



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:25 pm BST

PDB ID : 4R1Z  
Title : Zebra fish cytochrome P450 17A1 with Abiraterone  
Authors : Pallan, P.S.; Egli, M.  
Deposited on : 2014-08-08  
Resolution : 3.30 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.

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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

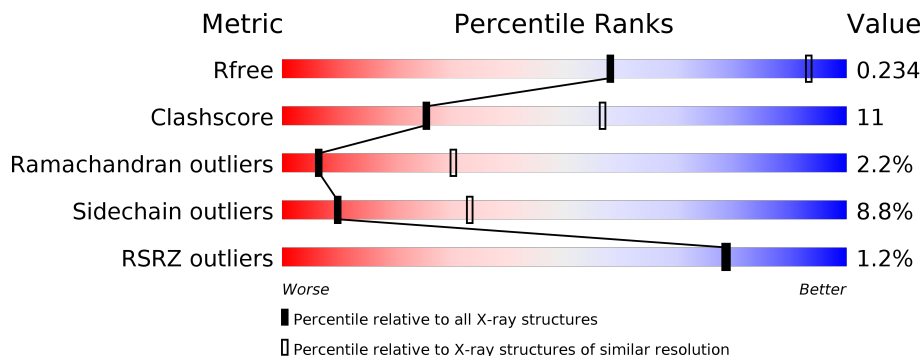
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	439	 % 71% 21% •• 5%
1	B	439	 2% 70% 18% 5% 6%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cyp17a1 protein.

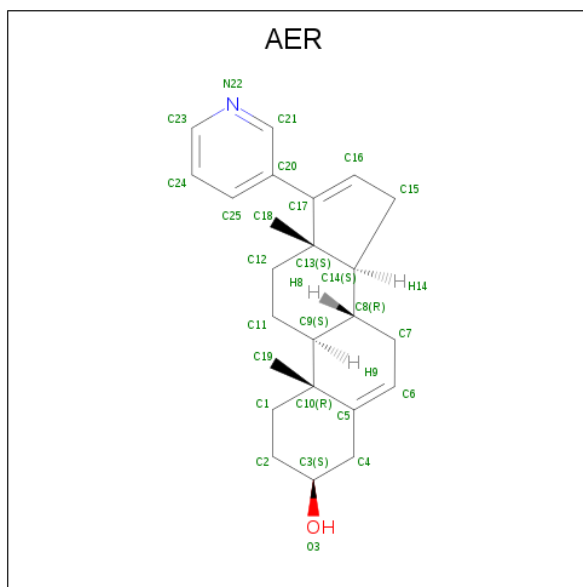
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	Total	C	N	O	S	4	0	0
			3310	2105	581	608	16			
1	B	411	Total	C	N	O	S	0	1	0
			3256	2068	571	601	16			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	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	N	O	0	0
			26	24	1	1		
3	B	1	Total	C	N	O	0	0
			26	24	1	1		

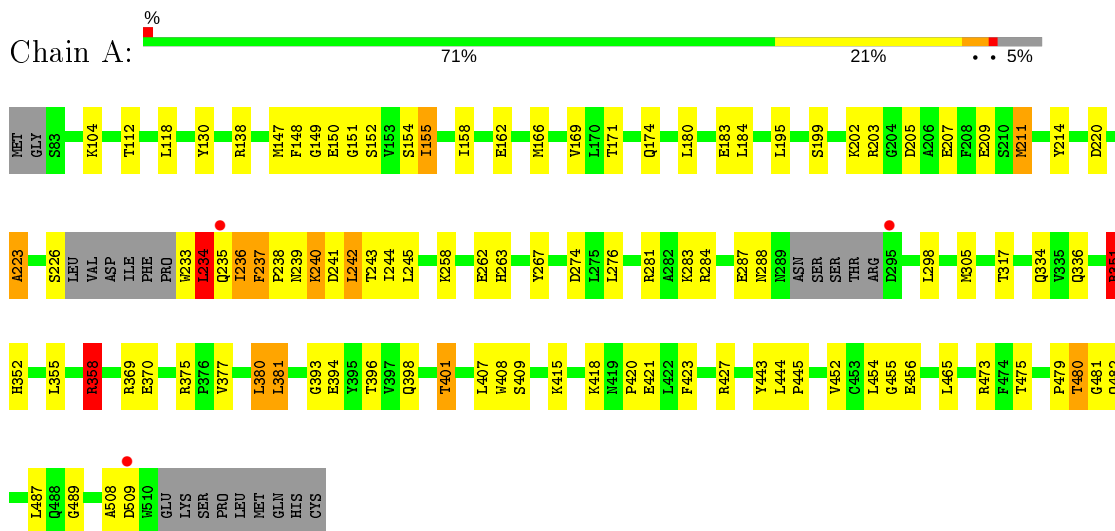
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	3	Total	O	0	0
			3	3		

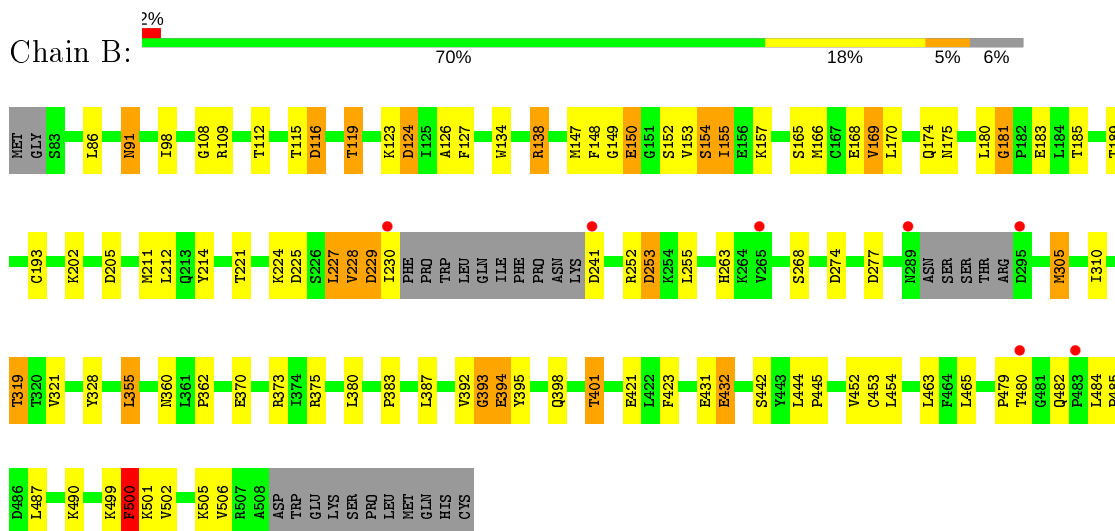
### 3 Residue-property plots [i](#)

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: Cyp17a1 protein



- Molecule 1: Cyp17a1 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.63Å 136.63Å 135.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 3.30 28.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.00-3.30) 100.0 (28.90-3.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.31 (at 3.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.168 , 0.238 0.166 , 0.234	Depositor DCC
$R_{free}$ test set	1682 reflections (7.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.9	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	0.69	0/3376	0.88	2/4562 (0.0%)
1	B	0.54	0/3317	0.79	0/4480
All	All	0.62	0/6693	0.84	2/9042 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	358	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	351	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	499	LYS	Peptide
1	B	500[B]	PHE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3310	0	3349	61	0
1	B	3256	0	3303	75	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	26	0	31	3	0
3	B	26	0	31	1	0
4	A	12	0	0	0	1
4	B	3	0	0	0	1
All	All	6719	0	6774	143	1

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 11.

All (143) 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:A:398:GLN:O	1:A:401:THR:HG22	1.56	1.05
1:B:112:THR:O	1:B:116:ASP:HB2	1.69	0.91
1:B:500[A]:PHE:HD1	1:B:500[A]:PHE:H	1.23	0.86
1:B:185:THR:HG22	1:B:319:THR:HG21	1.65	0.78
1:A:334:GLN:N	1:A:334:GLN:OE1	2.21	0.74
1:B:227:LEU:HB3	1:B:228:VAL:HG22	1.70	0.73
2:B:600:HEM:HHC	2:B:600:HEM:HBB2	1.70	0.73
1:A:138:ARG:NH2	1:A:452:VAL:O	2.19	0.69
1:B:370:GLU:OE2	1:B:373:ARG:NH1	2.25	0.69
1:A:240:LYS:HG2	1:A:241:ASP:HA	1.75	0.68
1:A:237:PHE:O	1:A:239:ASN:ND2	2.26	0.67
1:B:398:GLN:O	1:B:401:THR:HG23	1.95	0.66
1:B:500[A]:PHE:N	1:B:500[A]:PHE:CD1	2.64	0.66
1:B:112:THR:HG21	1:B:224:LYS:HG2	1.78	0.66
1:B:108:GLY:HA3	1:B:387:LEU:HD21	1.80	0.62
2:A:600:HEM:HHC	2:A:600:HEM:HBB2	1.82	0.62
1:A:171:THR:O	1:A:174:GLN:HB2	1.99	0.61
1:A:233:TRP:CZ3	1:A:235:GLN:HA	2.36	0.60
1:A:263:HIS:HE1	1:A:274:ASP:OD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:O	1:B:124:ASP:OD1	2.20	0.60
1:A:148:PHE:CE1	1:A:158:ILE:HD11	2.36	0.60
1:A:211:MET:HA	1:A:214:TYR:CE2	2.37	0.59
1:A:375:ARG:NH1	1:A:487:LEU:O	2.37	0.58
1:A:180:LEU:O	1:A:184:LEU:HB2	2.04	0.56
1:B:115:THR:O	1:B:119:THR:HG22	2.05	0.56
1:B:91:ASN:OD1	1:B:91:ASN:C	2.44	0.56
1:B:211:MET:HA	1:B:214:TYR:CE2	2.41	0.56
1:B:263:HIS:HE1	1:B:274:ASP:OD2	1.87	0.56
1:A:148:PHE:HE1	1:A:158:ILE:HD11	1.69	0.56
1:A:258:LYS:O	1:A:262:GLU:HG3	2.06	0.56
1:A:169:VAL:HG11	1:A:183:GLU:HG2	1.88	0.55
1:B:112:THR:HG21	1:B:224:LYS:CG	2.36	0.55
1:A:118:LEU:O	1:A:305:MET:HE1	2.07	0.55
1:B:431:GLU:O	1:B:432:GLU:HB2	2.07	0.55
1:B:224:LYS:HG3	1:B:225:ASP:HA	1.88	0.55
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.72	0.54
1:B:370:GLU:OE1	1:B:370:GLU:HA	2.06	0.54
1:B:112:THR:O	1:B:116:ASP:CB	2.49	0.54
1:B:147:MET:O	1:B:149:GLY:HA3	2.07	0.54
1:B:138:ARG:HG2	1:B:454:LEU:HD13	1.90	0.54
1:B:485:PRO:HB3	1:B:500[A]:PHE:HB3	1.90	0.54
1:A:235:GLN:C	1:A:236:ILE:HG12	2.28	0.53
1:B:355:LEU:HD13	1:B:465:LEU:HD11	1.90	0.52
1:B:112:THR:CG2	1:B:224:LYS:HG2	2.40	0.52
1:B:310:ILE:HG23	2:B:600:HEM:HBC1	1.92	0.51
1:A:420:PRO:O	1:A:421:GLU:CB	2.57	0.51
1:B:115:THR:OG1	1:B:116:ASP:N	2.44	0.51
1:B:392:VAL:O	1:B:393:GLY:O	2.28	0.51
1:B:230:ILE:HG22	1:B:230:ILE:O	2.11	0.50
1:A:240:LYS:CG	1:A:241:ASP:HA	2.41	0.50
1:B:360:ASN:C	1:B:362:PRO:HD3	2.32	0.50
1:B:174:GLN:NE2	1:B:506:VAL:HG23	2.26	0.50
1:B:431:GLU:O	1:B:432:GLU:CB	2.59	0.50
1:B:227:LEU:HA	1:B:228:VAL:HG13	1.94	0.50
1:B:109:ARG:HD2	1:B:126:ALA:O	2.12	0.50
1:A:138:ARG:HG2	1:A:454:LEU:HD13	1.93	0.49
1:A:380:LEU:C	1:A:381:LEU:O	2.48	0.49
1:B:153:VAL:H	1:B:154:SER:HA	1.76	0.49
1:A:237:PHE:O	1:A:239:ASN:N	2.44	0.49
1:B:147:MET:C	1:B:149:GLY:HA3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:MET:HA	1:B:169:VAL:HG12	1.94	0.49
1:B:252:ARG:O	1:B:255:LEU:N	2.46	0.49
1:B:375:ARG:NH2	1:B:421:GLU:OE2	2.45	0.49
1:A:479:PRO:O	1:A:481:GLY:N	2.46	0.49
1:B:175:ASN:OD1	1:B:505:LYS:HB3	2.12	0.48
1:A:147:MET:O	1:A:149:GLY:HA3	2.12	0.48
1:A:205:ASP:OD1	1:A:207:GLU:N	2.44	0.48
1:B:252:ARG:O	1:B:253:ASP:C	2.52	0.48
1:A:205:ASP:OD1	1:A:205:ASP:C	2.51	0.48
1:A:211:MET:HA	1:A:214:TYR:CD2	2.49	0.48
1:B:124:ASP:OD1	1:B:124:ASP:C	2.52	0.48
1:A:351:ARG:HG3	1:A:352:HIS:N	2.28	0.47
1:B:109:ARG:NH1	1:B:383:PRO:O	2.46	0.47
1:A:171:THR:O	1:A:174:GLN:CB	2.61	0.47
1:B:98:ILE:HD11	1:B:392:VAL:HG21	1.96	0.47
1:A:267:TYR:CE2	1:A:284:ARG:NH2	2.83	0.47
1:A:370:GLU:HG3	1:A:423:PHE:CE1	2.50	0.47
1:A:443:TYR:CZ	1:A:445:PRO:HG3	2.50	0.46
1:B:180:LEU:O	1:B:181:GLY:C	2.53	0.46
1:A:355:LEU:HG	1:A:358:ARG:HH11	1.80	0.46
1:A:415:LYS:HE3	1:A:415:LYS:HA	1.98	0.46
1:B:109:ARG:HD2	1:B:127:PHE:HA	1.97	0.46
1:B:214:TYR:CE1	1:B:252:ARG:HB2	2.50	0.46
1:B:305:MET:HA	1:B:305:MET:CE	2.45	0.46
1:B:165:SER:O	1:B:168:GLU:HG2	2.15	0.46
1:B:229:ASP:HA	1:B:230:ILE:HA	1.69	0.46
2:B:600:HEM:HBC2	2:B:600:HEM:HHD	1.97	0.46
2:A:600:HEM:C1B	3:A:601:AER:H23	2.51	0.46
1:A:239:ASN:HB3	1:A:240:LYS:HB3	1.99	0.45
1:B:214:TYR:OH	1:B:252:ARG:HG3	2.16	0.45
1:B:189:THR:O	1:B:193:CYS:N	2.46	0.45
1:B:321:VAL:HG11	1:B:463:LEU:HD11	1.99	0.45
1:B:214:TYR:CZ	1:B:252:ARG:HG3	2.52	0.45
1:A:408:TRP:C	1:A:408:TRP:CD1	2.90	0.45
2:A:600:HEM:HHD	2:A:600:HEM:HBC2	1.98	0.45
1:B:370:GLU:HG3	1:B:423:PHE:CD2	2.52	0.45
1:B:328:TYR:CZ	1:B:487:LEU:HD13	2.52	0.45
1:A:317:THR:HG21	3:A:601:AER:C23	2.46	0.45
1:A:284:ARG:O	1:A:287:GLU:HB3	2.17	0.44
1:A:150:GLU:HG3	1:A:151:GLY:HA2	1.98	0.44
1:B:392:VAL:O	1:B:393:GLY:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:CD1	1:A:148:PHE:C	2.90	0.44
1:A:150:GLU:CG	1:A:151:GLY:HA2	2.47	0.44
1:B:134:TRP:CZ2	1:B:138:ARG:HD2	2.52	0.44
1:B:444:LEU:O	1:B:445:PRO:C	2.56	0.44
1:A:155:ILE:HA	1:A:158:ILE:HD12	2.00	0.44
1:A:220:ASP:O	1:A:223:ALA:HB3	2.18	0.44
1:A:427:ARG:HG2	1:A:427:ARG:HH11	1.83	0.44
1:B:224:LYS:CG	1:B:225:ASP:HA	2.48	0.44
1:B:484:LEU:H	1:B:484:LEU:HD12	1.83	0.44
1:A:358:ARG:NH1	1:A:358:ARG:HG3	2.32	0.43
1:A:104:LYS:HE2	1:A:130:TYR:OH	2.18	0.43
1:A:480:THR:HG23	1:A:481:GLY:H	1.84	0.43
1:B:148:PHE:O	1:B:148:PHE:CD2	2.71	0.43
1:B:123:LYS:O	1:B:124:ASP:CB	2.67	0.43
1:A:162:GLU:HA	1:A:162:GLU:OE1	2.19	0.42
1:A:283:LYS:HG3	1:A:298:LEU:O	2.19	0.42
1:A:148:PHE:CE1	1:A:158:ILE:CD1	3.02	0.42
1:B:152:SER:HA	1:B:153:VAL:HA	1.83	0.42
1:B:479:PRO:HB2	1:B:482:GLN:HG3	2.00	0.42
1:A:240:LYS:CB	1:A:241:ASP:HA	2.50	0.42
1:A:381:LEU:HD21	1:A:407:LEU:HD13	2.02	0.41
2:A:600:HEM:C1D	3:A:601:AER:H21	2.55	0.41
1:A:205:ASP:O	1:A:209:GLU:HG2	2.21	0.41
1:A:455:GLY:O	1:A:456:GLU:C	2.56	0.41
1:B:180:LEU:HD13	1:B:502:VAL:HG22	2.00	0.41
2:B:600:HEM:ND	3:B:601:AER:H21	2.36	0.41
1:A:355:LEU:HD13	1:A:465:LEU:HD11	2.02	0.41
1:B:149:GLY:HA2	1:B:150:GLU:HA	1.68	0.41
1:B:166:MET:O	1:B:169:VAL:HG13	2.21	0.41
1:B:109:ARG:CD	1:B:126:ALA:O	2.69	0.41
1:B:452:VAL:HG22	1:B:453:CYS:N	2.36	0.41
1:B:153:VAL:N	1:B:154:SER:HA	2.35	0.41
1:B:181:GLY:O	1:B:185:THR:HG23	2.20	0.41
1:A:287:GLU:OE1	1:A:288:ASN:OD1	2.39	0.41
1:B:370:GLU:OE1	1:B:373:ARG:HD3	2.21	0.41
1:A:234:LEU:HG	1:A:234:LEU:O	2.21	0.40
1:B:394:GLU:HG2	1:B:395:TYR:N	2.36	0.40
1:B:202:LYS:O	1:B:205:ASP:HB2	2.21	0.40
1:A:169:VAL:HG22	1:A:203:ARG:NH2	2.36	0.40
1:A:242:LEU:C	1:A:242:LEU:HD23	2.42	0.40
1:B:149:GLY:N	1:B:152:SER:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:O	1:A:421:GLU:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:708:HOH:O	4:B:701:HOH:O[5_665]	2.17	0.03

## 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	411/439 (94%)	370 (90%)	32 (8%)	9 (2%)	6	30
1	B	406/439 (92%)	358 (88%)	38 (9%)	10 (2%)	5	27
All	All	817/878 (93%)	728 (89%)	70 (9%)	19 (2%)	6	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	A	480	THR
1	A	223	ALA
1	A	393	GLY
1	B	181	GLY
1	B	393	GLY
1	B	432	GLU
1	B	501	LYS
1	A	238	PRO
1	A	381	LEU
1	B	155	ILE
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	253	ASP
1	B	500[A]	PHE
1	B	500[B]	PHE
1	A	489	GLY
1	A	394	GLU
1	B	116	ASP
1	A	508	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/388 (95%)	332 (90%)	35 (10%)	8	29
1	B	362/388 (93%)	332 (92%)	30 (8%)	11	36
All	All	729/776 (94%)	664 (91%)	65 (9%)	10	32

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	152	SER
1	A	154	SER
1	A	155	ILE
1	A	166	MET
1	A	195	LEU
1	A	199	SER
1	A	202	LYS
1	A	211	MET
1	A	226	SER
1	A	234	LEU
1	A	236	ILE
1	A	237	PHE
1	A	240	LYS
1	A	242	LEU
1	A	243	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	244	ILE
1	A	245	LEU
1	A	276	LEU
1	A	281	ARG
1	A	336	GLN
1	A	351	ARG
1	A	358	ARG
1	A	369	ARG
1	A	377	VAL
1	A	380	LEU
1	A	396	THR
1	A	401	THR
1	A	409	SER
1	A	418	LYS
1	A	444	LEU
1	A	473	ARG
1	A	475	THR
1	A	482	GLN
1	A	509	ASP
1	B	86	LEU
1	B	91	ASN
1	B	119	THR
1	B	124	ASP
1	B	138	ARG
1	B	150	GLU
1	B	154	SER
1	B	155	ILE
1	B	157	LYS
1	B	169	VAL
1	B	170	LEU
1	B	183	GLU
1	B	212	LEU
1	B	221	THR
1	B	227	LEU
1	B	228	VAL
1	B	241	ASP
1	B	268	SER
1	B	277	ASP
1	B	305	MET
1	B	319	THR
1	B	355	LEU
1	B	380	LEU

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Mol	Chain	Res	Type
1	B	394	GLU
1	B	401	THR
1	B	442	SER
1	B	480	THR
1	B	490	LYS
1	B	500[A]	PHE
1	B	500[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	239	ASN
1	A	263	HIS
1	A	270	ASN
1	B	93	HIS
1	B	174	GLN
1	B	263	HIS
1	B	272	GLN
1	B	289	ASN
1	B	354	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	600	1,3	27,50,50	1.24	2 (7%)	17,82,82	1.17	2 (11%)
3	AER	B	601	2	30,30,30	2.36	2 (6%)	44,47,47	2.42	14 (31%)
3	AER	A	601	2	30,30,30	2.37	3 (10%)	44,47,47	2.22	9 (20%)
2	HEM	A	600	1,3	27,50,50	1.32	2 (7%)	17,82,82	1.40	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
2	HEM	B	600	1,3	-	0/6/54/54	-
3	AER	B	601	2	-	1/4/62/62	0/5/5/5
3	AER	A	601	2	-	2/4/62/62	0/5/5/5
2	HEM	A	600	1,3	-	0/6/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	AER	C16-C17	12.09	1.55	1.33
3	A	601	AER	C16-C17	11.93	1.54	1.33
2	B	600	HEM	C3B-C2B	-4.43	1.34	1.40
2	A	600	HEM	C3B-C2B	-4.34	1.34	1.40
2	A	600	HEM	C3C-C2C	-2.52	1.36	1.40
2	B	600	HEM	C3C-C2C	-2.36	1.37	1.40
3	B	601	AER	C20-C17	2.24	1.51	1.48
3	A	601	AER	C13-C14	-2.17	1.50	1.54
3	A	601	AER	C12-C13	-2.04	1.50	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	AER	C15-C16-C17	-9.72	104.88	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AER	C15-C16-C17	-8.55	105.84	112.87
3	B	601	AER	C20-C17-C16	-6.76	115.92	125.19
3	A	601	AER	C20-C17-C16	-5.49	117.65	125.19
3	B	601	AER	C14-C13-C17	5.00	103.96	99.70
3	A	601	AER	C14-C13-C17	4.90	103.88	99.70
3	B	601	AER	C15-C14-C13	3.95	107.00	104.05
3	A	601	AER	C15-C14-C8	-3.74	117.08	121.57
3	B	601	AER	C13-C17-C16	-3.47	105.50	109.72
3	B	601	AER	C7-C8-C9	3.26	113.66	109.71
3	B	601	AER	C4-C5-C6	-3.00	116.28	120.61
3	A	601	AER	C13-C17-C16	-2.95	106.13	109.72
2	A	600	HEM	C4A-C3A-C2A	2.74	108.91	107.00
3	B	601	AER	C15-C14-C8	-2.74	118.28	121.57
3	B	601	AER	C4-C5-C10	2.67	119.96	116.42
3	B	601	AER	C14-C8-C9	-2.63	105.57	109.09
2	A	600	HEM	C3C-C4C-NC	-2.62	106.01	110.94
2	B	600	HEM	C4A-C3A-C2A	2.58	108.79	107.00
2	B	600	HEM	C3C-C4C-NC	-2.49	106.24	110.94
2	A	600	HEM	C4C-C3C-C2C	2.44	108.60	106.90
3	B	601	AER	C18-C13-C12	-2.42	108.28	111.13
3	A	601	AER	C18-C13-C17	-2.40	102.94	108.00
3	B	601	AER	C23-N22-C21	2.28	120.78	116.85
3	B	601	AER	C12-C11-C9	2.24	117.00	113.11
3	A	601	AER	C14-C8-C9	-2.23	106.10	109.09
3	A	601	AER	C12-C13-C14	-2.20	105.52	108.99
3	B	601	AER	C12-C13-C14	-2.15	105.60	108.99
3	A	601	AER	C4-C5-C10	2.13	119.25	116.42

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	AER	C13-C17-C20-C25
3	A	601	AER	C13-C17-C20-C21
3	B	601	AER	C13-C17-C20-C25

There are no ring outliers.

4 monomers are involved in 9 short contacts:

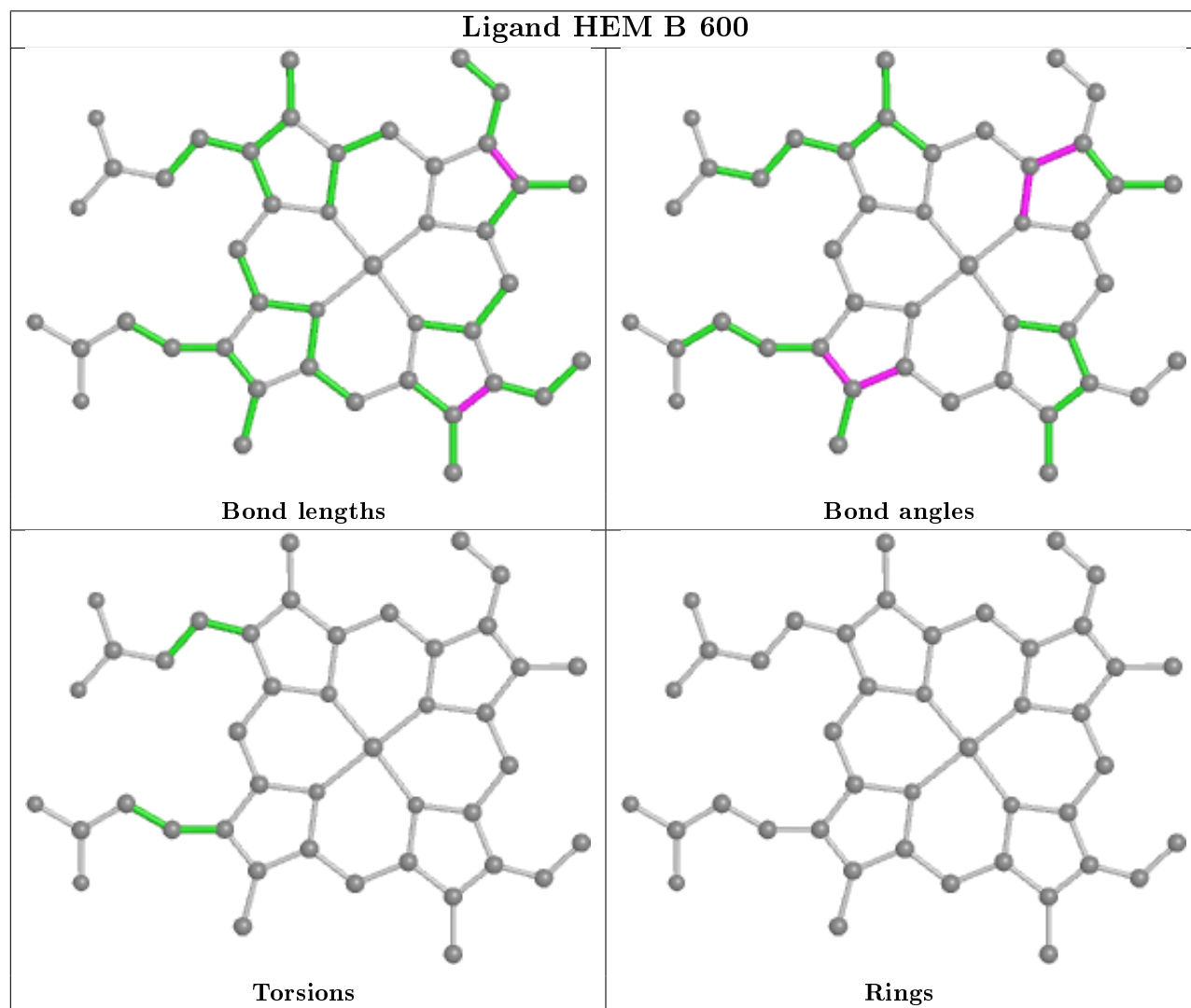
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	4	0

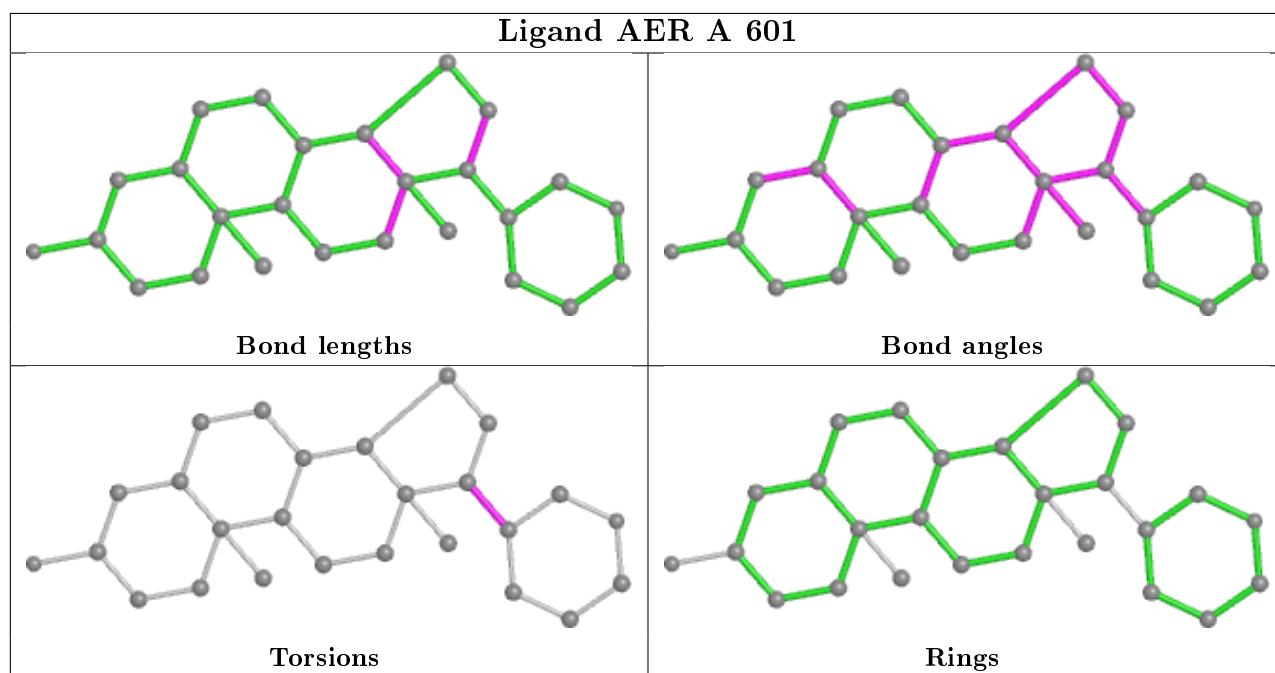
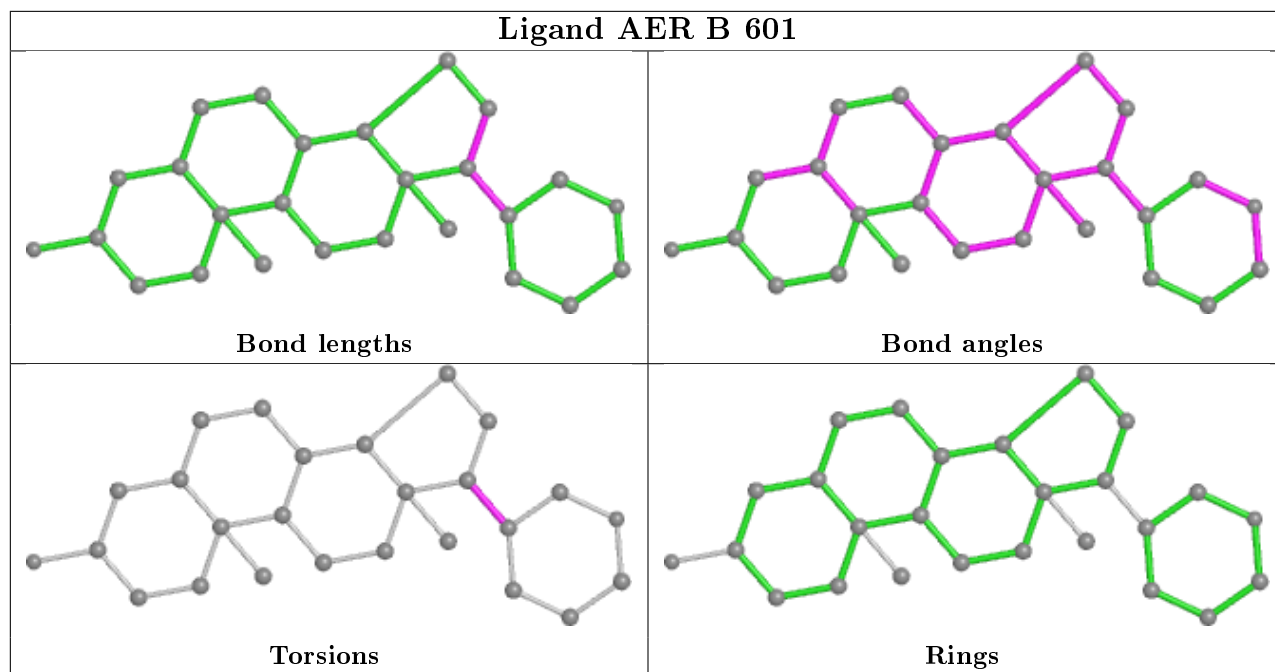
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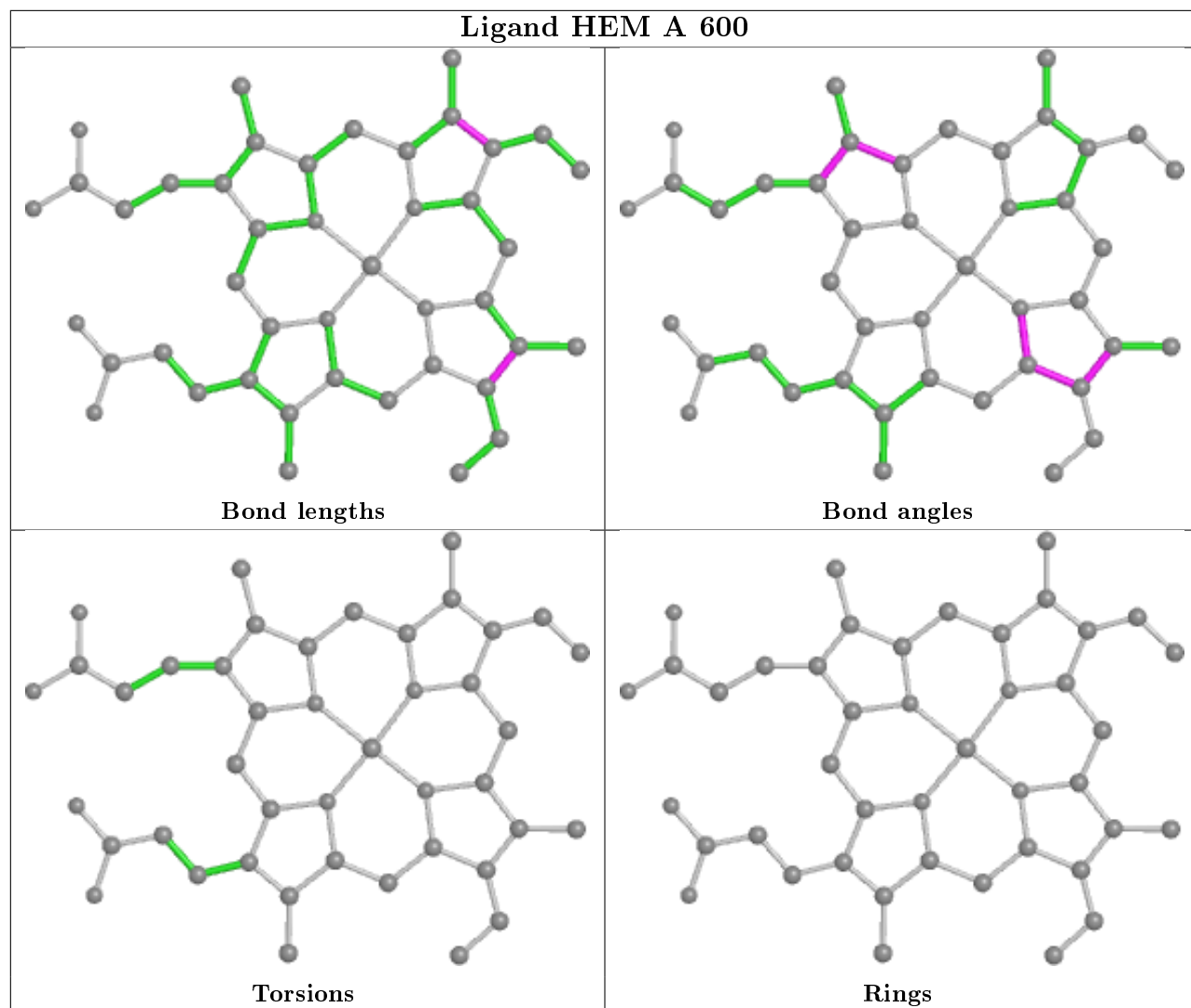
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	AER	1	0
3	A	601	AER	3	0
2	A	600	HEM	4	0

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







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	417/439 (94%)	-0.55	3 (0%) 87 88	35, 54, 107, 153	1 (0%)
1	B	411/439 (93%)	-0.31	7 (1%) 70 68	45, 85, 125, 143	0
All	All	828/878 (94%)	-0.43	10 (1%) 79 78	35, 67, 122, 153	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	ASP	4.8
1	A	295	ASP	3.2
1	B	483	PRO	2.9
1	B	265	VAL	2.8
1	B	480	THR	2.6
1	A	509	ASP	2.5
1	B	289	ASN	2.4
1	B	241	ASP	2.3
1	B	230	ILE	2.3
1	A	235	GLN	2.1

### 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](#)

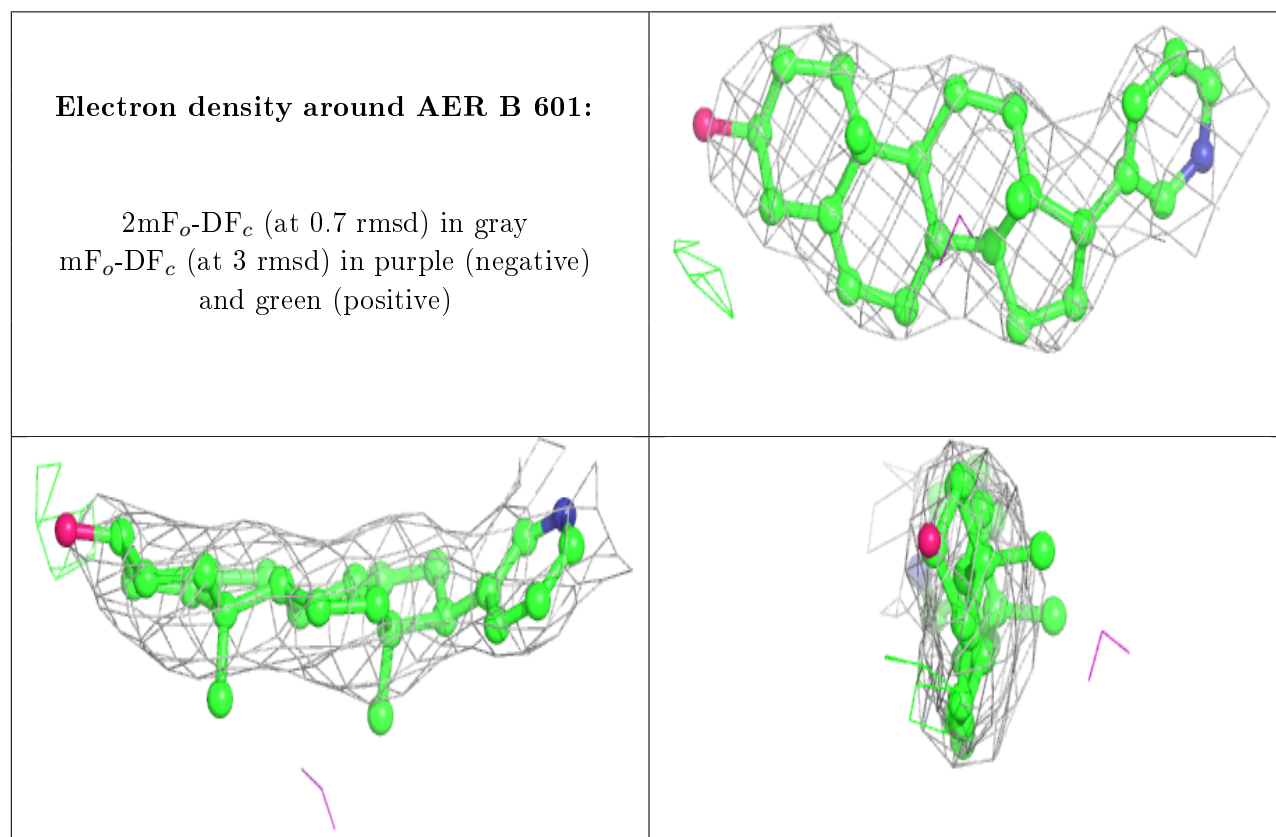
There are no carbohydrates in this entry.

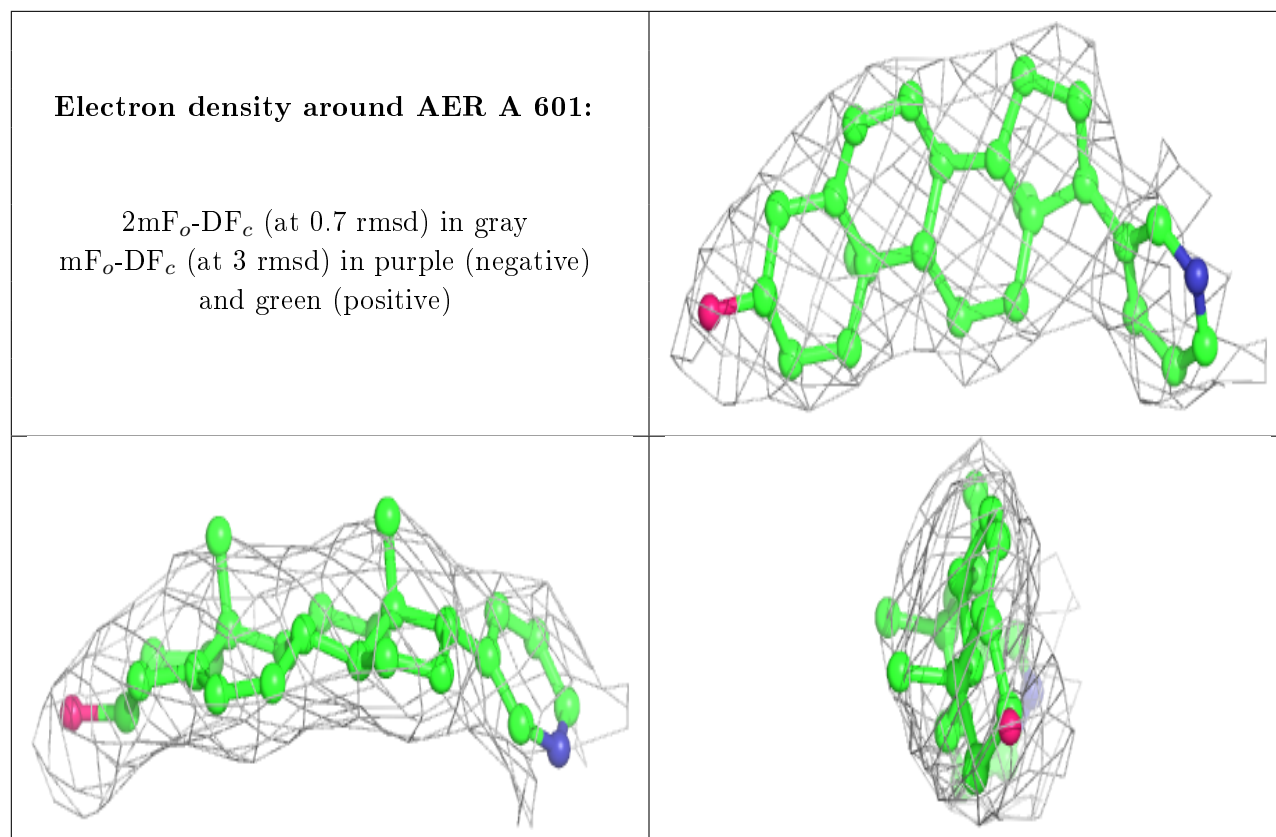
## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
3	AER	B	601	26/26	0.98	0.15	67,74,80,81	0
3	AER	A	601	26/26	0.98	0.17	37,41,48,51	0
2	HEM	B	600	43/43	0.99	0.14	46,53,58,65	0
2	HEM	A	600	43/43	0.99	0.17	35,49,54,62	0

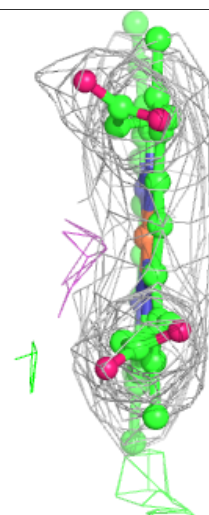
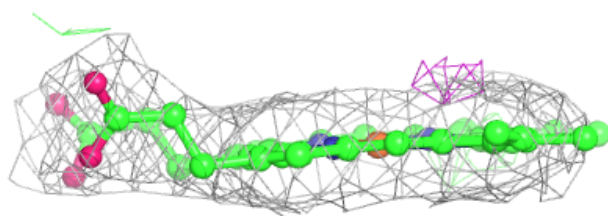
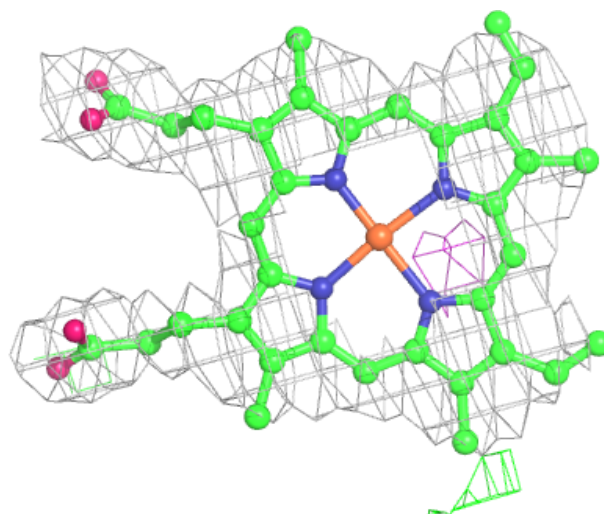
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



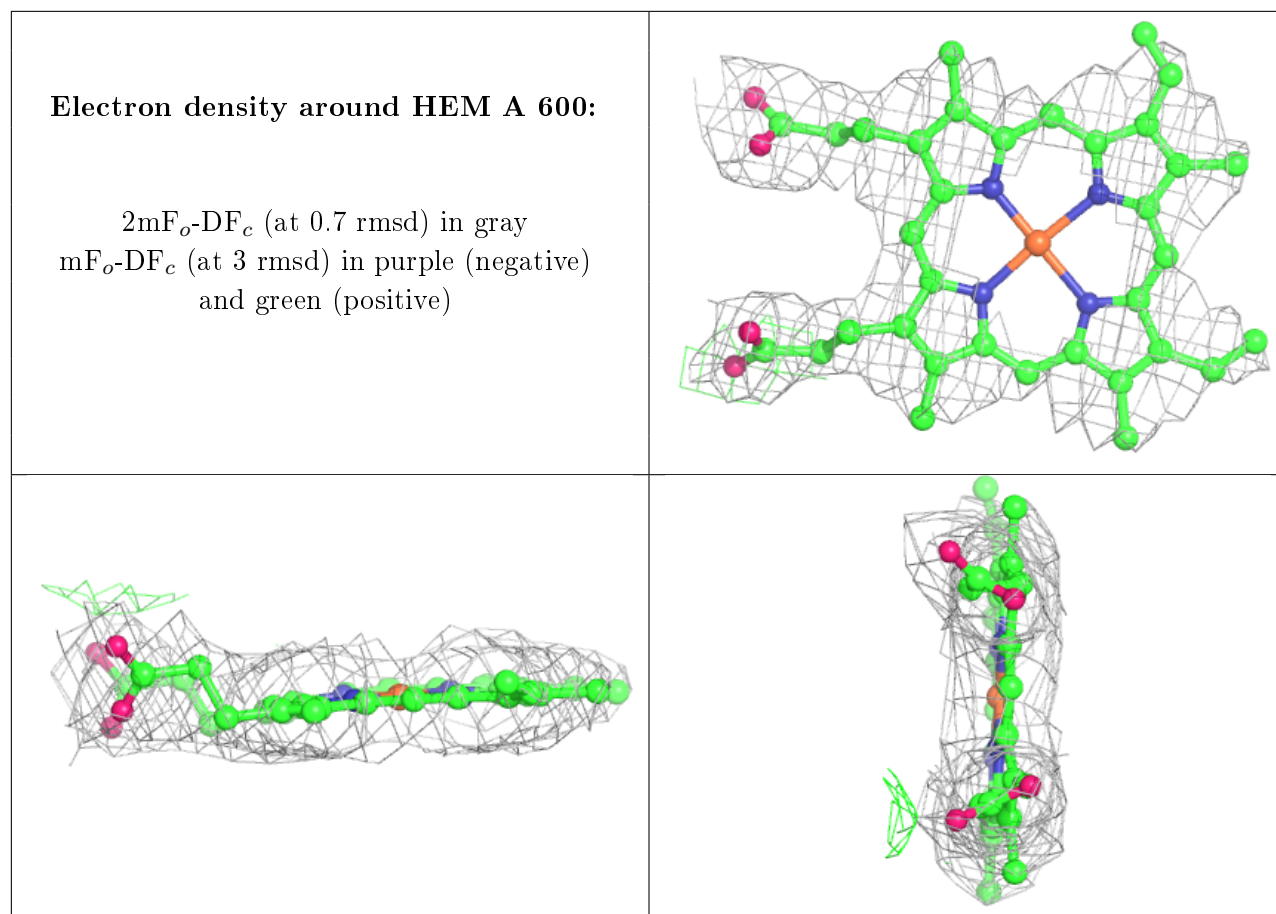


**Electron density around HEM B 600:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.