



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 4R1Z / pdb_00004r1z
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

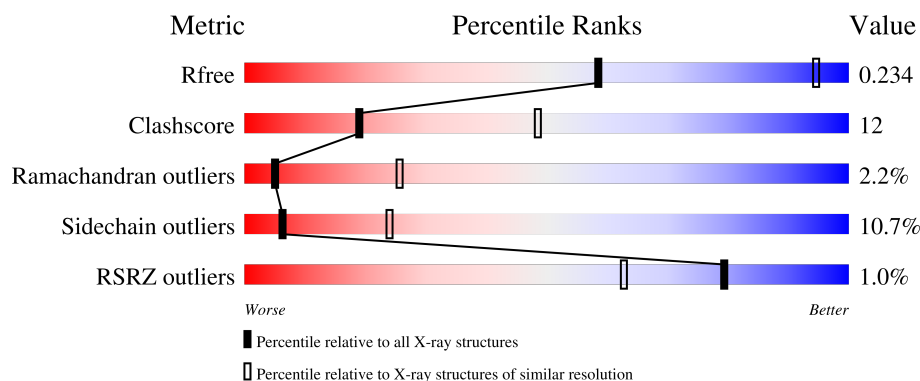
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 68% 23% • • 5%
1	B	439	% 68% 20% 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.

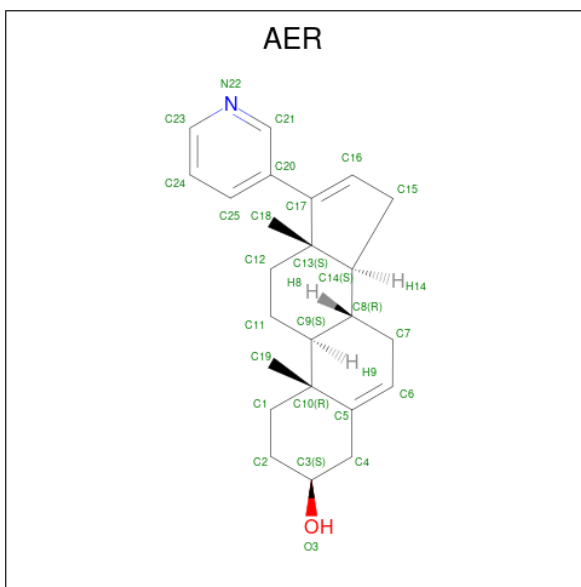
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	4	0	0
			3310	2105	581	608	16			
1	B	411	Total	C	N	O	S	0	1	0
			3256	2068	571	601	16			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: 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		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.63Å 136.63Å 135.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 3.30 29.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.00-3.30) 99.8 (29.00-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.31 (at 3.31Å)	Xtriage
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 (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6719	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	1/3376 (0.0%)	1.13	6/4562 (0.1%)
1	B	0.75	0/3317	1.05	4/4480 (0.1%)
All	All	0.88	1/6693 (0.0%)	1.09	10/9042 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	ASN	CA-C	-5.25	1.50	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ILE	CB-CA-C	-7.68	101.97	112.04
1	A	420	PRO	N-CA-C	-6.12	102.23	111.41
1	A	242	LEU	N-CA-C	-6.00	105.14	112.88
1	B	502	VAL	N-CA-C	5.98	117.53	108.80
1	A	502	VAL	CB-CA-C	-5.41	104.34	111.70
1	A	98	ILE	CB-CA-C	-5.37	104.85	111.94
1	A	374	ILE	N-CA-C	5.31	116.08	110.72
1	A	243	THR	N-CA-C	-5.30	105.55	112.23
1	B	397	VAL	N-CA-C	5.29	114.93	106.88
1	B	203	ARG	N-CA-C	5.25	117.07	110.24

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

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	68	0
1	B	3256	0	3303	84	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	159	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 12.

All (159) 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:H	1:B:500[A]:PHE:HD1	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
1:A:330:VAL:HG11	1:A:478:MET:HE3	1.71	0.73
2:B:600:HEM:HBB2	2:B:600:HEM:HHC	1.70	0.73
1:A:119:THR:HA	1:A:305:MET:HE2	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:B:500[A]:PHE:N	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:HBB2	2:A:600:HEM:HHC	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
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:B:91:ASN:OD1	1:B:91:ASN:C	2.44	0.59
1:A:211:MET:HA	1:A:214:TYR:CE2	2.37	0.59
1:B:305:MET:HE3	1:B:305:MET:HA	1.85	0.59
1:A:375:ARG:NH1	1:A:487:LEU:O	2.37	0.58
1:A:235:GLN:C	1:A:236:ILE:HG12	2.28	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: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: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:B:360:ASN:C	1:B:362:PRO:HD3	2.32	0.55
1:A:358:ARG:HG3	1:A:358:ARG:HH11	1.72	0.54
1:B:370:GLU:HA	1:B:370:GLU:OE1	2.06	0.54
1:A:380:LEU:C	1:A:381:LEU:O	2.48	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:140:MET:HA	1:B:140:MET:HE2	1.90	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:B:147:MET:C	1:B:149:GLY:HA3	2.33	0.53
1:B:252:ARG:O	1:B:253:ASP:C	2.52	0.53
1:B:124:ASP:OD1	1:B:124:ASP:C	2.52	0.52
1:A:205:ASP:OD1	1:A:205:ASP:C	2.51	0.52
1:B:355:LEU:HD13	1:B:465:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:LEU:O	1:B:181:GLY:C	2.53	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: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:408:TRP:C	1:A:408:TRP:CD1	2.90	0.49
1:A:138:ARG:HG2	1:A:454:LEU:HD13	1.93	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: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:B:392:VAL:O	1:B:393:GLY:C	2.56	0.49
1:A:148:PHE:C	1:A:148:PHE:CD1	2.90	0.49
1:A:479:PRO:O	1:A:481:GLY:N	2.46	0.49
1:B:444:LEU:O	1:B:445:PRO:C	2.56	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:A:211:MET:HA	1:A:214:TYR:CD2	2.49	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: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:A:478:MET:HE1	1:A:500:PHE:CD2	2.50	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:A:455:GLY:O	1:A:456:GLU:C	2.56	0.46
1:B:165:SER:O	1:B:168:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:HA	1:B:230:ILE:HA	1.69	0.46
2:B:600:HEM:HHD	2:B:600:HEM:HBC2	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:242:LEU:C	1:A:242:LEU:HD23	2.42	0.45
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.98	0.45
1:B:328:TYR:CZ	1:B:487:LEU:HD13	2.52	0.45
1:B:370:GLU:HG3	1:B:423:PHE:CD2	2.52	0.45
1:A:317:THR:HG21	3:A:601:AER:C23	2.46	0.45
1:A:305:MET:HA	1:A:305:MET:HE3	1.98	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:255:LEU:C	1:B:255:LEU:HD23	2.42	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: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:B:100:ILE:O	1:B:101:LYS:C	2.59	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:HD12	1:B:484:LEU:H	1.83	0.44
1:A:358:ARG:HG3	1:A:358:ARG:NH1	2.32	0.43
1:A:104:LYS:HE2	1:A:130:TYR:OH	2.18	0.43
1:B:345:SER:C	1:B:346:LYS:HG2	2.43	0.43
1:A:480:THR:HG23	1:A:481:GLY:H	1.84	0.43
1:B:148:PHE:CD2	1:B:148:PHE:O	2.71	0.43
1:A:162:GLU:OE1	1:A:162:GLU:HA	2.19	0.42
1:A:283:LYS:HG3	1:A:298:LEU:O	2.19	0.42
1:B:214:TYR:CD1	1:B:214:TYR:C	2.97	0.42
1:A:235:GLN:C	1:A:236:ILE:CG1	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:C	1:B:119:THR:HG22	2.45	0.41
1:B:123:LYS:O	1:B:124:ASP:CB	2.67	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:252:ARG:NH2	1:B:305:MET:HE1	2.36	0.41
1:A:140:MET:HA	1:A:140:MET:HE2	2.02	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:123:LYS:O	1:B:124:ASP:CG	2.64	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:150:GLU:C	1:B:152:SER:N	2.79	0.41
1:B:370:GLU:OE1	1:B:373:ARG:HD3	2.21	0.41
1:A:234:LEU:O	1:A:234:LEU:HG	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:357:ASP:O	1:A:358:ARG:C	2.64	0.40
1:A:452:VAL:O	1:A:453:CYS:C	2.64	0.40
1:A:169:VAL:HG22	1:A:203:ARG:NH2	2.36	0.40
1:B:149:GLY:N	1:B:152:SER:O	2.55	0.40
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%)	5	26
1	B	406/439 (92%)	358 (88%)	38 (9%)	10 (2%)	4	23
All	All	817/878 (93%)	728 (89%)	70 (9%)	19 (2%)	5	25

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
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 ⓘ

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%)	324 (88%)	43 (12%)	5	20
1	B	362/388 (93%)	326 (90%)	36 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	729/776 (94%)	650 (89%)	79 (11%)	6 23

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	132	SER
1	A	147	MET
1	A	152	SER
1	A	154	SER
1	A	155	ILE
1	A	166	MET
1	A	178	VAL
1	A	180	LEU
1	A	195	LEU
1	A	199	SER
1	A	202	LYS
1	A	211	MET
1	A	212	LEU
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
1	A	244	ILE
1	A	245	LEU
1	A	265	VAL
1	A	276	LEU
1	A	281	ARG
1	A	330	VAL
1	A	336	GLN
1	A	351	ARG
1	A	369	ARG
1	A	373	ARG
1	A	375	ARG
1	A	377	VAL
1	A	380	LEU
1	A	381	LEU
1	A	396	THR
1	A	401	THR

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Mol	Chain	Res	Type
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	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	245	LEU
1	B	268	SER
1	B	277	ASP
1	B	287	GLU
1	B	298	LEU
1	B	300	GLU
1	B	305	MET
1	B	319	THR
1	B	355	LEU
1	B	373	ARG
1	B	377	VAL
1	B	380	LEU
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
1	B	505	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	175	ASN
1	A	239	ASN
1	A	263	HIS
1	A	472	GLN
1	A	482	GLN
1	B	93	HIS
1	B	174	GLN
1	B	263	HIS
1	B	270	ASN
1	B	272	GLN
1	B	289	ASN
1	B	340	GLN
1	B	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	600	3,1	50,50,50	1.73	10 (20%)	67,82,82	1.74	15 (22%)
3	AER	A	601	2	30,30,30	2.46	3 (10%)	47,47,47	2.34	11 (23%)
3	AER	B	601	2	30,30,30	2.45	2 (6%)	47,47,47	2.56	17 (36%)
2	HEM	B	600	3,1	50,50,50	1.68	8 (16%)	67,82,82	1.79	18 (26%)

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	A	600	3,1	-	6/14/54/54	-
3	AER	A	601	2	-	2/4/62/62	0/5/5/5
3	AER	B	601	2	-	0/4/62/62	0/5/5/5
2	HEM	B	600	3,1	-	4/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	AER	C16-C17	12.58	1.55	1.33
3	A	601	AER	C16-C17	12.41	1.54	1.33
2	B	600	HEM	FE-NB	5.68	2.12	1.94
2	A	600	HEM	FE-NB	5.07	2.10	1.94
2	B	600	HEM	FE-NC	4.09	2.08	1.95
2	A	600	HEM	FE-NC	4.08	2.08	1.95
2	B	600	HEM	C1B-NB	-4.06	1.33	1.40
2	A	600	HEM	C1B-NB	-3.89	1.33	1.40
2	B	600	HEM	C4D-ND	-3.45	1.34	1.40
2	A	600	HEM	C4B-NB	-3.26	1.32	1.38
2	A	600	HEM	C4D-ND	-3.18	1.34	1.40
2	B	600	HEM	C1C-C2C	-3.16	1.39	1.45
2	A	600	HEM	C1C-C2C	-3.07	1.39	1.45
2	B	600	HEM	C4B-NB	-2.76	1.33	1.38
2	A	600	HEM	C1C-NC	-2.70	1.34	1.39
3	B	601	AER	C20-C17	2.32	1.51	1.48
2	B	600	HEM	FE-ND	-2.28	1.87	1.94
3	A	601	AER	C13-C14	-2.23	1.50	1.54
2	A	600	HEM	C3B-C4B	2.23	1.49	1.44
3	A	601	AER	C12-C13	-2.13	1.50	1.54
2	A	600	HEM	O2D-CGD	-2.09	1.23	1.30
2	B	600	HEM	C1D-ND	-2.07	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C2A-C3A	-2.06	1.33	1.38

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	AER	C15-C16-C17	-8.85	104.88	112.56
3	B	601	AER	C15-C16-C17	-7.74	105.84	112.56
3	B	601	AER	C20-C17-C16	-7.11	115.92	125.08
3	A	601	AER	C20-C17-C16	-5.76	117.65	125.08
3	B	601	AER	C13-C17-C20	-5.54	119.52	125.39
3	A	601	AER	C13-C17-C20	-5.43	119.63	125.39
3	B	601	AER	C14-C13-C17	5.27	103.96	99.50
3	A	601	AER	C14-C13-C17	5.17	103.88	99.50
2	B	600	HEM	CHD-C1D-ND	4.74	129.52	124.42
3	B	601	AER	C13-C17-C16	-4.68	105.50	109.66
2	B	600	HEM	CAC-C3C-C4C	4.41	135.34	124.82
3	A	601	AER	C15-C14-C8	-4.29	117.08	121.63
3	B	601	AER	C15-C14-C13	4.22	107.00	104.05
2	A	600	HEM	CHD-C1D-ND	4.04	128.78	124.42
2	A	600	HEM	CAC-C3C-C4C	4.00	134.37	124.82
3	A	601	AER	C13-C17-C16	-3.97	106.13	109.66
2	B	600	HEM	CHA-C4D-ND	3.78	129.04	124.37
2	A	600	HEM	CHA-C4D-ND	3.69	128.94	124.37
2	A	600	HEM	CAC-C3C-C2C	-3.57	116.82	128.43
2	B	600	HEM	CHC-C4B-NB	3.46	128.15	124.42
2	B	600	HEM	CAC-C3C-C2C	-3.44	117.24	128.43
3	B	601	AER	C7-C8-C9	3.41	113.66	109.72
2	B	600	HEM	C1B-NB-C4B	3.20	108.99	105.21
2	A	600	HEM	C4B-C3B-C2B	-3.19	104.35	107.28
3	B	601	AER	C4-C5-C6	-3.16	116.28	120.57
3	B	601	AER	C15-C14-C8	-3.16	118.28	121.63
2	A	600	HEM	C1B-NB-C4B	3.14	108.93	105.21
3	A	601	AER	C18-C13-C17	-3.10	102.94	107.81
2	B	600	HEM	CMB-C2B-C1B	3.08	129.84	125.03
2	A	600	HEM	CHA-C4D-C3D	-3.04	119.62	125.23
2	B	600	HEM	CHA-C4D-C3D	-2.86	119.95	125.23
2	B	600	HEM	CHC-C1C-NC	2.82	127.52	124.45
2	A	600	HEM	CMB-C2B-C1B	2.79	129.39	125.03
2	B	600	HEM	CHB-C1B-NB	2.77	127.79	124.37
3	B	601	AER	C4-C5-C10	2.76	119.96	116.42
3	B	601	AER	C14-C8-C9	-2.69	105.57	109.09
2	A	600	HEM	C3B-C2B-C1B	2.55	108.33	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	CHC-C4B-NB	2.55	127.16	124.42
2	A	600	HEM	CMB-C2B-C3B	-2.54	122.28	128.43
2	A	600	HEM	CHD-C4C-C3C	2.48	129.40	125.21
3	B	601	AER	C18-C13-C12	-2.47	108.28	111.10
2	B	600	HEM	C3B-C4B-NB	-2.41	107.73	109.47
3	B	601	AER	C12-C13-C17	2.39	122.07	119.30
2	A	600	HEM	O2D-CGD-O1D	-2.30	117.42	123.33
3	A	601	AER	C14-C8-C9	-2.29	106.10	109.09
3	B	601	AER	C12-C11-C9	2.28	117.00	113.14
3	B	601	AER	C23-N22-C21	2.25	120.78	116.85
2	B	600	HEM	CHD-C4C-C3C	2.24	128.99	125.21
2	B	600	HEM	C4C-NC-C1C	2.22	109.44	105.82
3	A	601	AER	C4-C5-C10	2.21	119.25	116.42
2	A	600	HEM	CHB-C1B-NB	2.20	127.08	124.37
3	A	601	AER	C12-C13-C14	-2.17	105.52	108.88
2	B	600	HEM	CMB-C2B-C3B	-2.15	123.22	128.43
2	B	600	HEM	CAB-C3B-C2B	-2.14	121.48	128.43
3	B	601	AER	C12-C13-C14	-2.12	105.60	108.88
2	B	600	HEM	CHD-C1D-C2D	-2.11	121.69	125.03
2	B	600	HEM	C4D-ND-C1D	2.08	107.67	105.21
2	B	600	HEM	O2A-CGA-O1A	-2.08	117.99	123.33
2	A	600	HEM	C4C-C3C-C2C	2.06	108.60	106.81
3	B	601	AER	C13-C14-C8	-2.03	110.99	113.13
3	A	601	AER	C24-C25-C20	-2.02	118.38	120.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

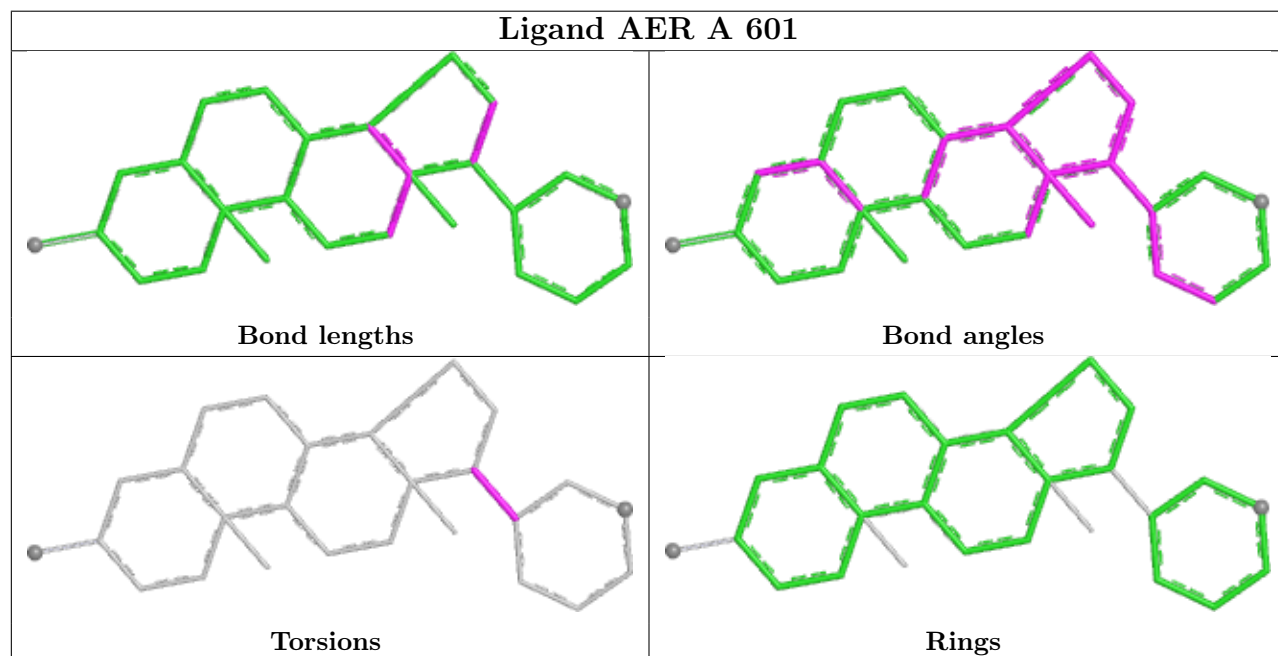
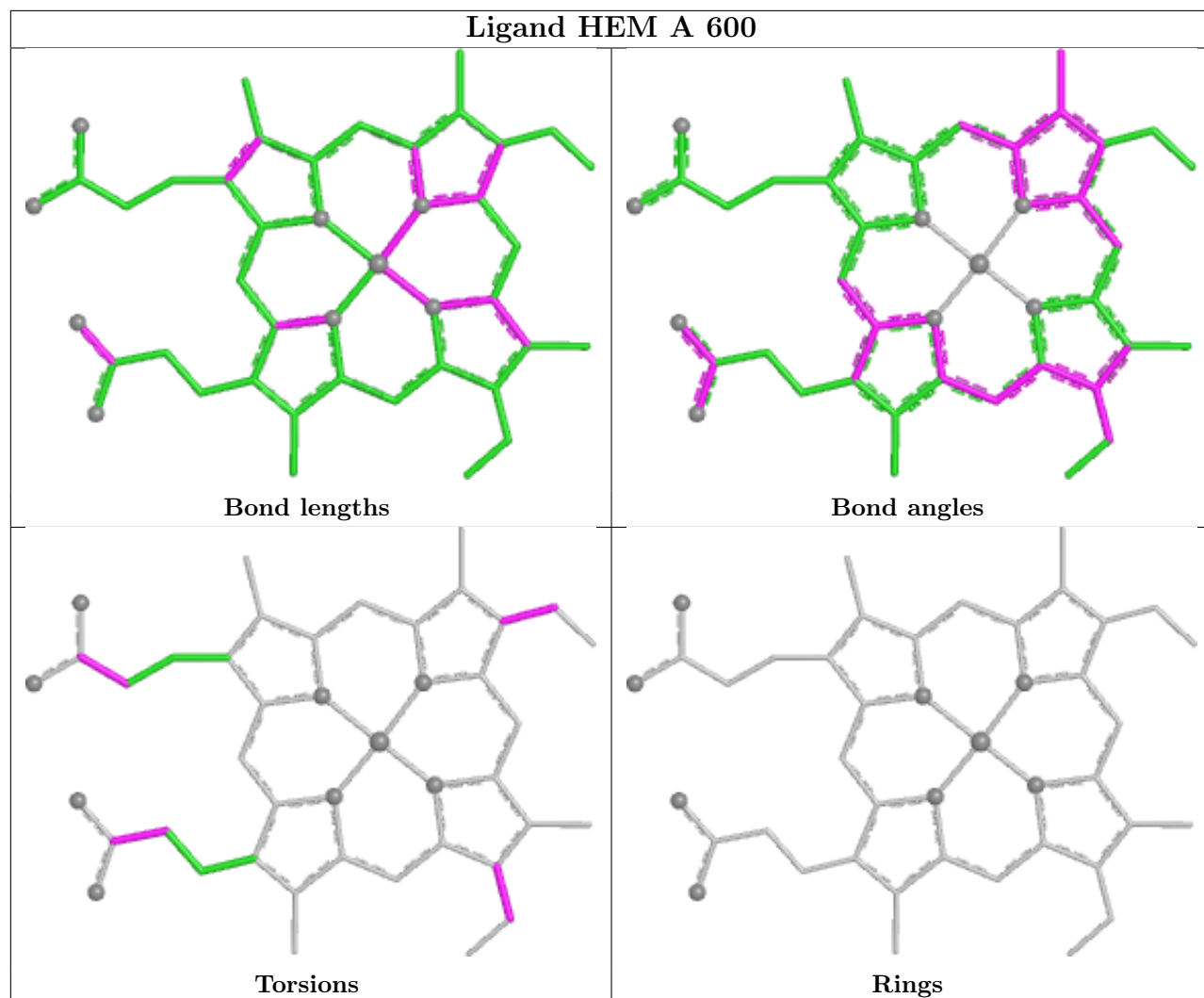
Mol	Chain	Res	Type	Atoms
2	B	600	HEM	C4B-C3B-CAB-CBB
2	A	600	HEM	C4B-C3B-CAB-CBB
2	A	600	HEM	C4C-C3C-CAC-CBC
2	B	600	HEM	C4C-C3C-CAC-CBC
3	A	601	AER	C13-C17-C20-C25
2	A	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAD-CBD-CGD-O1D
2	B	600	HEM	CAD-CBD-CGD-O1D
2	B	600	HEM	CAD-CBD-CGD-O2D
3	A	601	AER	C13-C17-C20-C21
2	A	600	HEM	CAD-CBD-CGD-O2D

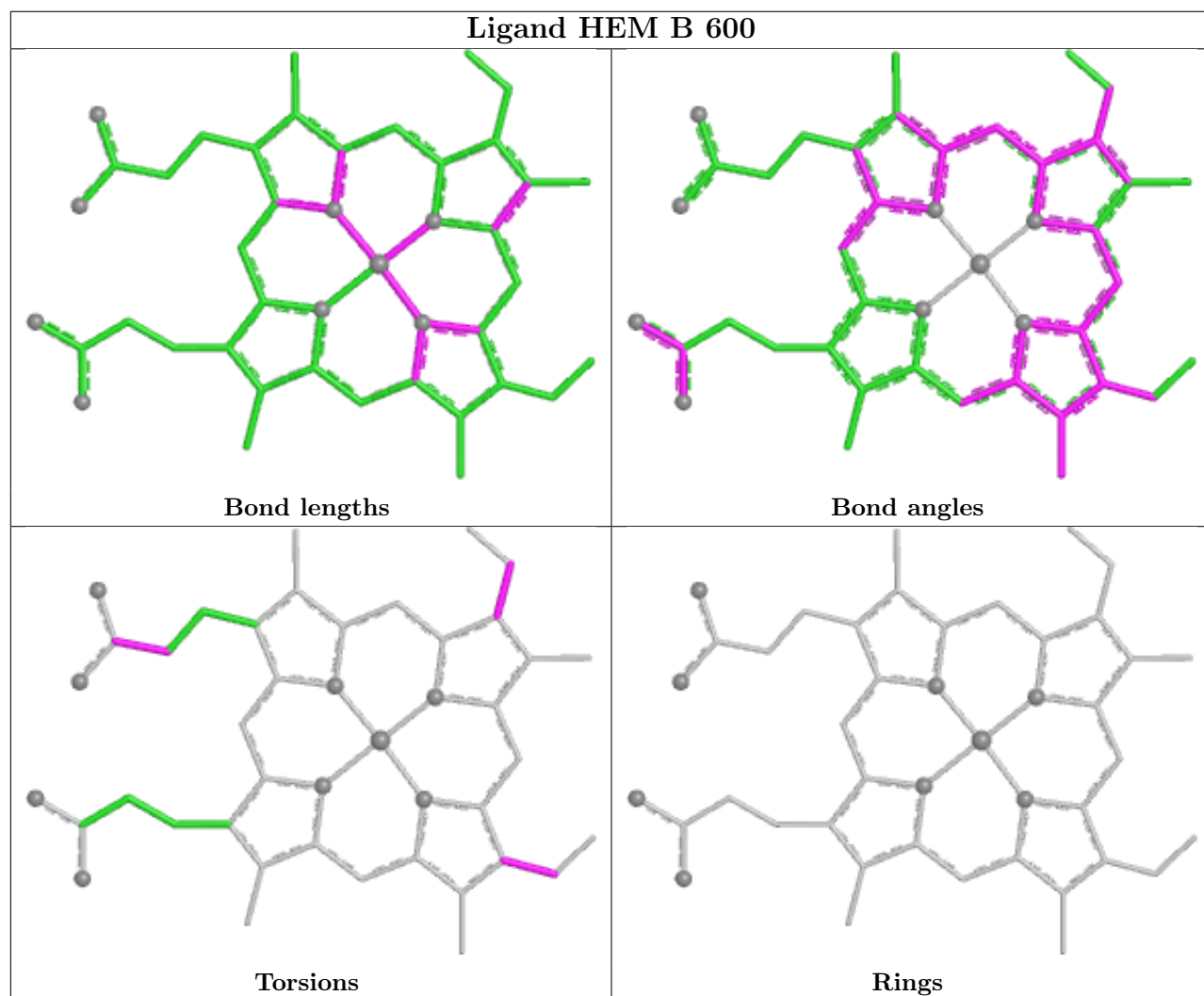
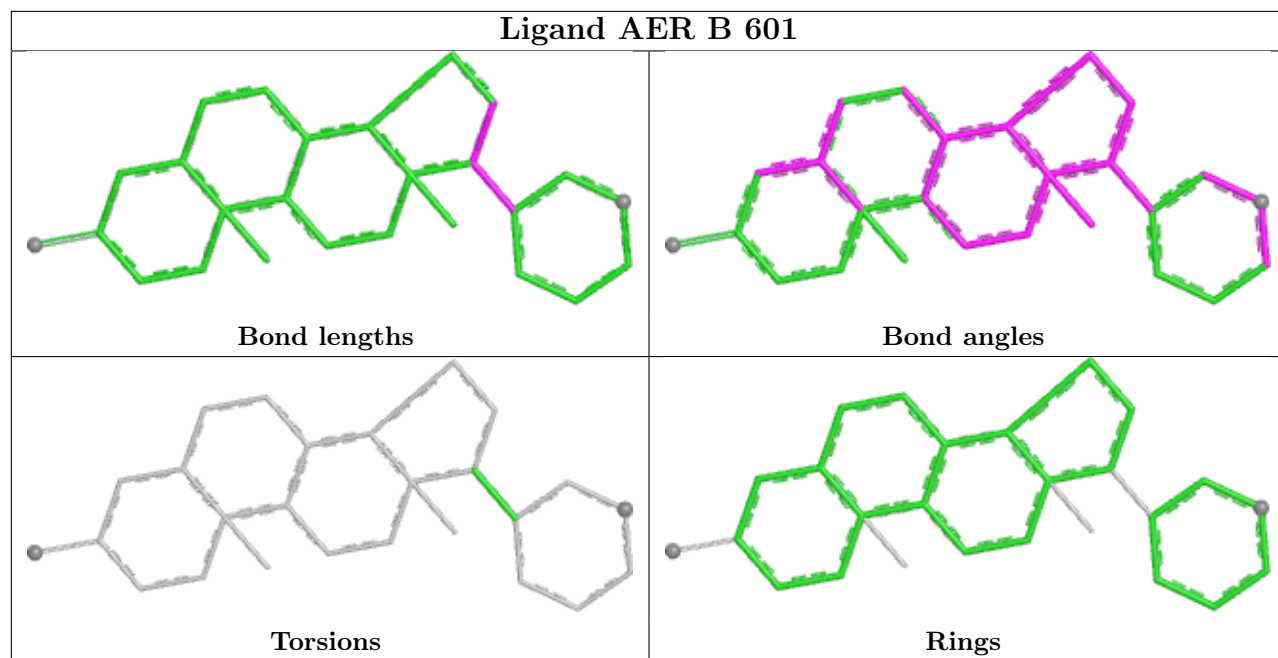
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	4	0
3	A	601	AER	3	0
3	B	601	AER	1	0
2	B	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, 95th 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 ²)	Q < 0.9
1	A	417/439 (94%)	-0.59	3 (0%)	84 70	33, 54, 107, 153	1 (0%)
1	B	411/439 (93%)	-0.36	5 (1%)	76 58	44, 85, 125, 143	1 (0%)
All	All	828/878 (94%)	-0.48	8 (0%)	79 63	33, 67, 122, 153	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	LEU	4.2
1	A	226	SER	3.3
1	A	234	LEU	3.3
1	B	500[A]	PHE	3.1
1	B	508	ALA	2.5
1	B	150	GLU	2.5
1	B	228	VAL	2.0
1	A	238	PRO	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 oligosaccharides in this entry.

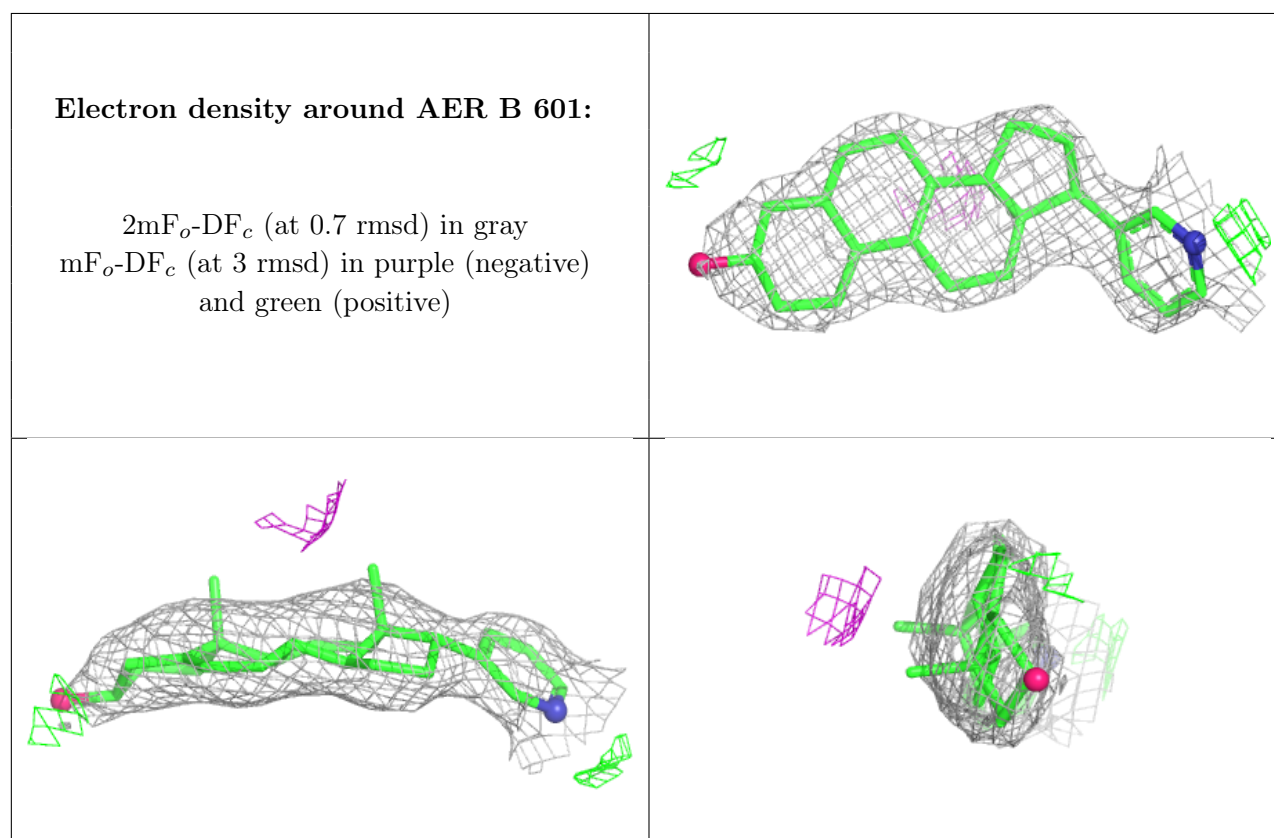
6.4 Ligands [i](#)

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, 95th 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.

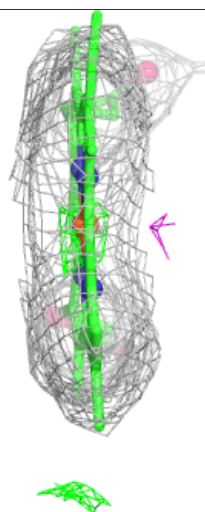
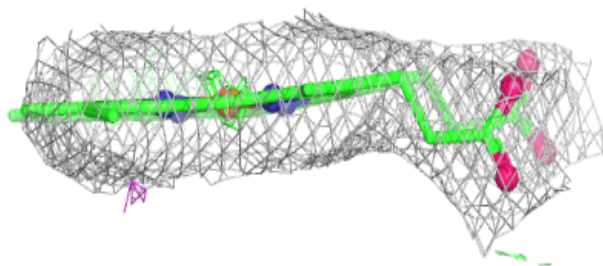
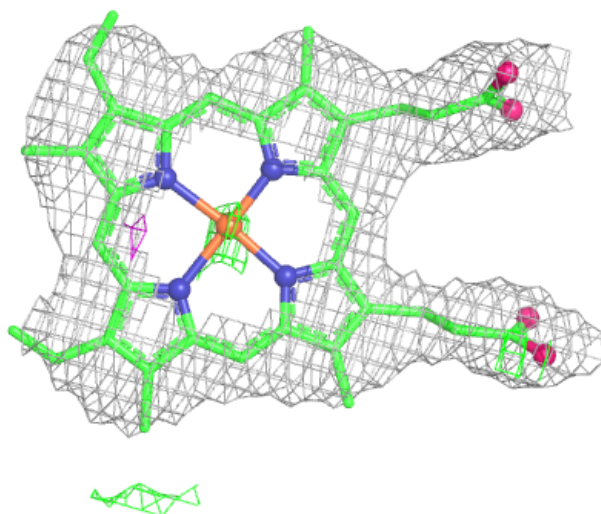
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AER	B	601	26/26	0.97	0.09	67,74,80,81	0
2	HEM	B	600	43/43	0.98	0.07	46,53,58,65	0
3	AER	A	601	26/26	0.98	0.08	37,41,48,51	0
2	HEM	A	600	43/43	0.98	0.07	35,49,54,62	0

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.



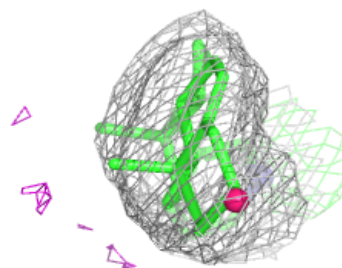
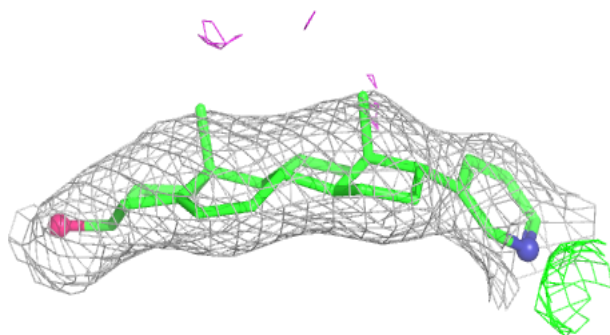
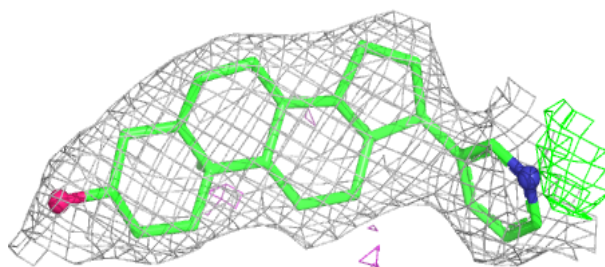
Electron density around HEM B 600:

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

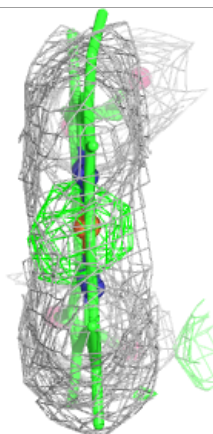
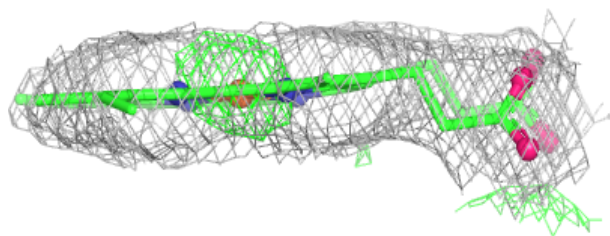
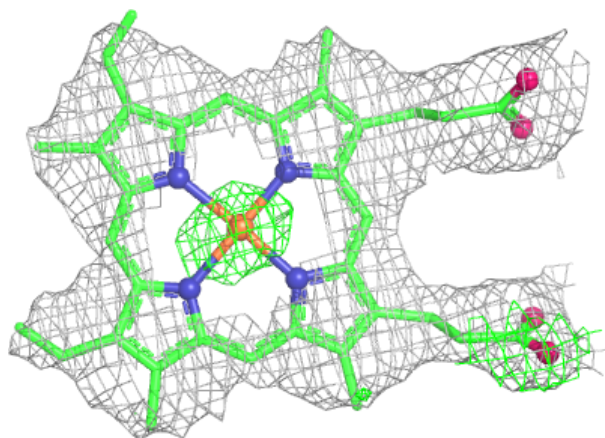


Electron density around AER A 601:

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

**Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.