



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:44 AM UTC

PDB ID : 6B82 / pdb_00006b82
Title : Zebra Fish CYP-450 17A1 Mutant Abiraterone Complex
Authors : Pallan, P.S.; Egli, M.
Deposited on : 2017-10-05
Resolution : 3.03 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

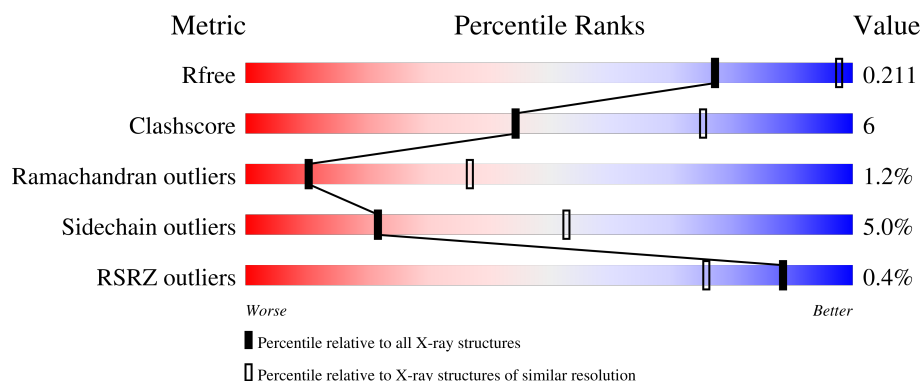
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	509	 76% 15% • 9%
1	B	509	 77% 14% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7579 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 Cytochrome P450, family 17, subfamily A, polypeptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	41	0	0
			3678	2342	637	677	22			
1	B	470	Total	C	N	O	S	46	0	0
			3712	2360	645	685	22			

There are 42 discrepancies between the modelled and reference sequences:

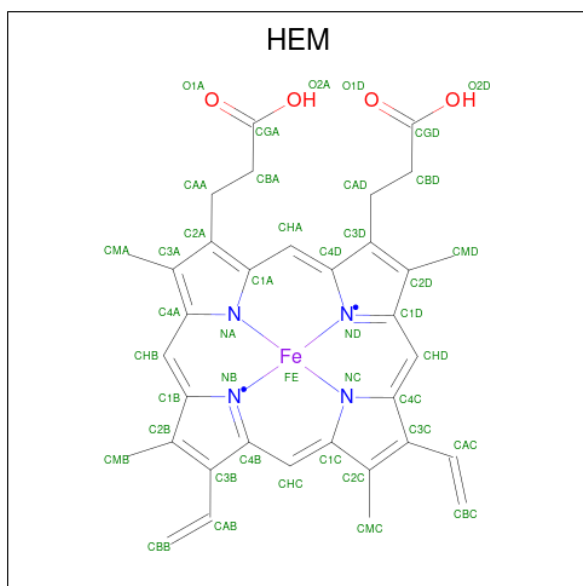
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP A2ATX9
A	18	ALA	-	expression tag	UNP A2ATX9
A	19	LYS	-	expression tag	UNP A2ATX9
A	20	LYS	-	expression tag	UNP A2ATX9
A	21	THR	-	expression tag	UNP A2ATX9
A	22	SER	-	expression tag	UNP A2ATX9
A	23	SER	-	expression tag	UNP A2ATX9
A	24	LYS	-	expression tag	UNP A2ATX9
A	25	GLY	-	expression tag	UNP A2ATX9
A	26	LYS	-	expression tag	UNP A2ATX9
A	309	GLU	ASP	engineered mutation	UNP A2ATX9
A	321	THR	VAL	engineered mutation	UNP A2ATX9
A	369	CYS	ARG	engineered mutation	UNP A2ATX9
A	372	MET	LEU	engineered mutation	UNP A2ATX9
A	407	MET	LEU	engineered mutation	UNP A2ATX9
A	520	HIS	-	expression tag	UNP A2ATX9
A	521	HIS	-	expression tag	UNP A2ATX9
A	522	HIS	-	expression tag	UNP A2ATX9
A	523	HIS	-	expression tag	UNP A2ATX9
A	524	HIS	-	expression tag	UNP A2ATX9
A	525	HIS	-	expression tag	UNP A2ATX9
B	17	MET	-	initiating methionine	UNP A2ATX9
B	18	ALA	-	expression tag	UNP A2ATX9
B	19	LYS	-	expression tag	UNP A2ATX9
B	20	LYS	-	expression tag	UNP A2ATX9

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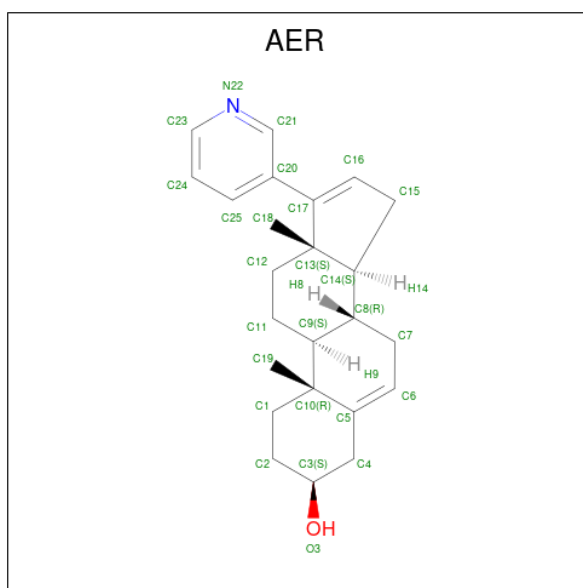
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	THR	-	expression tag	UNP A2ATX9
B	22	SER	-	expression tag	UNP A2ATX9
B	23	SER	-	expression tag	UNP A2ATX9
B	24	LYS	-	expression tag	UNP A2ATX9
B	25	GLY	-	expression tag	UNP A2ATX9
B	26	LYS	-	expression tag	UNP A2ATX9
B	309	GLU	ASP	engineered mutation	UNP A2ATX9
B	321	THR	VAL	engineered mutation	UNP A2ATX9
B	369	CYS	ARG	engineered mutation	UNP A2ATX9
B	372	MET	LEU	engineered mutation	UNP A2ATX9
B	407	MET	LEU	engineered mutation	UNP A2ATX9
B	520	HIS	-	expression tag	UNP A2ATX9
B	521	HIS	-	expression tag	UNP A2ATX9
B	522	HIS	-	expression tag	UNP A2ATX9
B	523	HIS	-	expression tag	UNP A2ATX9
B	524	HIS	-	expression tag	UNP A2ATX9
B	525	HIS	-	expression tag	UNP A2ATX9

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



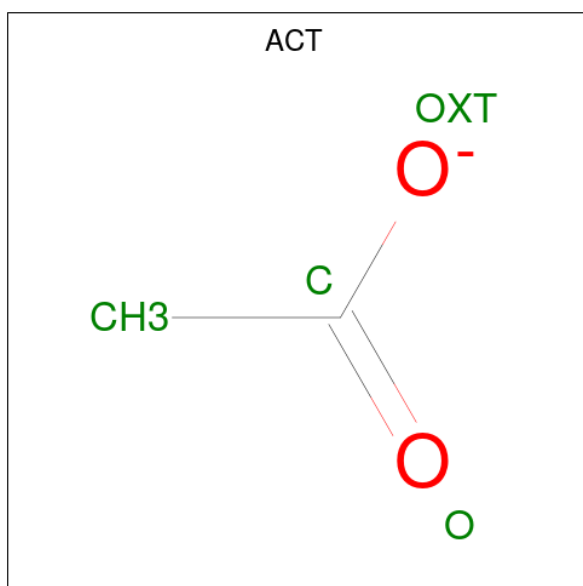
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

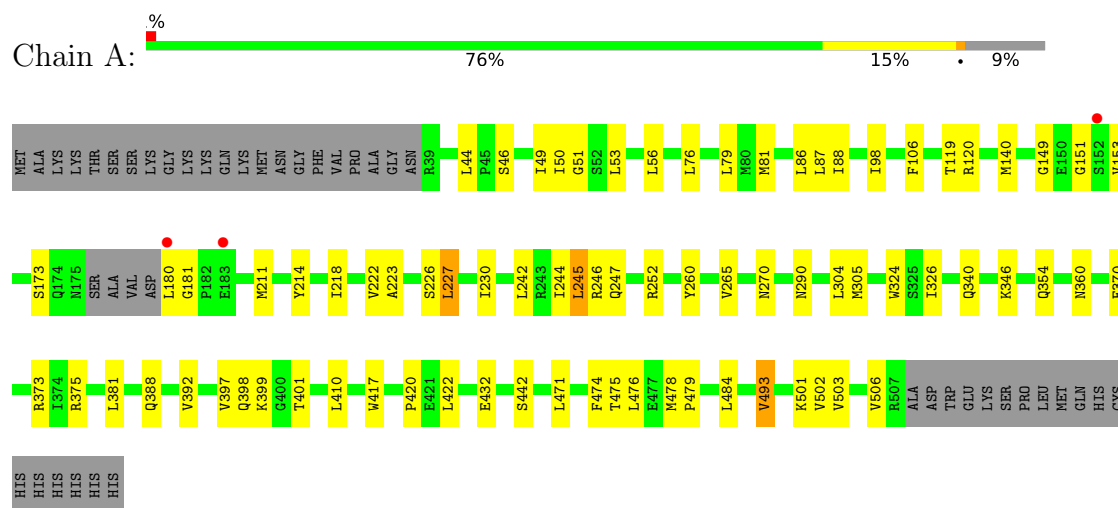
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	13	Total	O	0	0
			13	13		

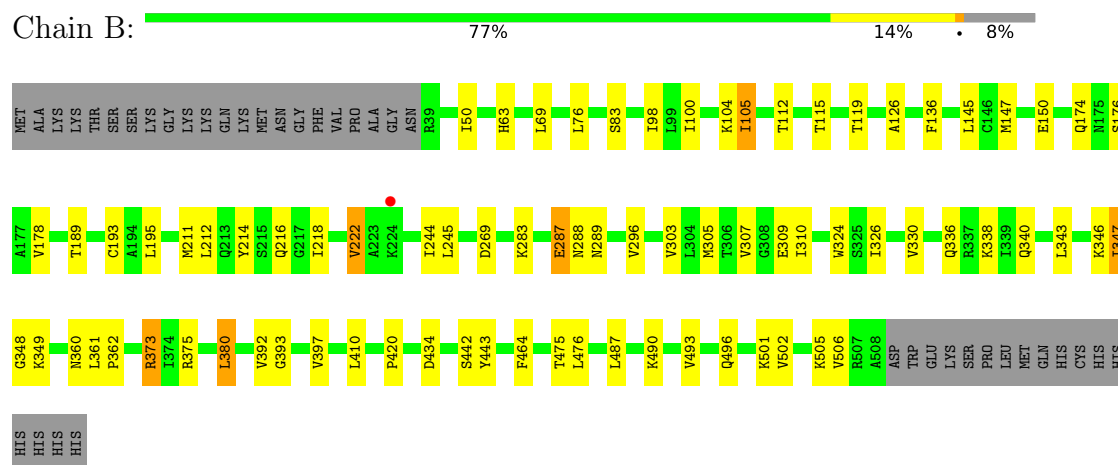
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytochrome P450, family 17, subfamily A, polypeptide 1



- Molecule 1: Cytochrome P450, family 17, subfamily A, polypeptide 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	104.92Å 104.92Å 235.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.26 – 3.03 51.26 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.26-3.03) 99.5 (51.26-3.03)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.255 (Not available) , 0.211	Depositor DCC
R_{free} test set	1330 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7579	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.05% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.77	0/3756	0.93	0/5078
1	B	0.79	0/3791	0.94	0/5127
All	All	0.78	0/7547	0.93	0/10205

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	347	ILE	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	3678	0	3717	49	1
1	B	3712	0	3748	37	1
2	A	43	0	30	4	0
2	B	43	0	30	7	0
3	A	26	0	31	2	0
3	B	26	0	31	3	0
4	A	4	0	3	0	0
4	B	12	0	9	0	0
5	B	1	0	0	0	0
6	A	21	0	0	0	1
6	B	13	0	0	0	1
All	All	7579	0	7599	89	3

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 6.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLN:HE22	1:B:496:GLN:HE22	1.03	0.98
1:B:216:GLN:HE22	1:B:496:GLN:NE2	1.74	0.83
1:B:216:GLN:NE2	1:B:496:GLN:HE22	1.79	0.79
1:B:119:THR:HA	1:B:305:MET:HE2	1.72	0.71
1:A:218:ILE:O	1:A:222:VAL:HG23	1.92	0.70
1:A:373:ARG:NH2	1:A:420:PRO:O	2.25	0.70
1:B:104:LYS:O	1:B:105:ILE:HG13	1.92	0.69
2:B:601:HEM:NB	3:B:602:AER:H23	2.06	0.69
1:A:270:ASN:HD21	1:B:288:ASN:HD22	1.40	0.69
1:A:245:LEU:O	1:A:247:GLN:N	2.28	0.66
1:B:373:ARG:NH2	1:B:420:PRO:O	2.30	0.64
2:A:601:HEM:HHD	2:A:601:HEM:HBC2	1.80	0.62
2:B:601:HEM:C1B	3:B:602:AER:H23	2.35	0.61
1:B:98:ILE:HD11	1:B:392:VAL:HG21	1.83	0.60
2:B:601:HEM:HHC	2:B:601:HEM:HBB2	1.86	0.57
1:B:392:VAL:HG23	1:B:397:VAL:HG21	1.86	0.57
1:B:346:LYS:HD2	1:B:360:ASN:O	2.04	0.56
1:A:226:SER:O	1:A:227:LEU:HB2	2.05	0.56
1:A:478:MET:HE1	1:A:484:LEU:HA	1.86	0.56
1:A:44:LEU:HD13	1:A:79:LEU:HB3	1.88	0.56
1:A:503:VAL:O	1:A:503:VAL:HG23	2.06	0.54
1:A:252:ARG:HH22	1:A:305:MET:HE1	1.72	0.53
1:A:398:GLN:O	1:A:401:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.90	0.52
1:B:63:HIS:HB3	1:B:380:LEU:HD13	1.92	0.52
1:A:346:LYS:HD3	1:A:360:ASN:O	2.10	0.52
1:A:326:ILE:HG23	1:A:476:LEU:HD13	1.92	0.52
1:A:223:ALA:HB3	1:A:493:VAL:CG1	2.40	0.51
1:B:283:LYS:O	1:B:287:GLU:HG2	2.10	0.51
1:A:56:LEU:CD2	1:A:79:LEU:HD13	2.41	0.51
1:B:343:LEU:O	1:B:348:GLY:N	2.43	0.51
2:A:601:HEM:HBB2	2:A:601:HEM:HHC	1.92	0.51
1:A:373:ARG:HD2	1:A:417:TRP:CZ3	2.46	0.50
2:A:601:HEM:C1B	3:A:602:AER:H23	2.46	0.50
1:A:180:LEU:N	1:A:502:VAL:O	2.44	0.50
1:A:370:GLU:OE1	1:A:373:ARG:NH1	2.45	0.50
1:A:79:LEU:HD21	1:A:88:ILE:HD13	1.95	0.49
1:A:49:ILE:CG2	1:A:50:ILE:HG23	2.43	0.49
1:A:119:THR:HA	1:A:305:MET:HE2	1.95	0.48
1:B:174:GLN:OE1	1:B:505:LYS:HG2	2.13	0.48
1:A:211:MET:HA	1:A:214:TYR:CD2	2.48	0.48
1:A:223:ALA:HB3	1:A:493:VAL:HG13	1.96	0.48
1:A:340:GLN:HG2	1:A:471:LEU:O	2.14	0.48
1:A:290:ASN:HD21	1:B:150:GLU:HG2	1.79	0.47
1:A:49:ILE:HG22	1:A:50:ILE:HG23	1.96	0.47
1:A:242:LEU:O	1:A:246:ARG:HG3	2.15	0.47
1:B:189:THR:O	1:B:193:CYS:HB2	2.15	0.46
1:B:218:ILE:O	1:B:222:VAL:HG23	2.16	0.46
1:B:347:ILE:HD11	1:B:361:LEU:HD11	1.98	0.46
1:A:76:LEU:CD2	1:A:87:LEU:HD11	2.46	0.46
1:B:326:ILE:HG21	1:B:502:VAL:HG11	1.97	0.46
2:A:601:HEM:NB	3:A:602:AER:H23	2.30	0.46
1:A:98:ILE:HD11	1:A:392:VAL:HG21	1.98	0.46
1:B:340:GLN:HE22	1:B:475:THR:HB	1.81	0.46
1:B:361:LEU:HD12	1:B:464:PHE:CZ	2.51	0.45
1:A:410:LEU:O	1:A:442:SER:OG	2.34	0.45
1:B:373:ARG:HB2	1:B:443:TYR:CE1	2.51	0.45
1:A:479:PRO:HD3	1:A:503:VAL:HG22	1.99	0.45
1:B:112:THR:HB	1:B:115:THR:OG1	2.17	0.45
1:A:140:MET:HA	1:B:147:MET:HE1	1.98	0.44
1:A:180:LEU:HD12	1:A:181:GLY:N	2.33	0.44
1:B:336:GLN:OE1	1:B:476:LEU:N	2.39	0.44
1:A:53:LEU:HD21	1:A:230:ILE:HD13	2.00	0.44
1:A:340:GLN:NE2	1:A:474:PHE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:C1D	3:B:602:AER:H21	2.52	0.44
1:A:81:MET:HG3	1:A:86:LEU:HG	2.00	0.43
1:A:388:GLN:HA	1:A:399:LYS:HD3	2.00	0.43
1:B:375:ARG:NH1	1:B:487:LEU:O	2.51	0.43
1:B:310:ILE:HG23	2:B:601:HEM:HBC1	1.99	0.43
1:A:76:LEU:HD21	1:A:87:LEU:HD11	2.00	0.43
1:B:410:LEU:O	1:B:442:SER:OG	2.36	0.43
1:A:180:LEU:HG	1:A:502:VAL:CG1	2.49	0.43
1:B:126:ALA:HB2	2:B:601:HEM:HAD1	2.01	0.43
1:A:270:ASN:ND2	1:B:288:ASN:HD22	2.12	0.42
1:A:244:ILE:C	1:A:245:LEU:O	2.63	0.42
1:A:324:TRP:CE3	1:A:375:ARG:HG3	2.54	0.41
1:A:360:ASN:HB2	1:B:100:ILE:HG21	2.03	0.41
1:B:324:TRP:CE3	1:B:375:ARG:HG3	2.56	0.41
1:A:106:PHE:HE1	1:A:397:VAL:HG11	1.86	0.41
1:B:211:MET:HA	1:B:214:TYR:CD2	2.55	0.41
1:A:149:GLY:O	1:A:153:VAL:HB	2.21	0.41
1:B:136:PHE:CD2	1:B:296:VAL:HG11	2.56	0.41
1:A:46:SER:HB2	1:A:51:GLY:HA2	2.03	0.41
1:B:303:VAL:O	1:B:307:VAL:HG23	2.21	0.41
1:A:260:TYR:CD1	1:A:304:LEU:HD21	2.56	0.41
1:A:354:GLN:NE2	1:B:104:LYS:HE2	2.36	0.41
1:B:360:ASN:C	1:B:362:PRO:HD3	2.45	0.40
1:A:173:SER:OG	1:A:506:VAL:HG23	2.22	0.40
1:A:120:ARG:HG3	1:A:305:MET:SD	2.61	0.40

All (3) 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)
6:A:708:HOH:O	6:A:708:HOH:O[5_655]	1.45	0.75
6:B:708:HOH:O	6:B:708:HOH:O[6_554]	1.75	0.45
1:A:265:VAL:O	1:B:289:ASN:ND2[6_554]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/509 (91%)	425 (92%)	31 (7%)	5 (1%)	11	39
1	B	468/509 (92%)	434 (93%)	28 (6%)	6 (1%)	9	35
All	All	929/1018 (91%)	859 (92%)	59 (6%)	11 (1%)	10	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ILE
1	A	227	LEU
1	A	245	LEU
1	B	178	VAL
1	B	222	VAL
1	B	349	LYS
1	A	381	LEU
1	A	501	LYS
1	B	501	LYS
1	A	151	GLY
1	B	393	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/451 (19%)	80 (95%)	4 (5%)	23	54
1	B	416/451 (92%)	395 (95%)	21 (5%)	22	53
All	All	500/902 (55%)	475 (95%)	25 (5%)	22	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	432	GLU
1	A	475	THR
1	A	493	VAL
1	B	50	ILE
1	B	69	LEU
1	B	76	LEU
1	B	83	SER
1	B	145	LEU
1	B	176	SER
1	B	195	LEU
1	B	212	LEU
1	B	244	ILE
1	B	245	LEU
1	B	269	ASP
1	B	287	GLU
1	B	309	GLU
1	B	330	VAL
1	B	338	LYS
1	B	373	ARG
1	B	380	LEU
1	B	434	ASP
1	B	490	LYS
1	B	493	VAL
1	B	506	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	B	91	ASN
1	B	92	HIS
1	B	216	GLN
1	B	270	ASN
1	B	332	ASN
1	B	354	GLN
1	B	406	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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$
4	ACT	B	606	-	3,3,3	0.75	0	3,3,3	0.94	0
2	HEM	B	601	3,1	50,50,50	1.64	9 (18%)	67,82,82	1.66	14 (20%)
4	ACT	A	603	-	3,3,3	0.76	0	3,3,3	0.95	0
4	ACT	B	605	-	3,3,3	0.93	0	3,3,3	0.27	0
2	HEM	A	601	3,1	50,50,50	1.65	11 (22%)	67,82,82	1.75	22 (32%)
3	AER	B	602	2	30,30,30	2.44	2 (6%)	47,47,47	2.48	17 (36%)
3	AER	A	602	2	30,30,30	2.37	1 (3%)	47,47,47	2.50	11 (23%)
4	ACT	B	604	-	3,3,3	0.91	0	3,3,3	1.02	0

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	602	2	-	2/4/62/62	0/5/5/5
2	HEM	A	601	3,1	-	4/14/54/54	-
3	AER	A	602	2	-	2/4/62/62	0/5/5/5
2	HEM	B	601	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	602	AER	C16-C17	12.50	1.54	1.33
3	A	602	AER	C16-C17	12.28	1.54	1.33
2	B	601	HEM	FE-NB	5.80	2.12	1.94
2	A	601	HEM	FE-NB	5.30	2.11	1.94
2	A	601	HEM	FE-NC	4.16	2.08	1.95
2	B	601	HEM	C4B-NB	-3.52	1.31	1.38
2	B	601	HEM	FE-NC	3.47	2.06	1.95
2	B	601	HEM	C1B-NB	-3.11	1.34	1.40
2	A	601	HEM	C3B-C4B	2.96	1.50	1.44
2	A	601	HEM	C1B-NB	-2.94	1.35	1.40
2	A	601	HEM	C4D-ND	-2.89	1.35	1.40
2	B	601	HEM	C4D-ND	-2.57	1.35	1.40
2	B	601	HEM	C1D-ND	-2.50	1.33	1.38
2	A	601	HEM	C1C-C2C	-2.47	1.40	1.45
3	B	602	AER	C15-C14	-2.42	1.50	1.54
2	B	601	HEM	C1C-NC	-2.36	1.35	1.39
2	A	601	HEM	C4B-NB	-2.32	1.34	1.38
2	A	601	HEM	C3C-C4C	-2.29	1.42	1.46
2	A	601	HEM	C4A-NA	-2.19	1.35	1.39
2	B	601	HEM	C4D-C3D	2.05	1.48	1.45
2	A	601	HEM	C1C-NC	-2.02	1.35	1.39
2	B	601	HEM	C3B-C4B	2.02	1.48	1.44
2	A	601	HEM	C1D-ND	-2.00	1.34	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	AER	C15-C16-C17	-10.30	103.62	112.56
3	B	602	AER	C15-C14-C8	-8.06	113.08	121.63
3	B	602	AER	C20-C17-C16	-7.17	115.84	125.08
3	A	602	AER	C20-C17-C16	-7.09	115.94	125.08
3	B	602	AER	C15-C16-C17	-6.40	107.01	112.56
3	A	602	AER	C15-C14-C8	-5.38	115.93	121.63
3	B	602	AER	C13-C17-C16	-4.29	105.84	109.66
3	A	602	AER	C13-C17-C20	-4.01	121.14	125.39
2	A	601	HEM	C1B-NB-C4B	3.99	109.93	105.21
2	B	601	HEM	CMD-C2D-C1D	3.84	131.04	125.03
2	B	601	HEM	CAC-C3C-C4C	3.71	133.67	124.82
2	A	601	HEM	CMD-C2D-C1D	3.47	130.46	125.03
3	B	602	AER	C13-C17-C20	-3.38	121.81	125.39
3	A	602	AER	C14-C15-C16	-3.32	96.15	101.25
2	B	601	HEM	O2A-CGA-CBA	3.27	124.32	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CAD-C3D-C4D	3.16	130.21	124.70
2	A	601	HEM	O2D-CGD-CBD	3.15	123.97	114.00
2	A	601	HEM	CHD-C1D-C2D	-3.15	120.06	125.03
3	B	602	AER	C15-C14-C13	3.13	106.24	104.05
3	A	602	AER	C13-C17-C16	-3.09	106.91	109.66
2	A	601	HEM	C3B-C4B-NB	-3.09	107.25	109.47
3	A	602	AER	C15-C14-C13	2.91	106.09	104.05
2	B	601	HEM	C1B-NB-C4B	2.90	108.64	105.21
2	A	601	HEM	CHD-C1D-ND	2.89	127.54	124.42
2	B	601	HEM	CMB-C2B-C1B	2.88	129.53	125.03
2	B	601	HEM	CHA-C4D-ND	2.79	127.82	124.37
2	A	601	HEM	O2D-CGD-O1D	-2.77	116.21	123.33
2	A	601	HEM	CAC-C3C-C4C	2.73	131.33	124.82
3	B	602	AER	C14-C13-C17	2.71	101.80	99.50
2	B	601	HEM	CAC-C3C-C2C	-2.69	119.67	128.43
3	B	602	AER	C18-C13-C12	-2.66	108.07	111.10
2	A	601	HEM	CMB-C2B-C1B	2.62	129.14	125.03
2	B	601	HEM	O1A-CGA-CBA	-2.62	114.77	123.09
2	A	601	HEM	CHC-C4B-NB	2.62	127.25	124.42
2	B	601	HEM	CHA-C4D-C3D	-2.50	120.62	125.23
3	B	602	AER	C10-C9-C8	-2.49	109.08	112.71
2	A	601	HEM	CAD-C3D-C4D	2.39	128.85	124.70
2	A	601	HEM	CHD-C4C-NC	2.38	127.04	124.45
2	A	601	HEM	CAB-C3B-C2B	-2.36	120.76	128.43
3	B	602	AER	C7-C8-C9	2.36	112.44	109.72
2	A	601	HEM	CHA-C4D-ND	2.29	127.20	124.37
2	A	601	HEM	C4C-NC-C1C	2.27	109.52	105.82
2	B	601	HEM	C4C-NC-C1C	2.27	109.52	105.82
3	B	602	AER	C12-C11-C9	2.22	116.91	113.14
3	B	602	AER	C2-C3-C4	-2.20	107.19	110.29
2	B	601	HEM	CAA-CBA-CGA	-2.19	107.85	113.67
2	A	601	HEM	CHB-C1B-NB	2.19	127.08	124.37
3	B	602	AER	C18-C13-C17	-2.17	104.40	107.81
3	A	602	AER	C10-C9-C8	-2.16	109.55	112.71
3	A	602	AER	C11-C9-C10	2.14	115.73	113.08
2	A	601	HEM	C2D-C1D-ND	2.14	112.38	109.90
3	B	602	AER	C4-C5-C6	-2.13	117.68	120.57
2	A	601	HEM	CBA-CAA-C2A	-2.13	106.65	112.53
3	B	602	AER	C13-C14-C8	2.13	115.37	113.13
2	B	601	HEM	O2D-CGD-CBD	2.12	120.71	114.00
2	A	601	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
2	A	601	HEM	CAC-C3C-C2C	-2.08	121.67	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	AER	C11-C9-C8	2.08	114.68	111.78
3	A	602	AER	C18-C13-C12	-2.05	108.77	111.10
2	B	601	HEM	CMC-C2C-C1C	2.04	128.31	124.73
2	A	601	HEM	O1A-CGA-CBA	-2.03	116.66	123.09
2	A	601	HEM	CAB-C3B-C4B	2.01	133.28	124.39
3	A	602	AER	C11-C9-C8	2.01	114.58	111.78
3	B	602	AER	C24-C25-C20	-2.01	118.39	120.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C4B-C3B-CAB-CBB
2	A	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	C4B-C3B-CAB-CBB
2	B	601	HEM	C4C-C3C-CAC-CBC
3	B	602	AER	C13-C17-C20-C25
3	B	602	AER	C13-C17-C20-C21
3	A	602	AER	C13-C17-C20-C25
3	A	602	AER	C13-C17-C20-C21
2	B	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAA-CBA-CGA-O1A

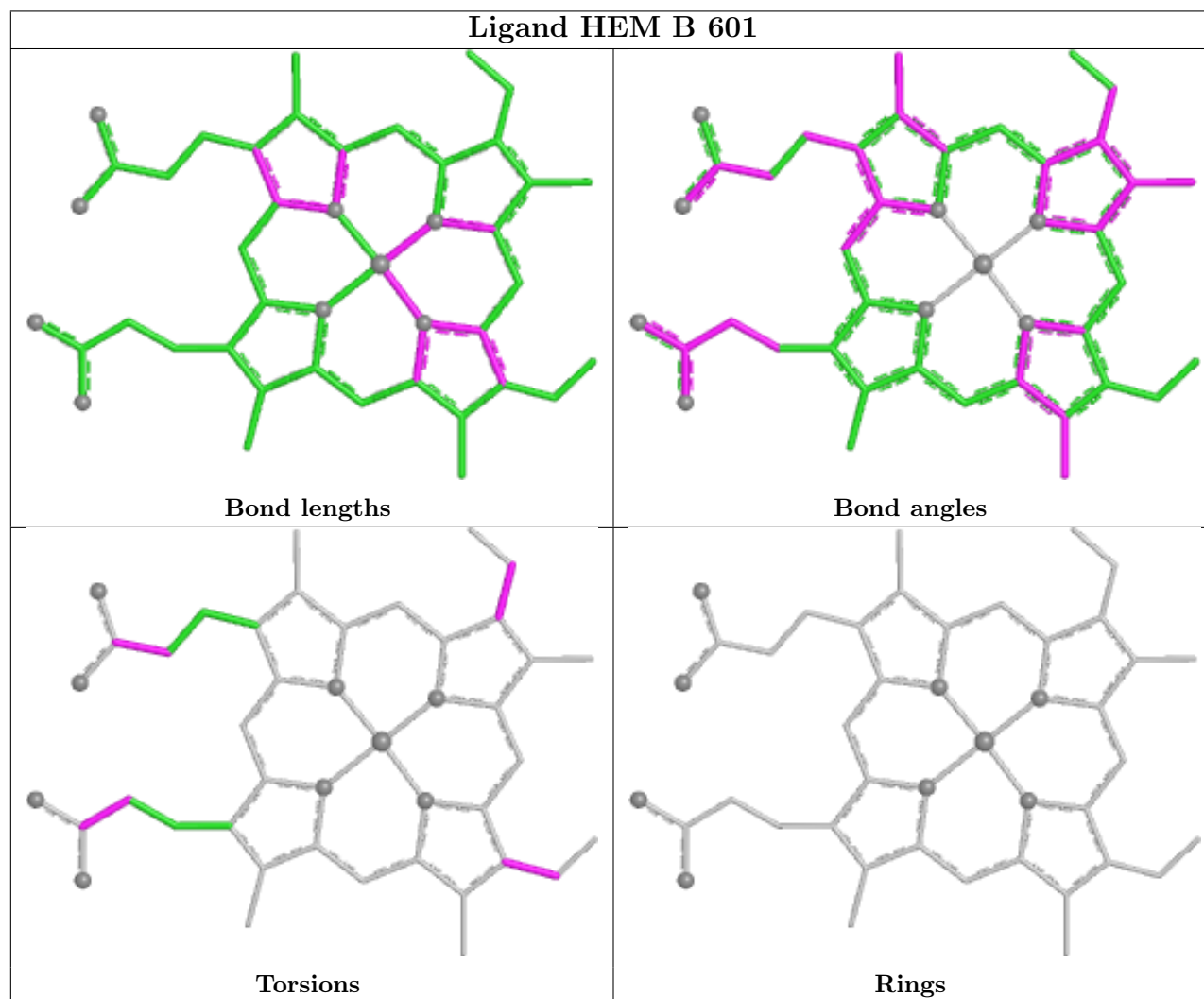
There are no ring outliers.

4 monomers are involved in 11 short contacts:

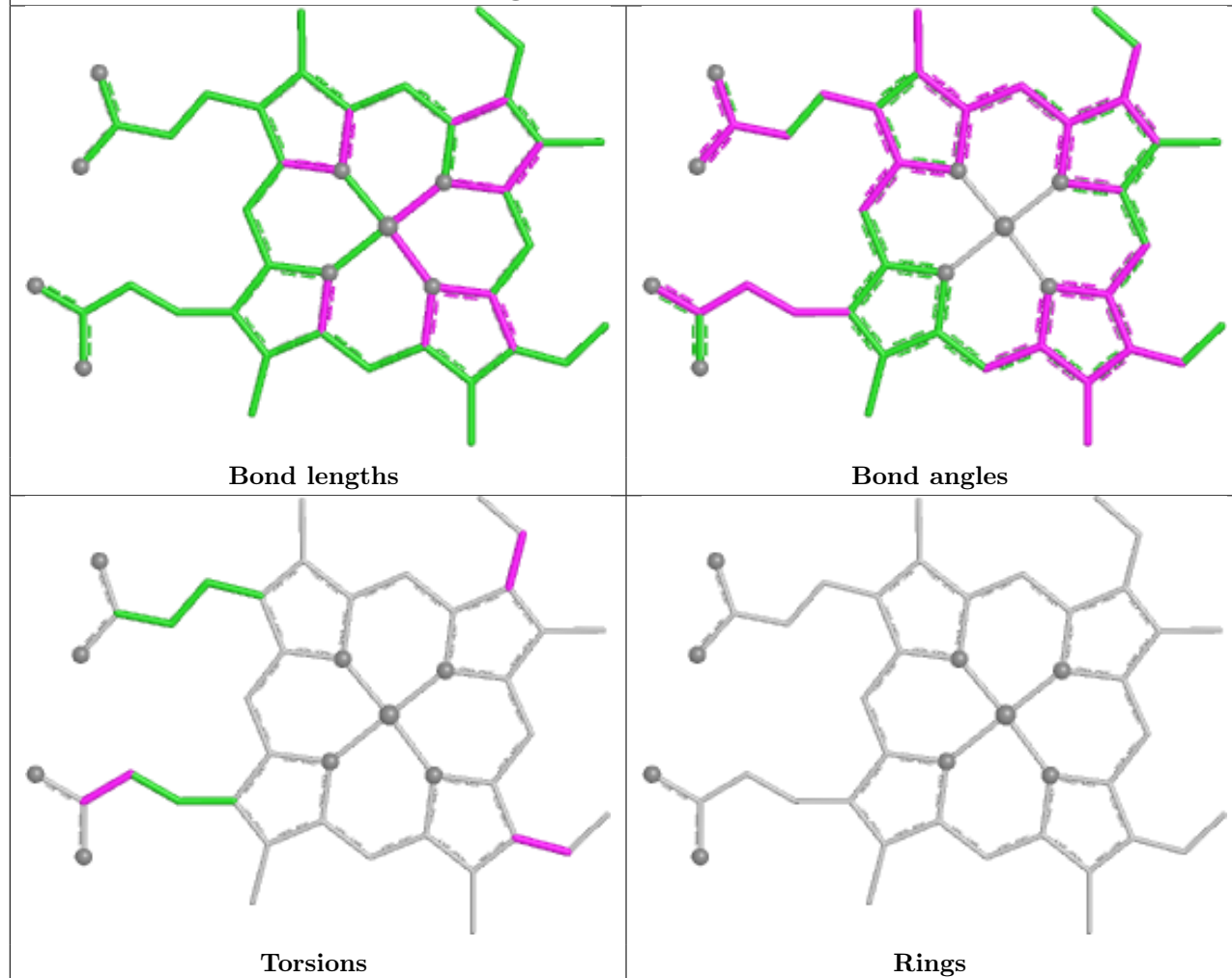
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	7	0
2	A	601	HEM	4	0
3	B	602	AER	3	0
3	A	602	AER	2	0

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

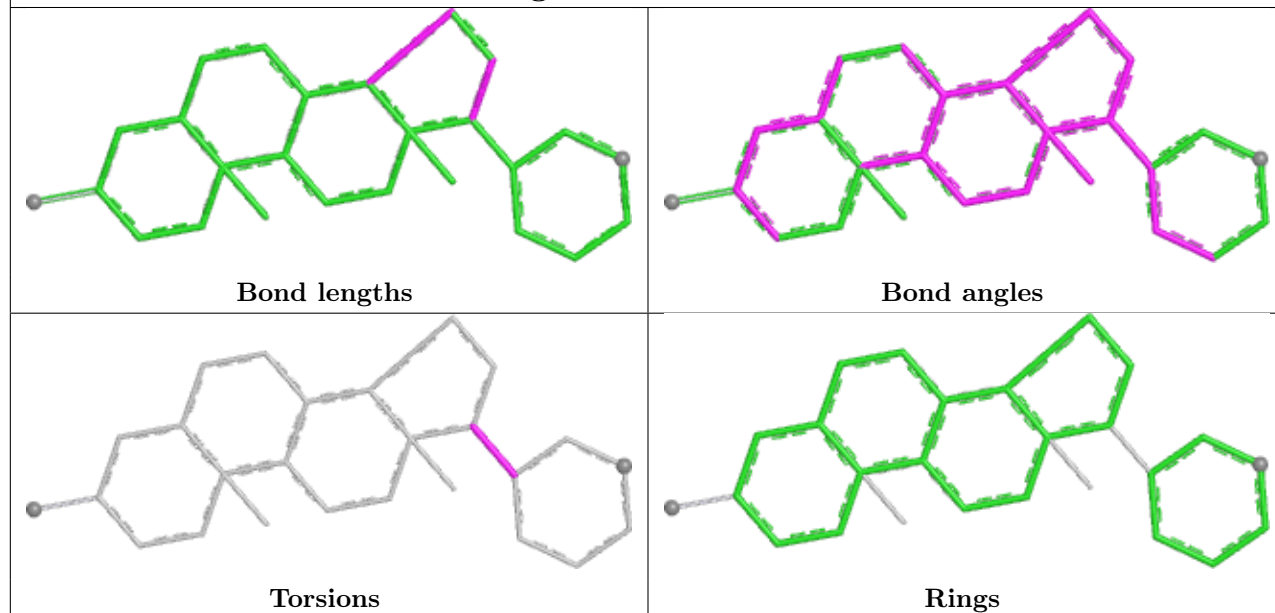
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

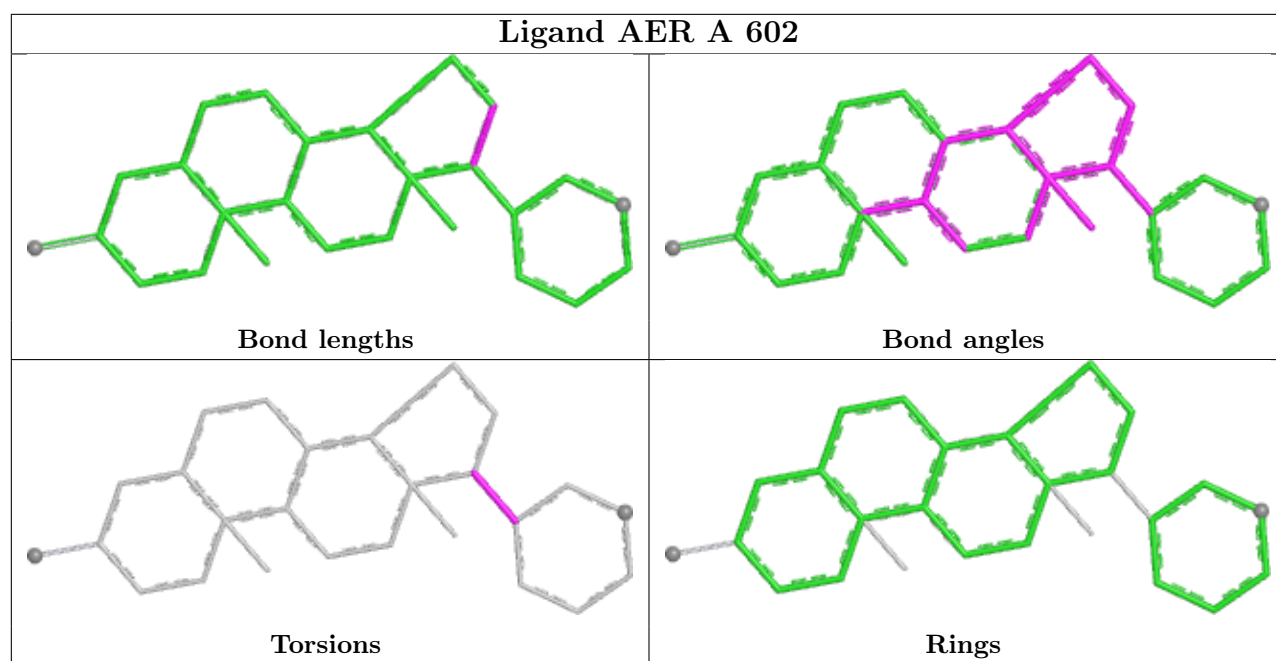


Ligand HEM A 601



Ligand AER B 602





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	465/509 (91%)	-0.40	3 (0%) 85 69	32, 76, 109, 140	9 (1%)
1	B	470/509 (92%)	-0.40	1 (0%) 91 83	42, 73, 109, 166	11 (2%)
All	All	935/1018 (91%)	-0.40	4 (0%) 88 76	32, 74, 109, 166	20 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	2.9
1	B	224	LYS	2.2
1	A	152	SER	2.1
1	A	183	GLU	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.

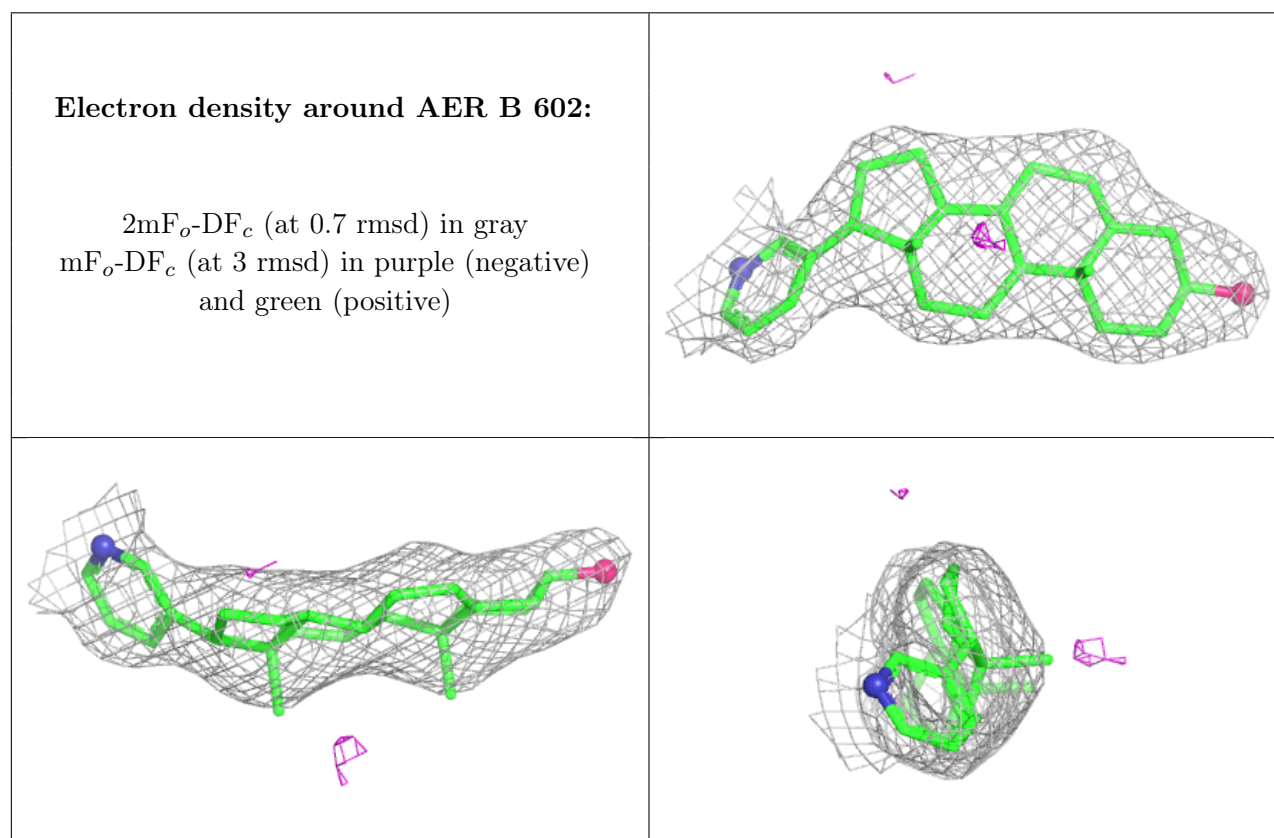
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	B	604	4/4	0.51	0.24	93,97,100,103	0

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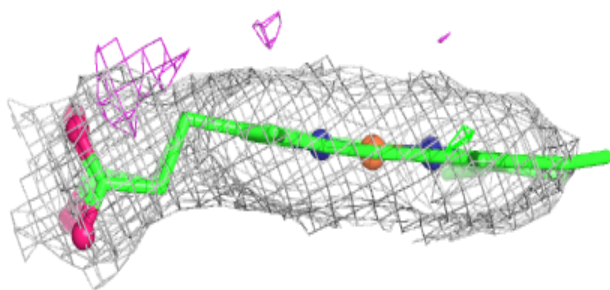
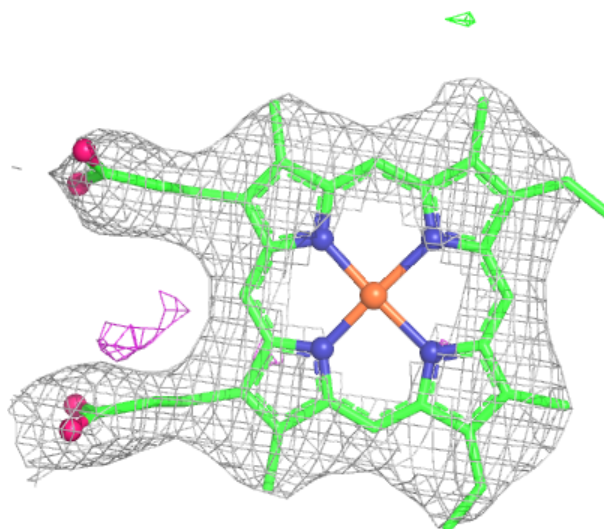
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	B	606	4/4	0.88	0.17	85,93,95,99	0
4	ACT	B	605	4/4	0.93	0.20	71,90,92,94	0
4	ACT	A	603	4/4	0.94	0.16	67,80,81,83	0
5	CL	B	603	1/1	0.96	0.06	94,94,94,94	0
3	AER	B	602	26/26	0.97	0.08	53,58,61,66	0
2	HEM	A	601	43/43	0.97	0.09	50,56,70,75	0
3	AER	A	602	26/26	0.97	0.08	58,63,68,71	0
2	HEM	B	601	43/43	0.98	0.07	51,56,65,74	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.



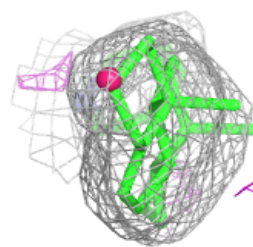
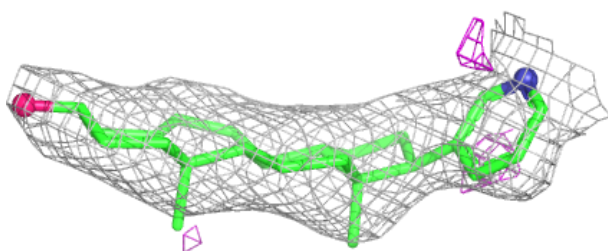
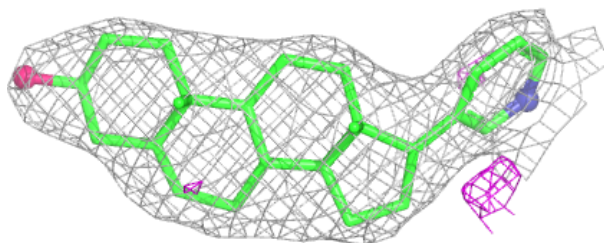
Electron density around HEM A 601:

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

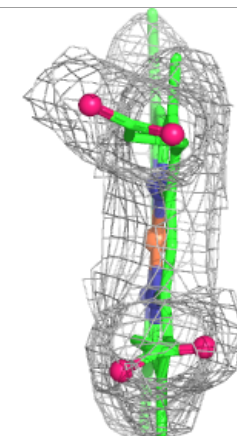
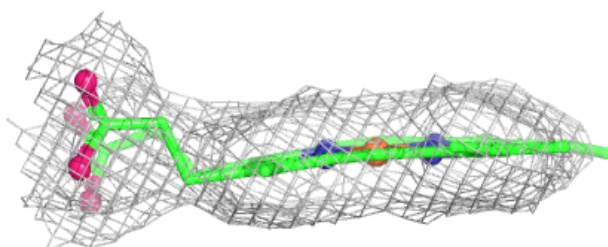
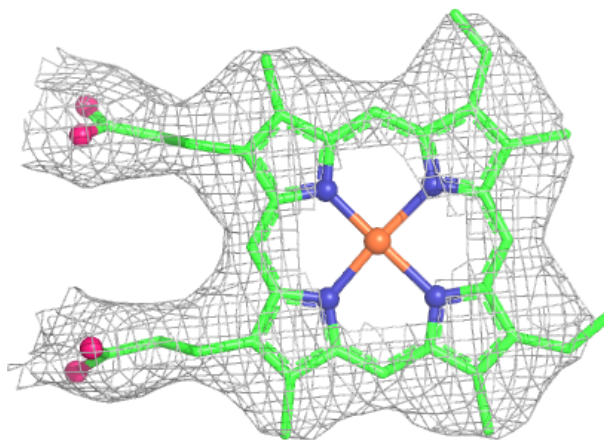


Electron density around AER A 602:

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

**Electron density around HEM B 601:**

$2mF_o-DF_c$ (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.