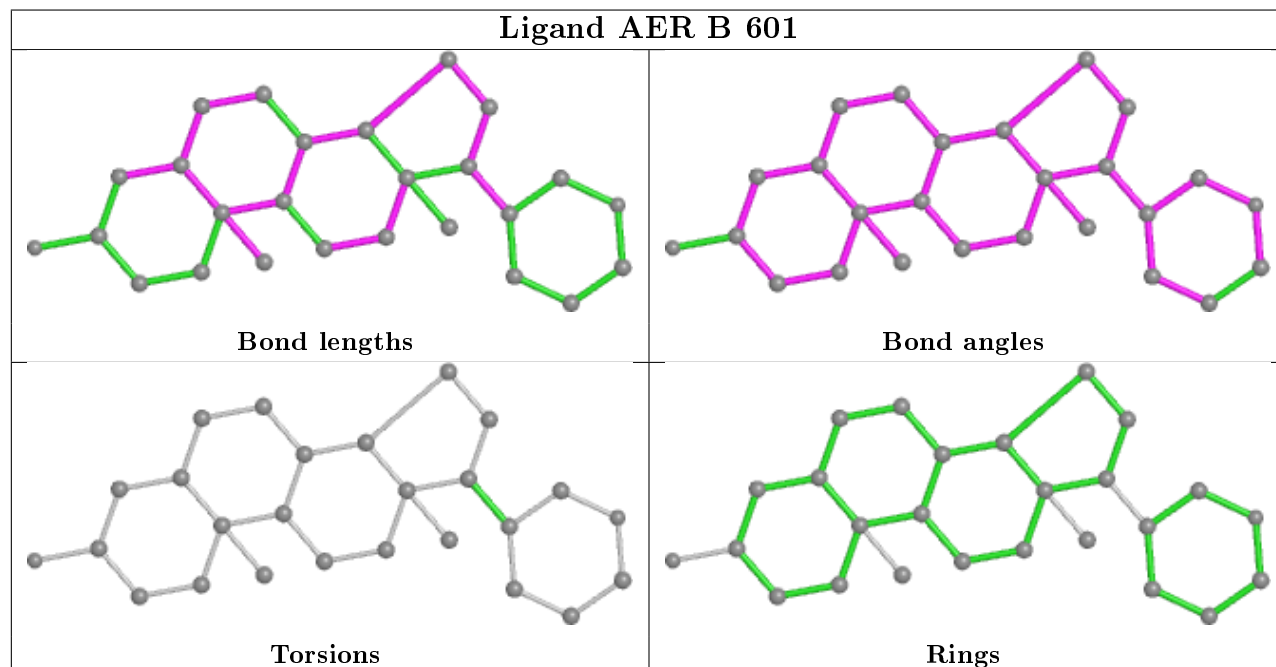
There are no ring outliers.

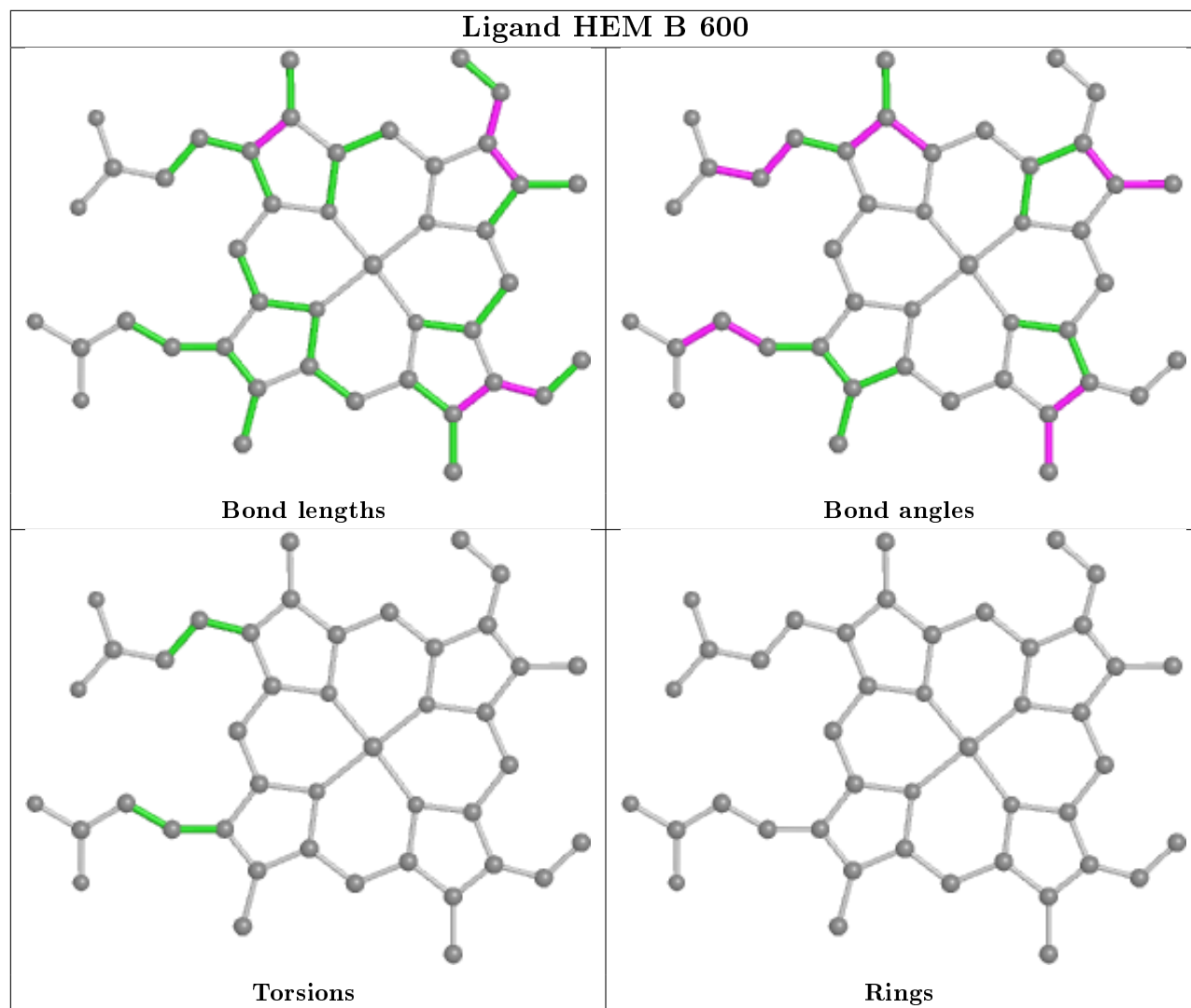
7 monomers are involved in 17 short contacts:

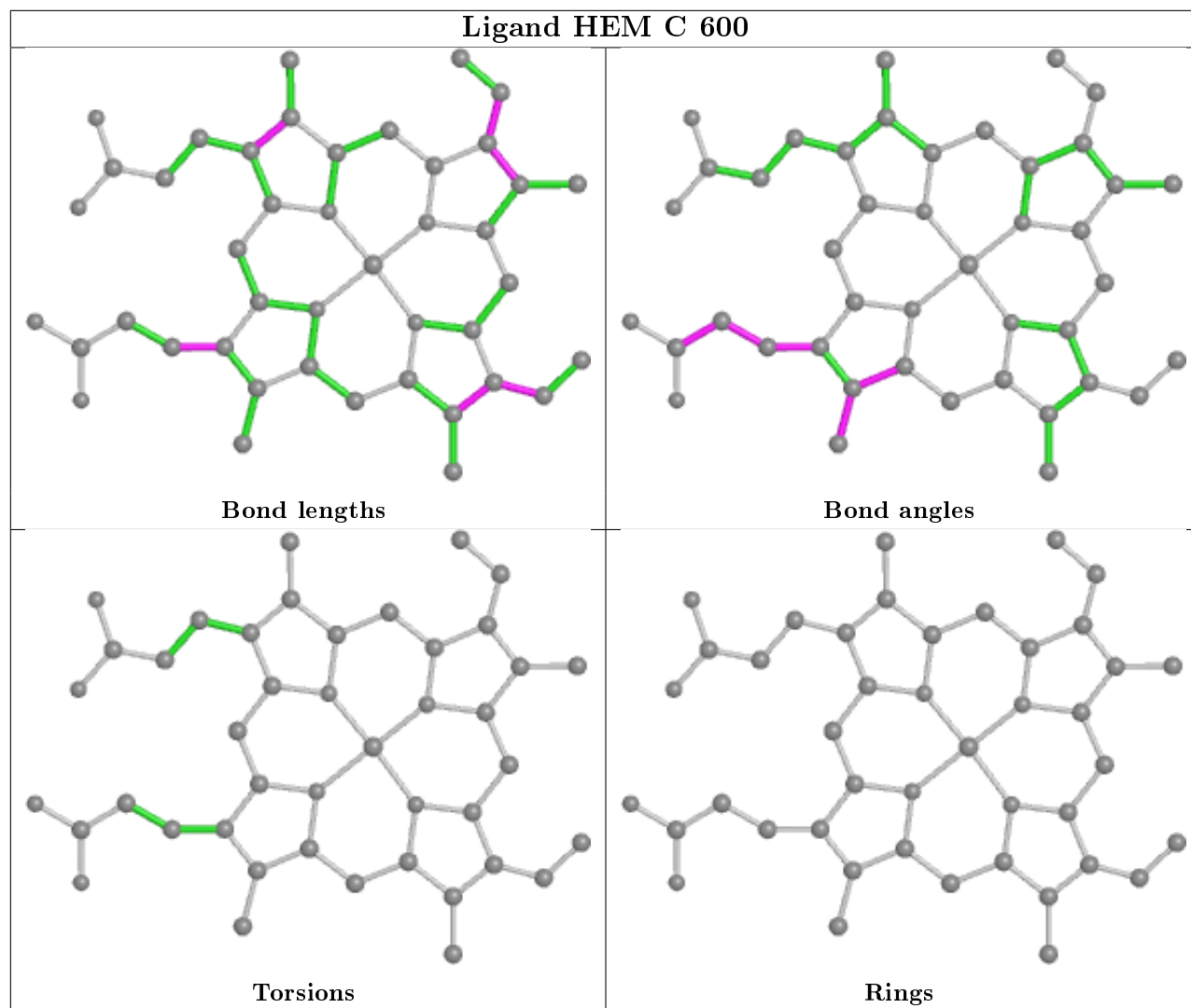
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	AER	4	0
2	B	600	HEM	4	0
2	C	600	HEM	2	0
2	D	600	HEM	2	0
3	D	601	AER	3	0
3	A	601	AER	2	0
2	A	600	HEM	2	0

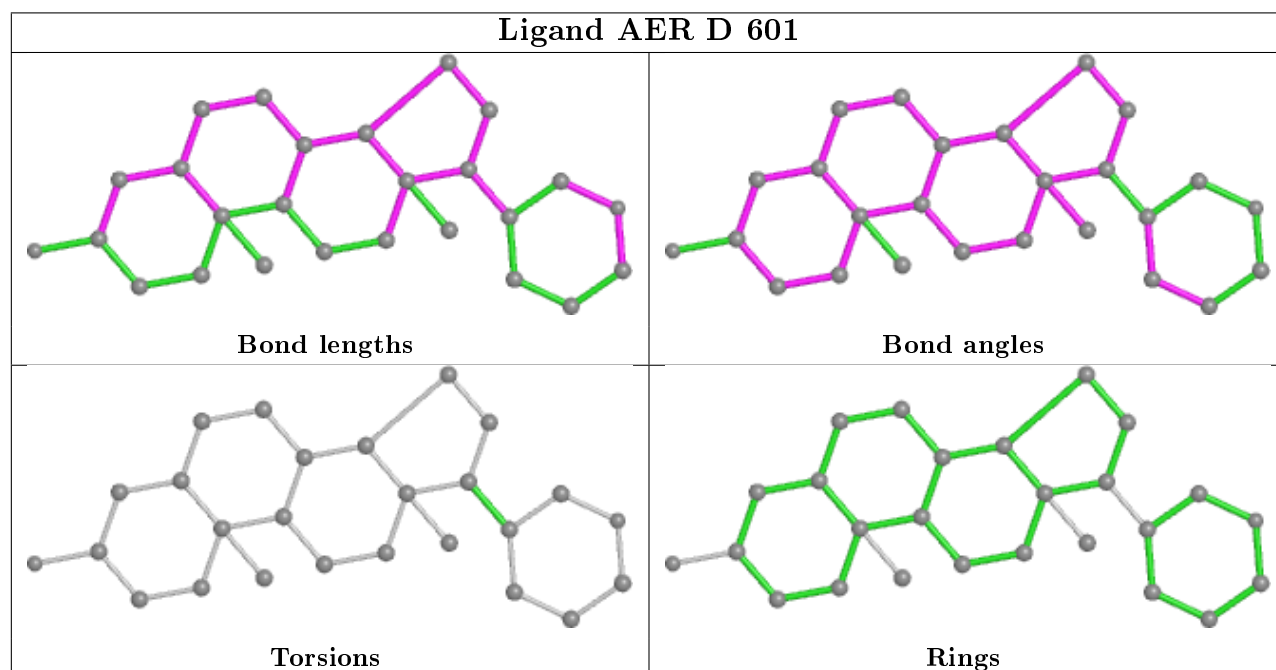
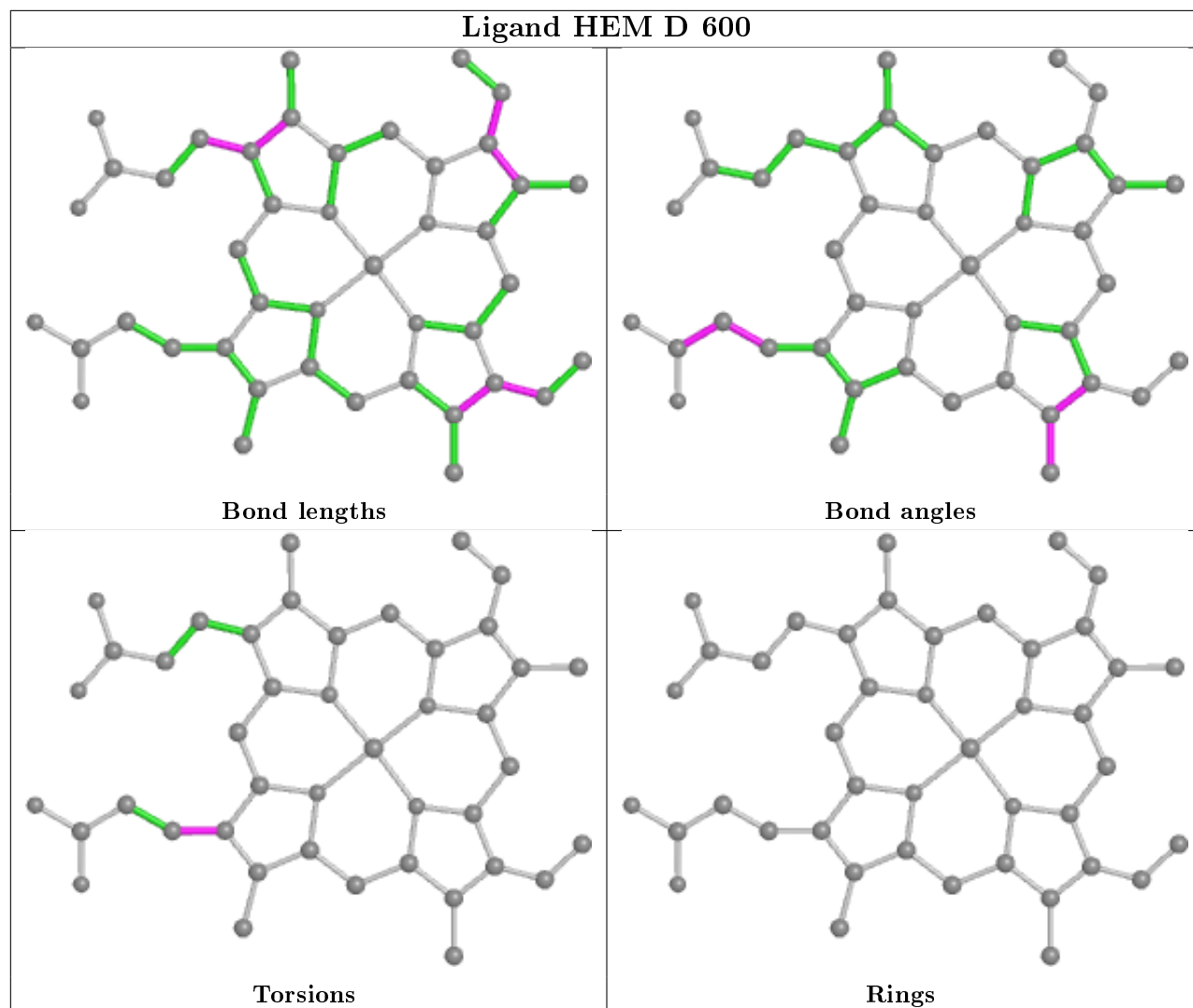
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

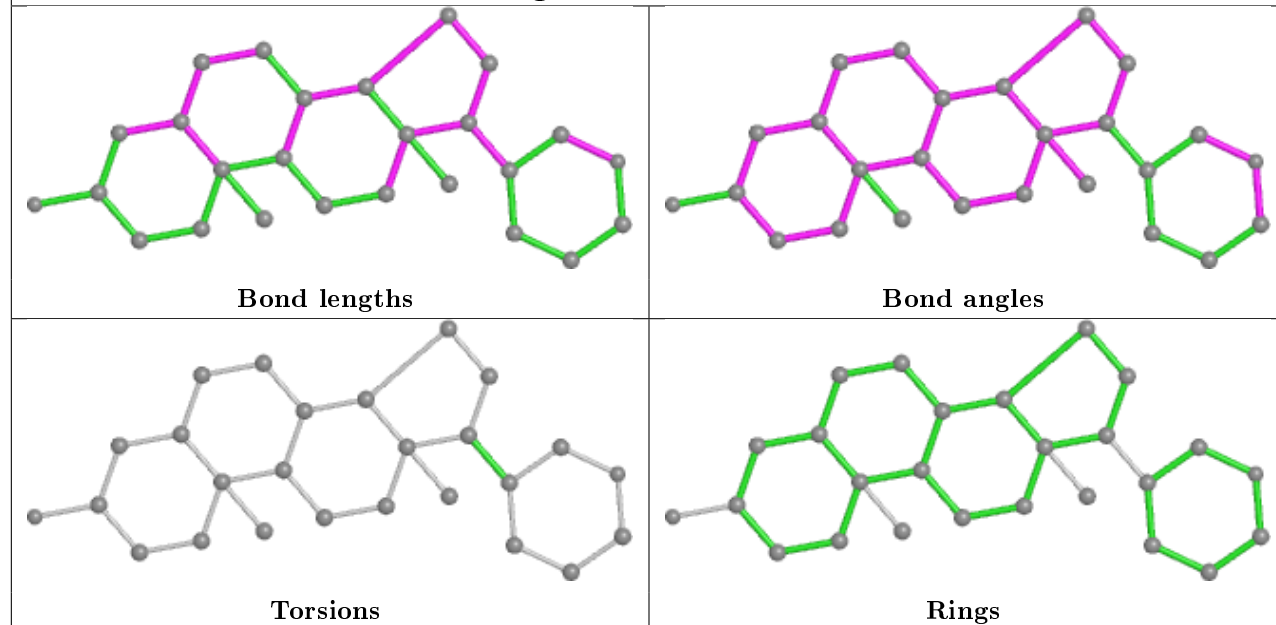




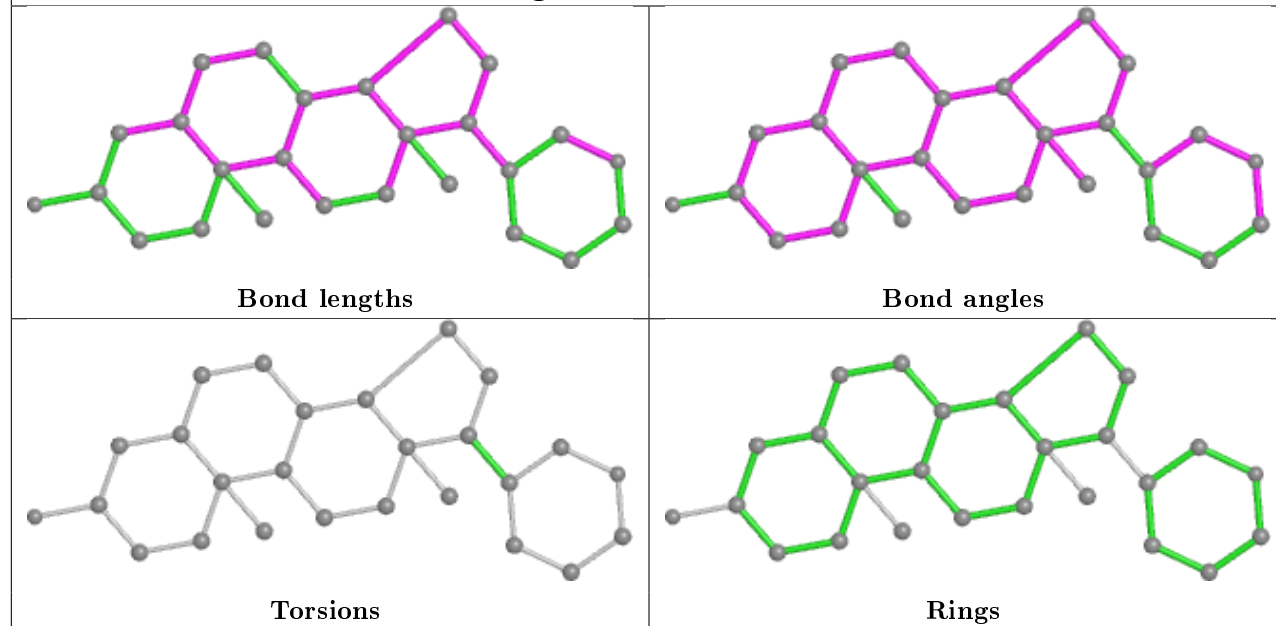


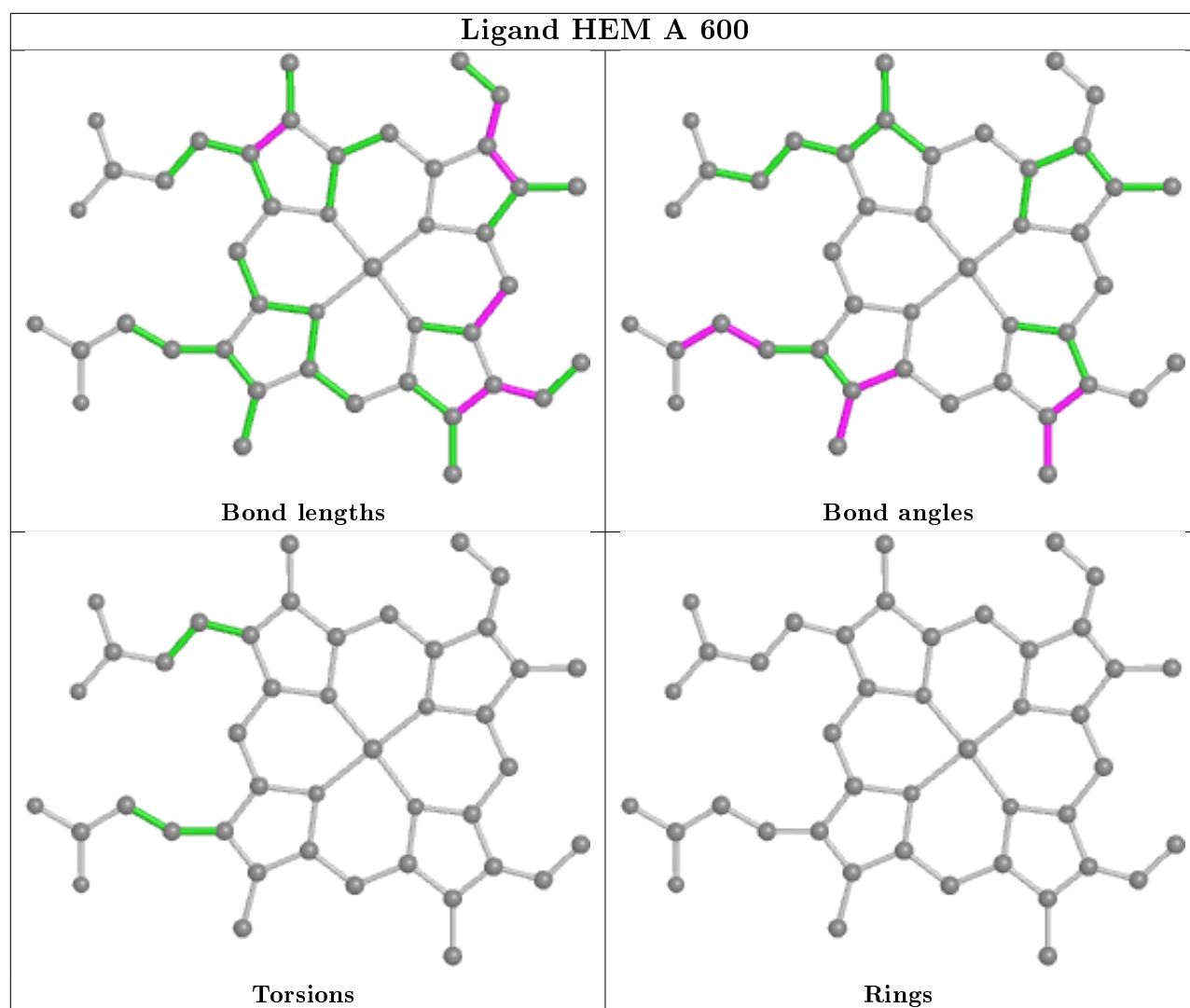


## Ligand AER C 601



## Ligand AER A 601





## 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%)	0.24	29 (6%) 20 17	38, 57, 94, 135	0
1	B	467/494 (94%)	0.12	16 (3%) 45 41	37, 56, 90, 121	0
1	C	471/494 (95%)	0.35	34 (7%) 15 12	37, 57, 99, 133	0
1	D	466/494 (94%)	0.51	47 (10%) 7 5	40, 68, 120, 150	0
All	All	1870/1976 (94%)	0.30	126 (6%) 17 15	37, 59, 108, 150	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLN	6.0
1	A	139	ASP	5.6
1	D	136	LYS	5.6
1	D	491	VAL	5.4
1	B	139	ASP	5.1
1	D	163	GLN	5.0
1	D	469	ASP	5.0
1	C	366	VAL	4.7
1	D	468	PRO	4.6
1	D	139	ASP	4.3
1	D	471	GLY	4.0
1	C	470	ASP	4.0
1	B	252	GLU	4.0
1	A	283	ASP	3.8
1	B	253	LYS	3.7
1	A	285	GLU	3.7
1	D	137	ASP	3.6
1	D	492	LYS	3.6
1	A	247	LEU	3.6
1	C	280	PRO	3.4
1	C	367	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	368	PRO	3.3
1	C	306	THR	3.3
1	A	302	ALA	3.3
1	D	161	ASN	3.2
1	C	140	GLN	3.2
1	D	465	LEU	3.2
1	A	271	MET	3.2
1	A	255	ARG	3.1
1	A	254	PHE	3.1
1	C	139	ASP	3.1
1	C	484	PHE	3.1
1	A	140	GLN	3.1
1	D	133	ALA	3.1
1	D	366	VAL	3.1
1	D	337	GLY	3.1
1	D	340	ARG	3.0
1	C	471	GLY	3.0
1	D	272	ASN	3.0
1	D	159	THR	3.0
1	A	249	ASN	3.0
1	D	158	ALA	2.9
1	D	306	THR	2.9
1	C	365	PRO	2.9
1	B	275	ASN	2.9
1	D	333	ASP	2.8
1	A	286	LEU	2.8
1	C	279	GLY	2.8
1	C	309	SER	2.8
1	B	140	GLN	2.8
1	C	308	THR	2.8
1	D	45	ARG	2.8
1	C	383	GLU	2.7
1	C	483	VAL	2.7
1	A	267	MET	2.7
1	A	284	SER	2.7
1	D	493	ILE	2.7
1	C	313	TRP	2.7
1	D	495	VAL	2.7
1	D	365	PRO	2.6
1	C	310	VAL	2.6
1	D	42	PHE	2.6
1	D	307	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	271	MET	2.6
1	B	255	ARG	2.6
1	B	257	ASP	2.6
1	B	340	ARG	2.6
1	A	137	ASP	2.5
1	D	138	GLY	2.5
1	C	137	ASP	2.5
1	C	138	GLY	2.5
1	C	136	LYS	2.5
1	A	287	LEU	2.5
1	D	499	TRP	2.5
1	C	45	ARG	2.5
1	D	140	GLN	2.4
1	D	134	LEU	2.4
1	C	305	GLU	2.4
1	A	256	SER	2.4
1	D	442	CYS	2.4
1	A	251	LYS	2.4
1	B	502	ALA	2.4
1	A	338	PHE	2.4
1	A	253	LYS	2.4
1	C	497	GLN	2.4
1	A	274	ASP	2.4
1	D	470	ASP	2.4
1	A	252	GLU	2.4
1	D	503	GLN	2.3
1	A	135	PHE	2.3
1	D	424	GLN	2.3
1	C	469	ASP	2.3
1	C	302	ALA	2.3
1	A	289	ASP	2.3
1	C	307	THR	2.3
1	B	271	MET	2.3
1	D	311	VAL	2.3
1	A	303	GLY	2.3
1	B	499	TRP	2.3
1	C	442	CYS	2.2
1	D	310	VAL	2.2
1	C	134	LEU	2.2
1	C	482	VAL	2.2
1	C	341	THR	2.2
1	A	501	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	165	ILE	2.2
1	D	367	ALA	2.2
1	D	339	SER	2.2
1	A	307	THR	2.2
1	C	281	ASP	2.2
1	B	303	GLY	2.1
1	B	304	VAL	2.1
1	D	419	ASN	2.1
1	D	144	LYS	2.1
1	C	472	GLN	2.1
1	D	418	LEU	2.1
1	B	248	GLU	2.1
1	C	369	MET	2.1
1	A	367	ALA	2.1
1	D	254	PHE	2.1
1	B	138	GLY	2.0
1	D	436	GLY	2.0
1	D	58	LYS	2.0
1	D	500	ARG	2.0
1	B	301	GLY	2.0
1	A	497	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

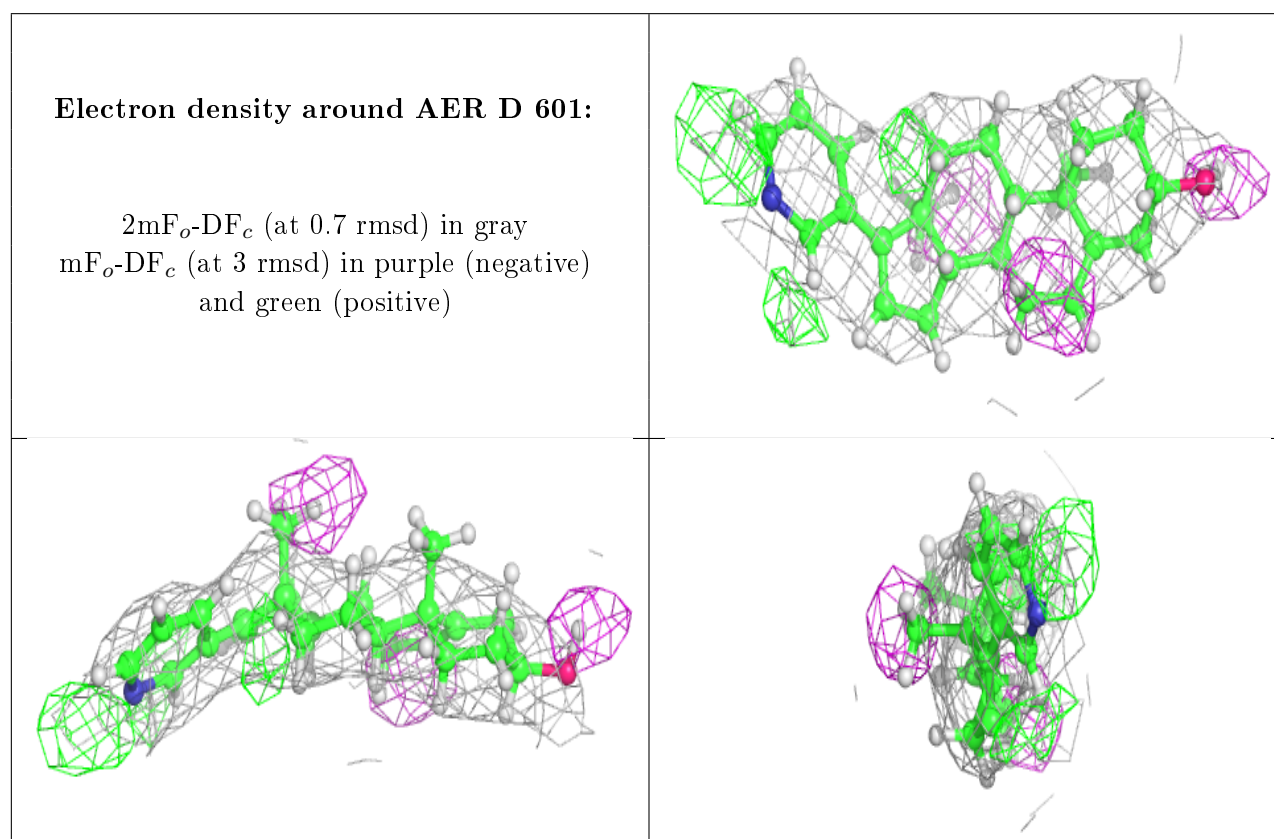
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AER	D	601	26/26	0.86	0.27	23,39,48,55	0
3	AER	B	601	26/26	0.93	0.22	24,37,49,56	0

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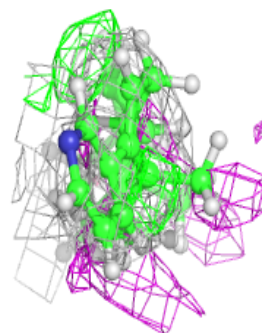
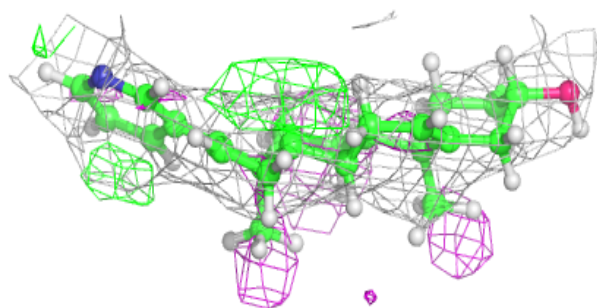
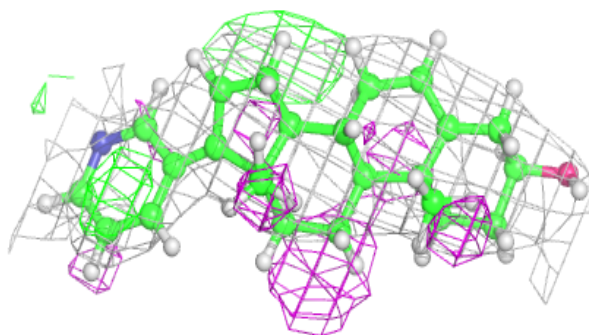
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AER	C	601	26/26	0.93	0.27	24,33,44,47	0
3	AER	A	601	26/26	0.95	0.23	23,35,45,50	0
2	HEM	B	600	43/43	0.98	0.28	31,46,57,67	0
2	HEM	C	600	43/43	0.98	0.33	33,47,60,70	0
2	HEM	D	600	43/43	0.98	0.33	38,54,72,81	0
2	HEM	A	600	43/43	0.98	0.34	32,51,69,76	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.

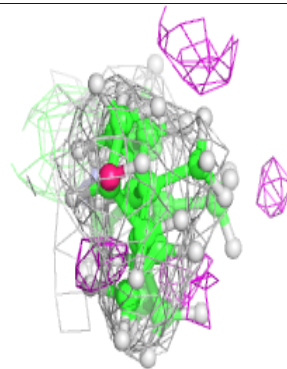
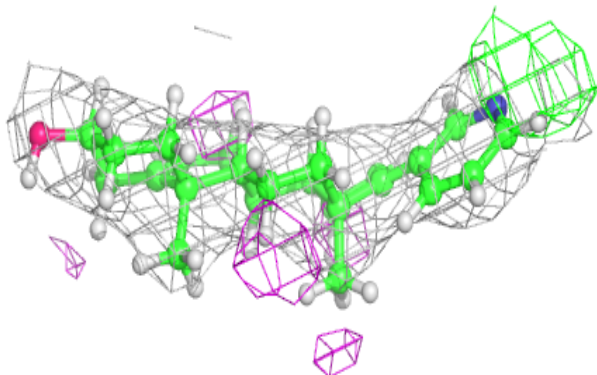
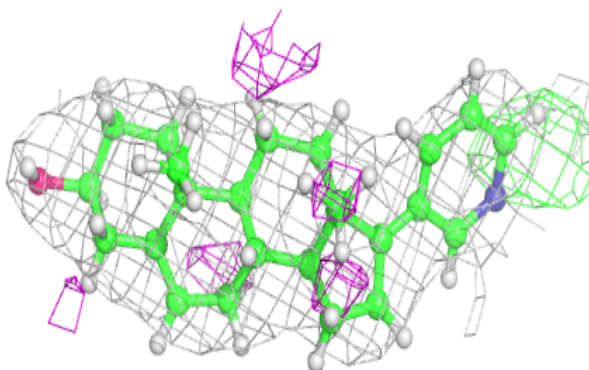


**Electron density around AER B 601:**

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

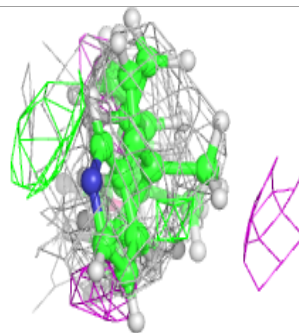
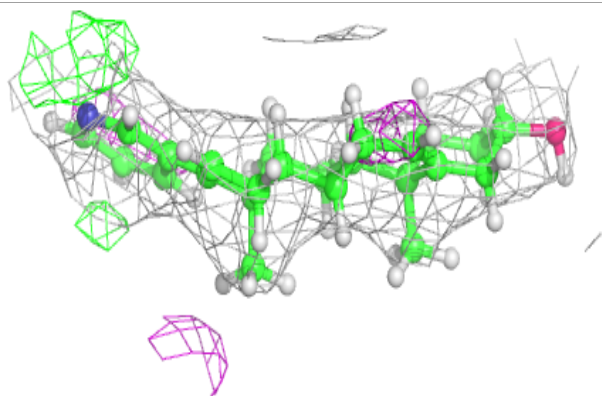
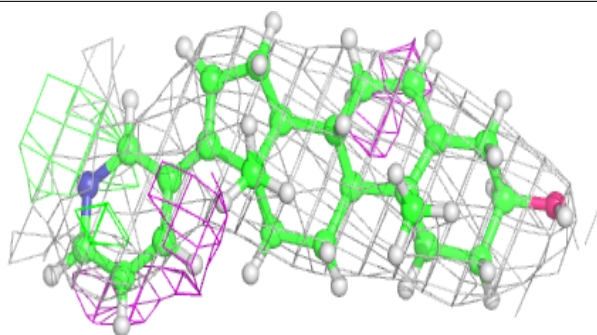
**Electron density around AER C 601:**

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

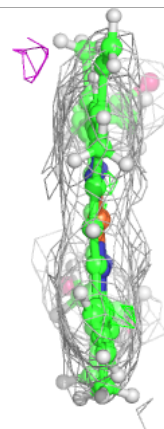
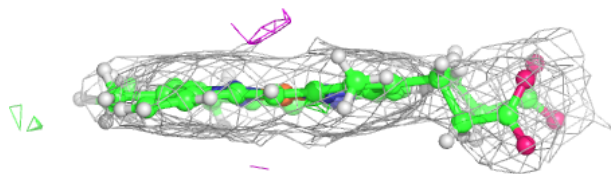
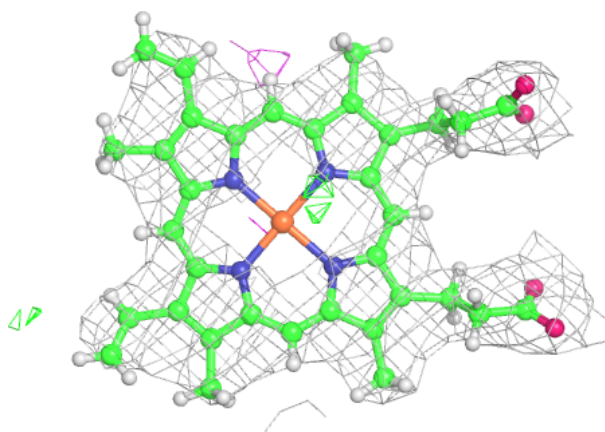


**Electron density around AER A 601:**

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

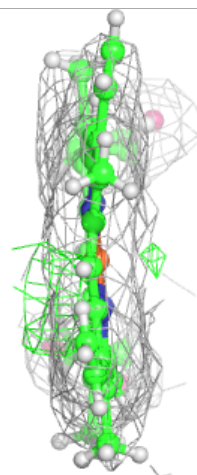
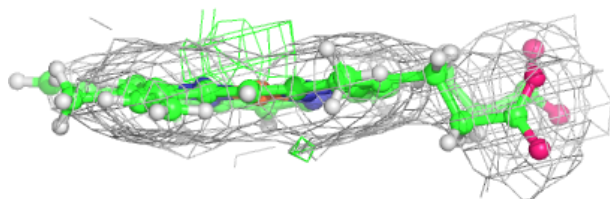
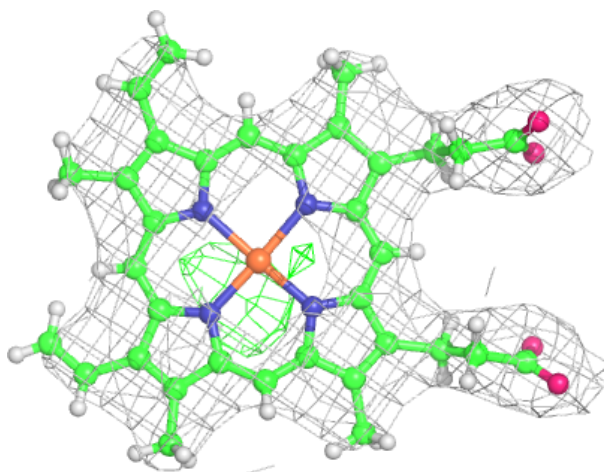
**Electron density around HEM B 600:**

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



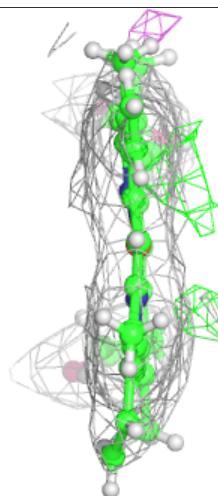
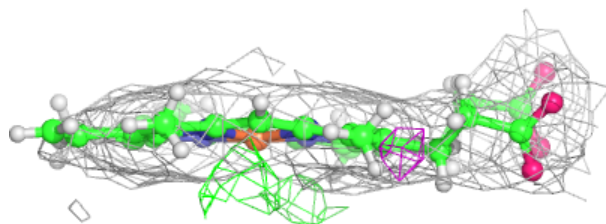
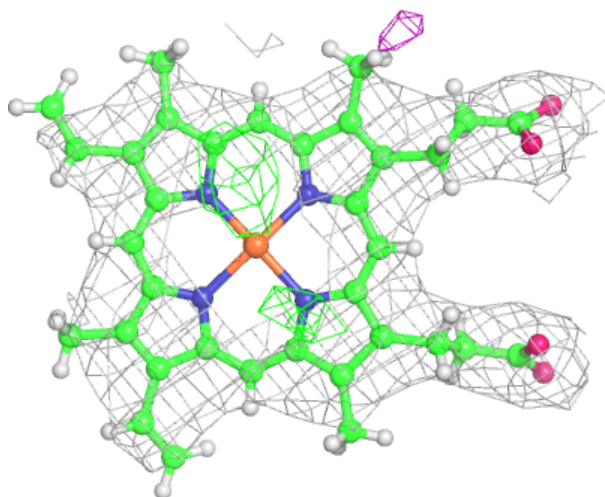
**Electron density around HEM C 600:**

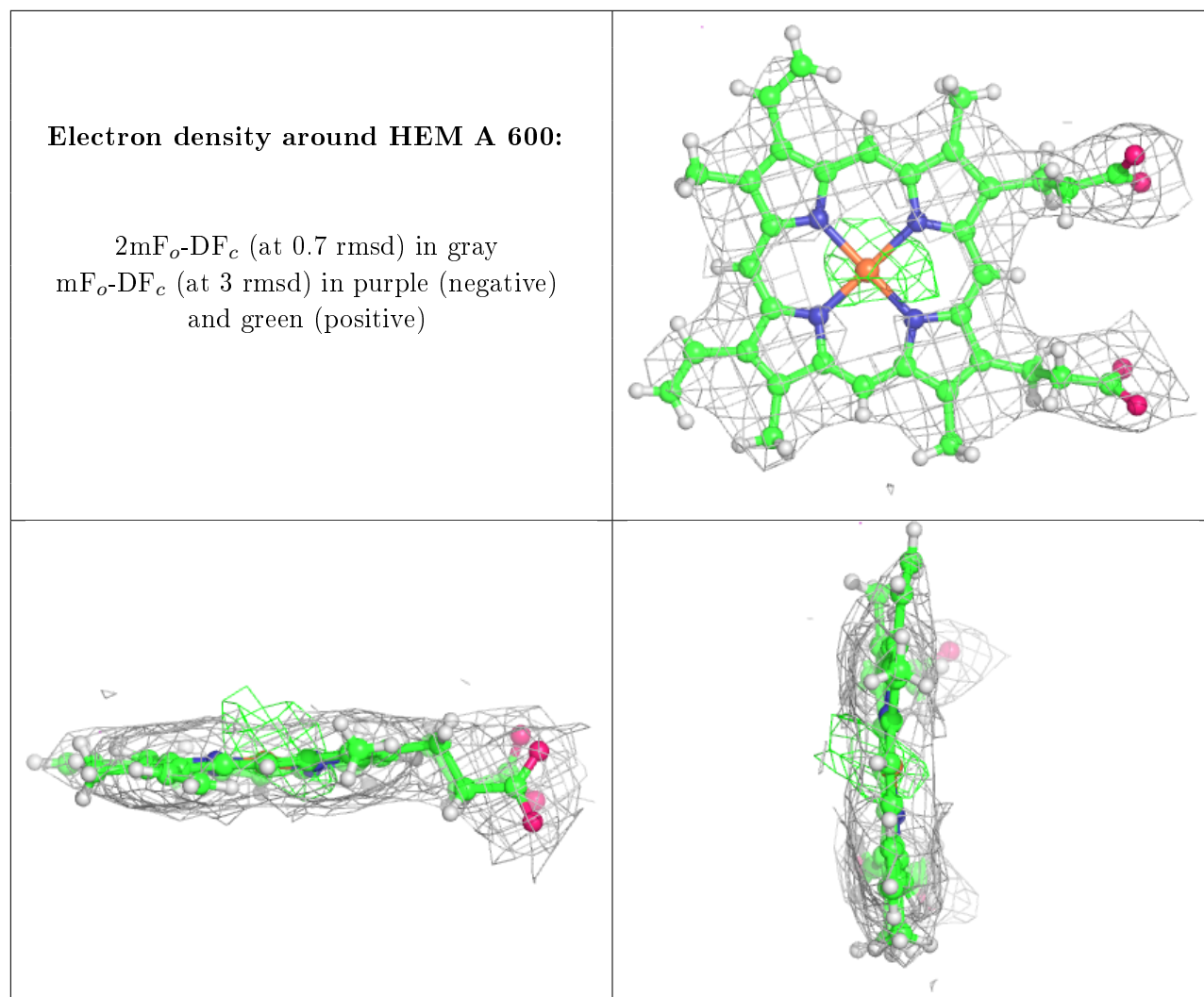
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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 ⓘ

There are no such residues in this entry.