



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2021 – 04:06 PM EST

PDB ID : 7KVN  
Title : Human CYP3A4 bound to an inhibitor  
Authors : Sevrioukova, I.  
Deposited on : 2020-11-28  
Resolution : 2.70 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 : 2.16  
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) : 2.16

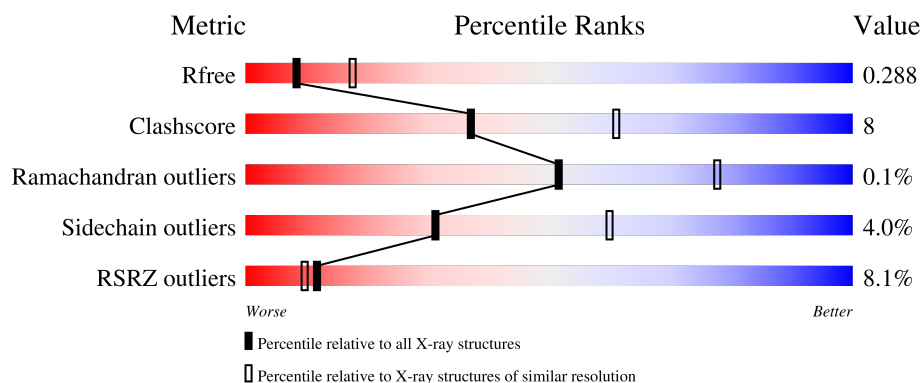
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	487	<div> <div>4%</div> <div>74%</div> <div>16%</div> <div>• 7%</div> </div>
1	B	487	<div> <div>11%</div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7488 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	2	0
			3653	2381	600	647	25			
1	B	448	Total	C	N	O	S	0	1	0
			3606	2353	587	642	24			

There are 48 discrepancies between the modelled and reference sequences:

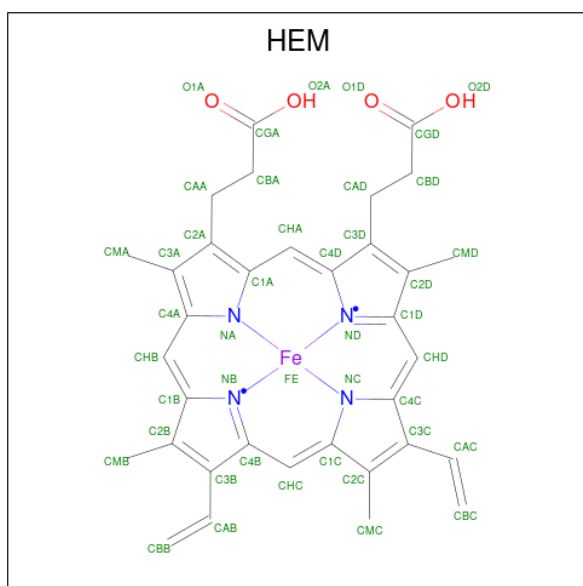
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	UNP P08684
A	?	-	TRP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	SER	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	?	-	LEU	deletion	UNP P08684

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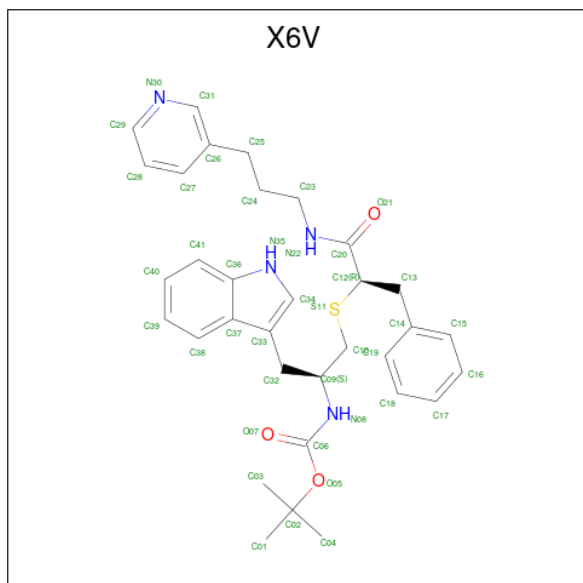
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	SER	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684

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



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

- Molecule 3 is tert-butyl [(2S)-1-(1H-indol-3-yl)-3-{[(2R)-1-oxo-3-phenyl-1-{[3-(pyridin-3-yl)propyl]amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (three-letter code: X6V) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 41	C 33	N 4	O 3	S 1	0	0
3	B	1	Total 41	C 33	N 4	O 3	S 1	0	0

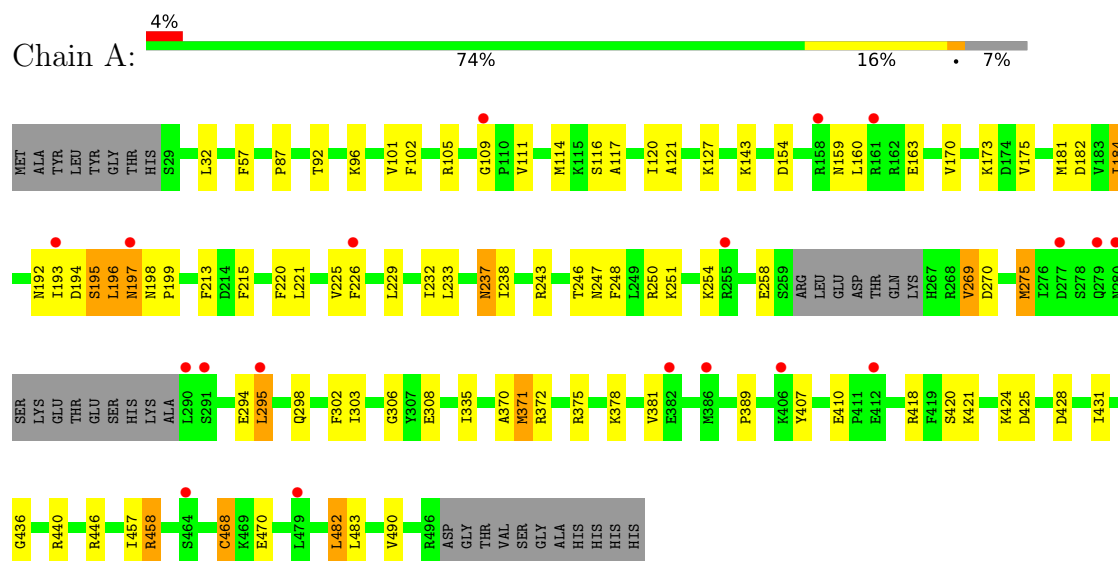
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	22	Total	O	0	0
			22	22		

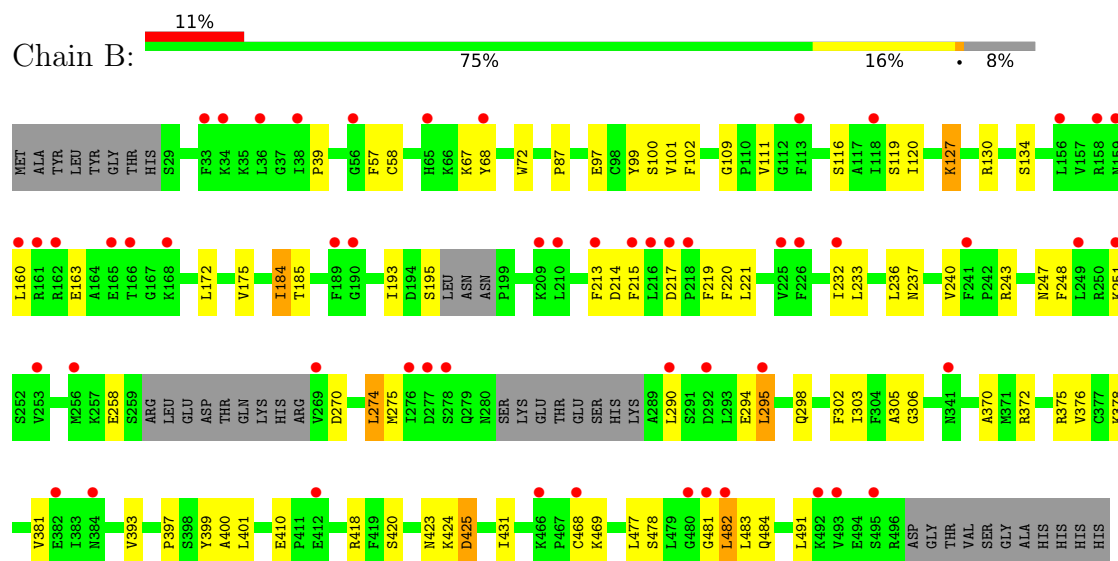
### 3 Residue-property plots [i](#)

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 3A4



#### • Molecule 1: Cytochrome P450 3A4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.76Å 95.61Å 93.02Å 90.00° 124.21° 90.00°	Depositor
Resolution (Å)	40.03 – 2.70 40.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.03-2.70) 90.8 (40.03-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.248 , 0.290 0.249 , 0.288	Depositor DCC
$R_{free}$ test set	1421 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.2	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.007 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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, X6V

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	0.30	0/3748	0.46	2/5068 (0.0%)
1	B	0.26	0/3696	0.42	0/4997
All	All	0.28	0/7444	0.44	2/10065 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	N-CA-CB	-5.38	100.91	110.60
1	A	269	VAL	N-CA-C	5.24	125.15	111.00

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	3653	0	3747	67	0
1	B	3606	0	3695	47	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
3	A	41	0	0	1	0
3	B	41	0	0	2	0
4	A	39	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	22	0	0	0	0
All	All	7488	0	7502	117	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 8.

All (117) 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:269:VAL:HG12	1:A:269:VAL:O	1.50	1.11
1:A:229:LEU:HD23	1:A:232:ILE:HD12	1.57	0.84
1:A:197:ASN:HA	1:A:198:ASN:HB2	1.58	0.83
1:A:197:ASN:HA	1:A:198:ASN:CB	2.08	0.82
1:A:269:VAL:O	1:A:269:VAL:CG1	2.26	0.79
1:A:195:SER:O	1:A:196:LEU:HB2	1.82	0.78
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.68	0.76
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.68	0.73
1:B:248:PHE:HA	1:B:251:LYS:HE2	1.71	0.73
1:B:219:PHE:HE2	1:B:240:VAL:HG12	1.53	0.72
1:A:248:PHE:HA	1:A:251:LYS:HE2	1.69	0.72
1:B:68:TYR:HB3	1:B:72:TRP:HB3	1.75	0.69
1:A:194:ASP:OD1	1:A:197:ASN:HA	1.93	0.68
1:B:420:SER:OG	1:B:423:ASN:ND2	2.28	0.67
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.78	0.66
1:B:214:ASP:HB3	1:B:217:ASP:HB2	1.79	0.64
1:B:270:ASP:O	1:B:274:LEU:HD12	1.97	0.64
1:A:197:ASN:CA	1:A:198:ASN:HB2	2.26	0.63
1:B:213:PHE:CE1	1:B:220:PHE:HB3	2.33	0.63
1:A:116:SER:O	1:A:298:GLN:NE2	2.31	0.63
1:B:120:ILE:HG12	3:B:602:X6V:S11	2.38	0.62
1:B:116:SER:O	1:B:298:GLN:NE2	2.33	0.61
1:A:194:ASP:OD1	1:A:197:ASN:CA	2.48	0.61
1:A:254:LYS:NZ	4:A:702:HOH:O	2.33	0.61
1:B:185:THR:HG21	1:B:193:ILE:HD12	1.83	0.60
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.84	0.59
1:B:160:LEU:HD21	1:B:175:VAL:HG11	1.86	0.57
1:A:197:ASN:HB3	4:A:718:HOH:O	2.02	0.57
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.88	0.56
1:B:233:LEU:HA	1:B:236:LEU:HB2	1.88	0.56
1:B:243:ARG:NE	1:B:247:ASN:HD21	2.04	0.56
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:HD23	1:B:482:LEU:H	1.70	0.55
1:A:194:ASP:OD1	1:A:197:ASN:N	2.39	0.55
1:A:109:GLY:HA2	1:A:111:VAL:HG13	1.89	0.54
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.89	0.54
1:A:225:VAL:HG12	1:A:226:PHE:HD2	1.72	0.54
1:A:482:LEU:H	1:A:482:LEU:HD23	1.73	0.54
1:A:121:ALA:O	1:A:440:ARG:NH2	2.38	0.53
1:A:159:ASN:HD21	1:A:197:ASN:HD22	1.55	0.53
1:A:213:PHE:CE1	1:A:220:PHE:HB3	2.44	0.53
1:B:119:SER:HB3	2:B:601:HEM:HAD1	1.89	0.53
1:B:68:TYR:CB	1:B:72:TRP:HB3	2.38	0.53
1:A:184:ILE:HG21	1:A:303:ILE:HA	1.90	0.52
1:A:420:SER:O	1:A:424:LYS:N	2.42	0.52
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.92	0.51
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.93	0.51
1:A:192:ASN:HD21	1:A:195:SER:HA	1.76	0.51
1:B:109:GLY:HA2	1:B:111:VAL:HG13	1.94	0.50
1:A:229:LEU:HA	1:A:232:ILE:HG13	1.93	0.50
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.93	0.50
1:A:421:LYS:HG3	1:A:424:LYS:HE3	1.95	0.49
1:A:184:ILE:HG13	1:A:306:GLY:HA3	1.95	0.48
1:A:181:MET:HG3	1:A:193:ILE:HD11	1.95	0.48
1:A:275:MET:HB3	1:A:295:LEU:HD12	1.95	0.48
1:B:294:GLU:O	1:B:298:GLN:HG2	2.14	0.48
1:B:97:GLU:OE1	1:B:100:SER:OG	2.21	0.48
1:A:371:MET:SD	1:A:483:LEU:HB2	2.54	0.47
1:A:92:THR:HA	1:A:96:LYS:HB2	1.97	0.47
1:A:294:GLU:O	1:A:298:GLN:HG2	2.15	0.46
1:B:57:PHE:HE2	1:B:481:GLY:HA2	1.79	0.46
1:A:160:LEU:HD21	1:A:175:VAL:HG11	1.97	0.46
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.97	0.46
1:A:196:LEU:O	1:A:197:ASN:ND2	2.48	0.46
1:A:173:LYS:NZ	1:A:308:GLU:OE2	2.37	0.46
1:A:243:ARG:NE	1:A:247:ASN:HD21	2.14	0.46
1:A:117:ALA:HB3	1:A:120:ILE:HG13	1.96	0.46
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.97	0.46
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.97	0.46
1:B:478:SER:N	1:B:484:GLN:O	2.42	0.46
1:A:159:ASN:ND2	1:A:197:ASN:ND2	2.63	0.45
1:A:468:CYS:O	1:A:470:GLU:N	2.49	0.45
1:A:246:THR:O	1:A:250:ARG:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MET:HB2	1:B:295:LEU:HD12	1.98	0.45
1:A:159:ASN:ND2	1:A:197:ASN:HD22	2.15	0.45
1:B:39:PRO:HB2	1:B:68:TYR:HD2	1.80	0.45
1:A:111:VAL:HB	1:A:114:MET:HB2	2.00	0.44
1:A:102:PHE:HB3	1:A:375:ARG:HB3	2.00	0.44
1:A:407:TYR:OH	1:A:428:ASP:N	2.48	0.44
1:B:290:LEU:HD23	1:B:295:LEU:HB2	2.00	0.44
1:A:143:LYS:NZ	4:A:706:HOH:O	2.37	0.44
1:A:87:PRO:HG3	1:A:431:ILE:HD11	2.00	0.44
1:A:154:ASP:OD1	1:A:458:ARG:NH1	2.51	0.43
1:B:410:GLU:O	1:B:418:ARG:NH2	2.48	0.43
1:A:57:PHE:HB2	1:A:371:MET:CE	2.49	0.43
1:A:407:TYR:OH	1:A:428:ASP:HB2	2.17	0.43
1:B:370:ALA:O	1:B:372:ARG:N	2.44	0.43
1:B:477:LEU:HD13	1:B:483:LEU:HD11	2.01	0.43
1:A:120:ILE:HG12	3:A:602:X6V:S11	2.59	0.43
1:A:233:LEU:HB3	1:A:238:ILE:HB	2.01	0.43
1:A:32:LEU:HD11	1:A:389:PRO:HG2	2.00	0.42
1:B:68:TYR:HB3	1:B:72:TRP:CB	2.46	0.42
1:A:199:PRO:HD2	4:A:712:HOH:O	2.18	0.42
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.54	0.42
1:A:193:ILE:HG13	1:A:193:ILE:H	1.75	0.42
1:B:99:TYR:CD2	1:B:127:LYS:HD2	2.54	0.42
1:A:410:GLU:O	1:A:418:ARG:NH2	2.51	0.42
1:B:130:ARG:O	1:B:134:SER:OG	2.23	0.42
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.54	0.42
1:B:219:PHE:CE2	1:B:240:VAL:HG12	2.44	0.42
1:A:237:ASN:ND2	1:A:237:ASN:O	2.42	0.42
1:A:170:VAL:O	1:A:490:VAL:HA	2.20	0.42
1:B:101:VAL:HA	1:B:378:LYS:HG2	2.01	0.42
1:A:182:ASP:OD1	1:A:194:ASP:HB3	2.20	0.41
1:A:370:ALA:O	1:A:372:ARG:N	2.47	0.41
1:A:101:VAL:HA	1:A:378:LYS:HG2	2.02	0.41
1:B:397:PRO:HB2	1:B:400:ALA:HB3	2.02	0.41
1:B:305:ALA:HB2	3:B:602:X6V:C25	2.51	0.41
1:A:335:ILE:HD13	1:A:457:ILE:HA	2.02	0.41
1:A:105:ARG:HH21	2:A:601:HEM:HAA1	1.85	0.41
1:A:225:VAL:HG12	1:A:226:PHE:CD2	2.55	0.41
1:A:446[A]:ARG:HE	1:B:425:ASP:HB3	1.85	0.41
1:B:376:VAL:HG22	1:B:393:VAL:HG22	2.03	0.41
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:HB3	1:B:431:ILE:HG23	2.03	0.40
1:B:275:MET:HB3	1:B:290:LEU:HD22	2.03	0.40
1:B:220:PHE:HE2	1:B:240:VAL:HB	1.86	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	448/487 (92%)	413 (92%)	34 (8%)	1 (0%)	47	73
1	B	441/487 (91%)	413 (94%)	28 (6%)	0	100	100
All	All	889/974 (91%)	826 (93%)	62 (7%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN

### 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	416/443 (94%)	400 (96%)	16 (4%)	33	62
1	B	410/443 (93%)	393 (96%)	17 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	826/886 (93%)	793 (96%)	33 (4%)	31	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	163	GLU
1	A	184	ILE
1	A	195	SER
1	A	196	LEU
1	A	215	PHE
1	A	221	LEU
1	A	237	ASN
1	A	258	GLU
1	A	275	MET
1	A	295	LEU
1	A	371	MET
1	A	425	ASP
1	A	458	ARG
1	A	468	CYS
1	A	482	LEU
1	B	67	LYS
1	B	127	LYS
1	B	163	GLU
1	B	184	ILE
1	B	195	SER
1	B	215	PHE
1	B	221	LEU
1	B	232	ILE
1	B	237	ASN
1	B	258	GLU
1	B	274	LEU
1	B	295	LEU
1	B	424	LYS
1	B	425	ASP
1	B	468	CYS
1	B	469	LYS
1	B	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
3	X6V	B	602	2	42,44,44	1.74	10 (23%)	47,59,59	2.11	11 (23%)
2	HEM	A	601	1,3	27,50,50	1.89	5 (18%)	17,82,82	1.44	2 (11%)
3	X6V	A	602	2	42,44,44	1.64	10 (23%)	47,59,59	2.19	13 (27%)
2	HEM	B	601	1,3	27,50,50	1.87	4 (14%)	17,82,82	1.42	1 (5%)

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	X6V	B	602	2	-	16/32/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1,3	-	0/6/54/54	-
3	X6V	A	602	2	-	16/32/33/33	0/4/4/4
2	HEM	B	601	1,3	-	0/6/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	X6V	C10-S11	4.90	1.87	1.82
2	A	601	HEM	C3C-C2C	-4.58	1.34	1.40
2	B	601	HEM	C3C-C2C	-4.54	1.34	1.40
3	B	602	X6V	C12-S11	4.08	1.87	1.83
3	A	602	X6V	C10-S11	4.03	1.86	1.82
2	A	601	HEM	C3B-CAB	3.82	1.55	1.47
2	B	601	HEM	C3B-CAB	3.78	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.73	1.35	1.40
2	B	601	HEM	C3C-CAC	3.71	1.55	1.47
2	A	601	HEM	C3C-CAC	3.71	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.66	1.35	1.40
3	B	602	X6V	C20-N22	3.48	1.41	1.33
3	A	602	X6V	C12-S11	3.45	1.86	1.83
3	A	602	X6V	C20-N22	3.25	1.40	1.33
3	A	602	X6V	C06-N08	2.88	1.41	1.34
3	B	602	X6V	C06-N08	2.64	1.41	1.34
3	A	602	X6V	O05-C06	2.30	1.39	1.34
3	B	602	X6V	O07-C06	2.26	1.25	1.21
3	B	602	X6V	C34-C33	2.23	1.43	1.37
3	A	602	X6V	O07-C06	2.22	1.25	1.21
3	B	602	X6V	C32-C09	2.21	1.58	1.53
3	A	602	X6V	C34-C33	2.18	1.43	1.37
3	B	602	X6V	O05-C02	-2.09	1.44	1.48
3	A	602	X6V	C32-C09	2.09	1.58	1.53
3	B	602	X6V	C37-C36	-2.08	1.37	1.42
2	A	601	HEM	CAA-C2A	2.08	1.55	1.52
3	A	602	X6V	C37-C36	-2.03	1.37	1.42
3	B	602	X6V	C34-N35	2.02	1.40	1.36
3	A	602	X6V	C09-N08	2.00	1.50	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	X6V	O05-C06-N08	7.95	123.37	110.02
3	B	602	X6V	O05-C06-N08	7.86	123.22	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	X6V	O05-C06-O07	-4.94	116.61	125.62
3	A	602	X6V	O05-C06-O07	-4.84	116.79	125.62
3	A	602	X6V	C32-C33-C37	4.57	133.36	126.25
3	B	602	X6V	C32-C33-C37	4.30	132.94	126.25
3	B	602	X6V	C38-C37-C33	-3.76	127.51	134.42
3	A	602	X6V	C32-C33-C34	-3.61	123.50	127.97
3	A	602	X6V	C38-C37-C33	-3.59	127.83	134.42
3	A	602	X6V	O21-C20-N22	-3.33	115.84	122.99
3	A	602	X6V	C39-C38-C37	-3.30	116.32	120.89
3	B	602	X6V	C32-C33-C34	-3.27	123.93	127.97
3	B	602	X6V	C39-C38-C37	-3.27	116.36	120.89
3	B	602	X6V	O21-C20-N22	-3.22	116.07	122.99
3	A	602	X6V	O07-C06-N08	-3.06	119.83	124.85
3	B	602	X6V	C40-C41-C36	-2.92	115.87	120.08
3	A	602	X6V	C40-C41-C36	-2.91	115.89	120.08
3	B	602	X6V	C38-C37-C36	2.87	121.97	118.17
3	B	602	X6V	O07-C06-N08	-2.86	120.16	124.85
3	A	602	X6V	C38-C37-C36	2.81	121.89	118.17
3	A	602	X6V	O21-C20-C12	-2.71	117.69	121.61
3	B	602	X6V	O21-C20-C12	-2.54	117.93	121.61
3	A	602	X6V	C14-C13-C12	2.53	116.95	113.32
2	A	601	HEM	CBD-CAD-C3D	-2.38	108.10	112.48
2	A	601	HEM	CMB-C2B-C3B	2.29	128.97	124.68
2	B	601	HEM	CMB-C2B-C3B	2.26	128.90	124.68
3	A	602	X6V	C09-N08-C06	2.23	125.73	122.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	X6V	C20-C12-S11-C10
3	B	602	X6V	O05-C06-N08-C09
3	B	602	X6V	O07-C06-N08-C09
3	B	602	X6V	C32-C09-C10-S11
3	B	602	X6V	C10-C09-C32-C33
3	B	602	X6V	C32-C09-N08-C06
3	B	602	X6V	C09-C10-S11-C12
3	A	602	X6V	C13-C12-S11-C10
3	A	602	X6V	C20-C12-S11-C10
3	A	602	X6V	O05-C06-N08-C09
3	A	602	X6V	O07-C06-N08-C09
3	A	602	X6V	C32-C09-C10-S11

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Mol	Chain	Res	Type	Atoms
3	A	602	X6V	C32-C09-N08-C06
3	A	602	X6V	C09-C10-S11-C12
3	B	602	X6V	O07-C06-O05-C02
3	B	602	X6V	N08-C06-O05-C02
3	A	602	X6V	N08-C06-O05-C02
3	A	602	X6V	O07-C06-O05-C02
3	B	602	X6V	C01-C02-O05-C06
3	B	602	X6V	C03-C02-O05-C06
3	B	602	X6V	C04-C02-O05-C06
3	B	602	X6V	C20-C12-C13-C14
3	B	602	X6V	N08-C09-C32-C33
3	A	602	X6V	C20-C12-C13-C14
3	A	602	X6V	C01-C02-O05-C06
3	A	602	X6V	C04-C02-O05-C06
3	A	602	X6V	N22-C23-C24-C25
3	B	602	X6V	N22-C23-C24-C25
3	A	602	X6V	C03-C02-O05-C06
3	B	602	X6V	N08-C09-C10-S11
3	A	602	X6V	N08-C09-C10-S11
3	A	602	X6V	C10-C09-C32-C33

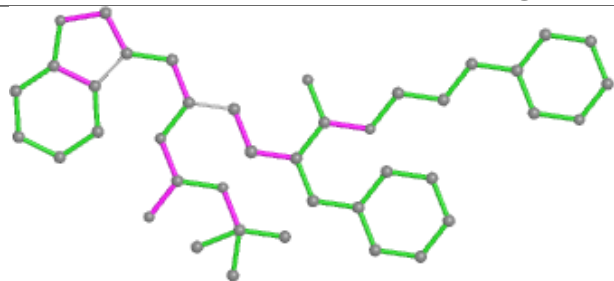
There are no ring outliers.

4 monomers are involved in 12 short contacts:

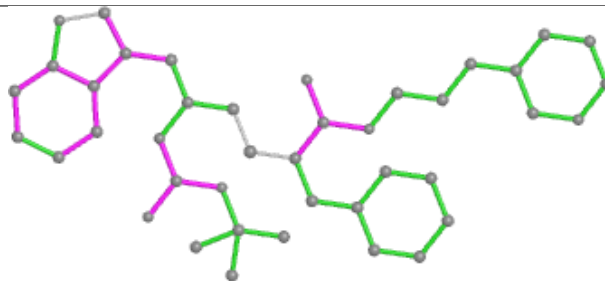
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	X6V	2	0
2	A	601	HEM	5	0
3	A	602	X6V	1	0
2	B	601	HEM	4	0

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.

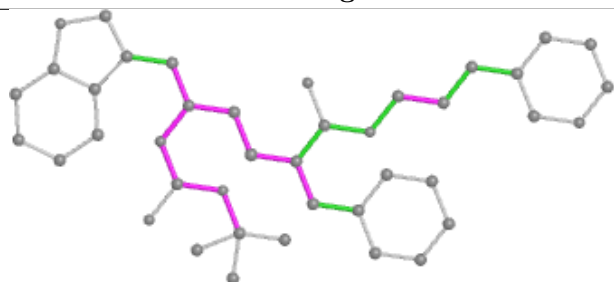
## Ligand X6V B 602



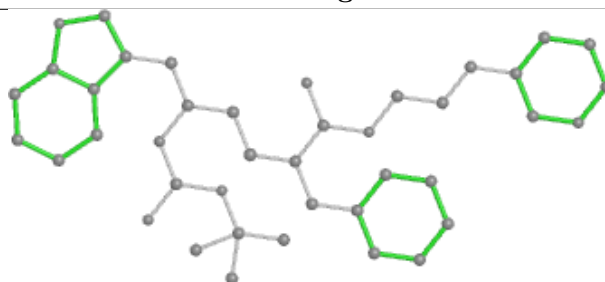
Bond lengths



Bond angles

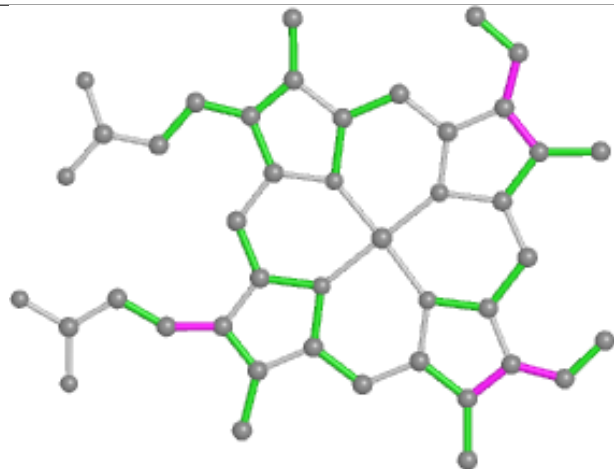


Torsions

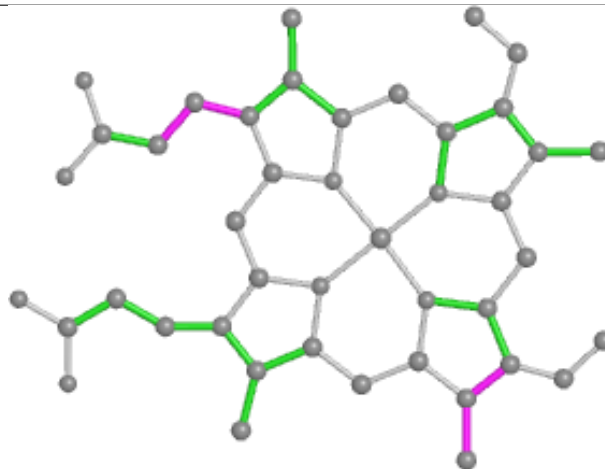


Rings

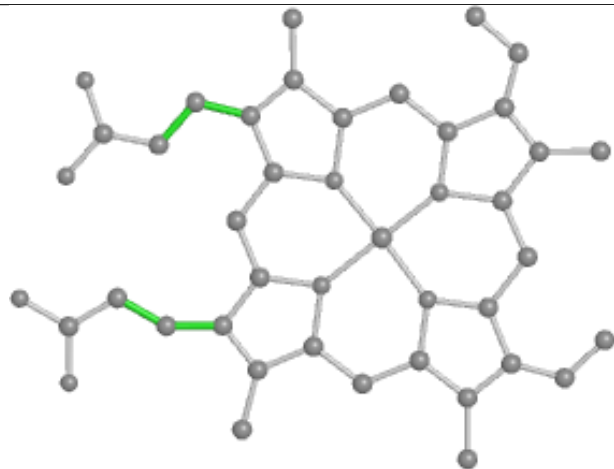
## Ligand HEM A 601



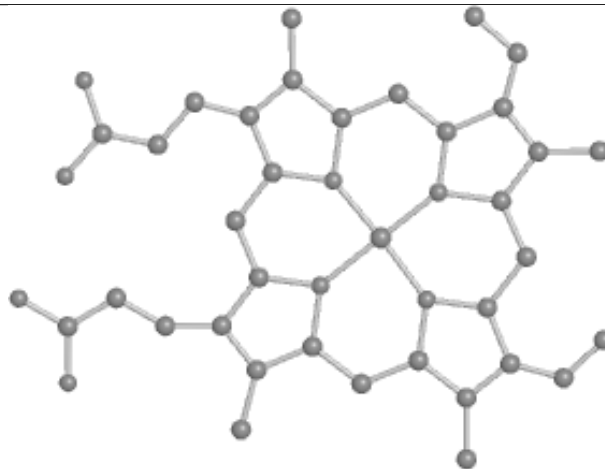
Bond lengths



Bond angles

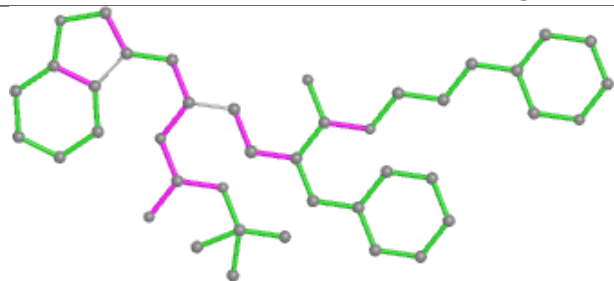


Torsions

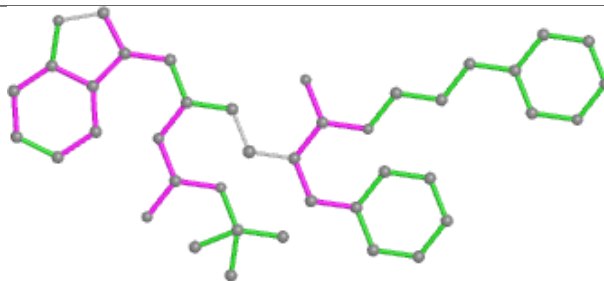


Rings

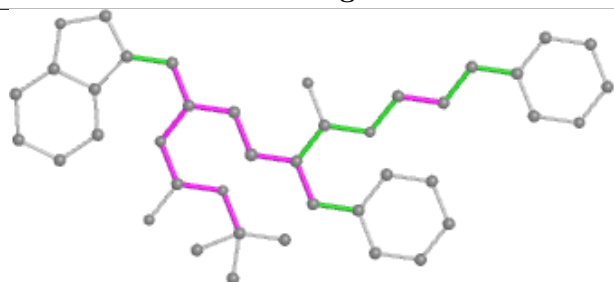
## Ligand X6V A 602



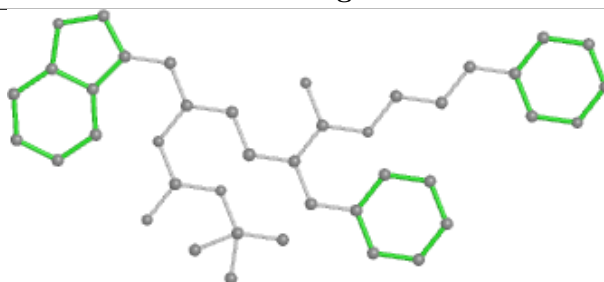
Bond lengths



Bond angles

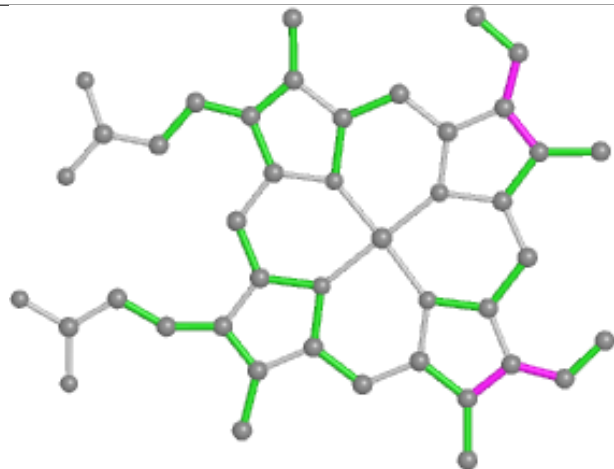


Torsions

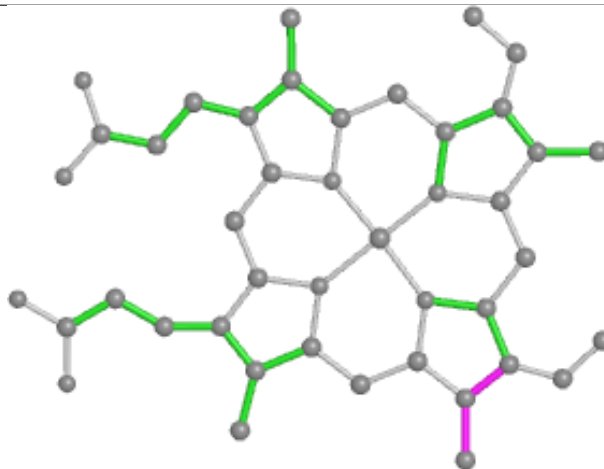


Rings

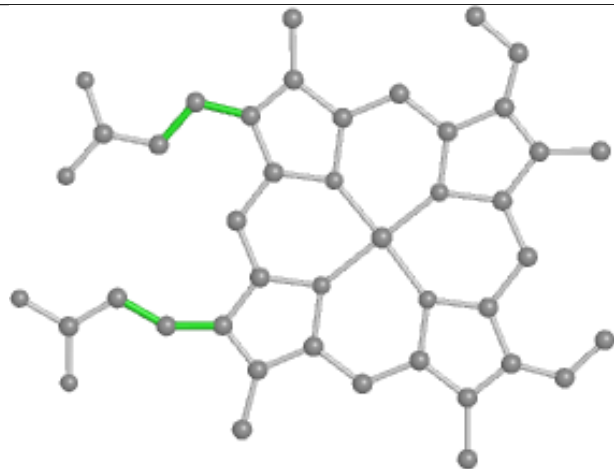
## Ligand HEM B 601



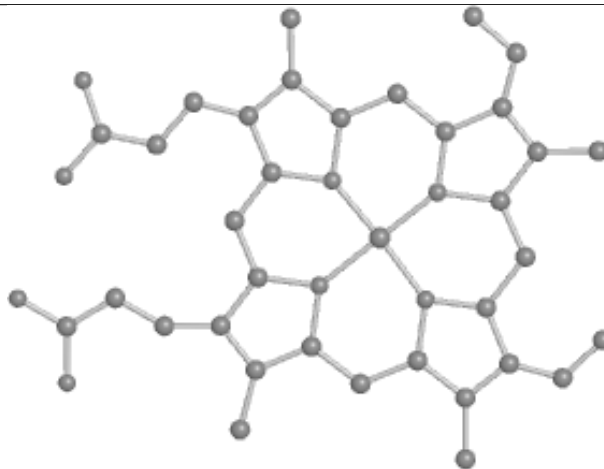
Bond lengths



Bond angles



Torsions



Rings

## 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	452/487 (92%)	0.25	19 (4%) 36 35	40, 73, 112, 182	0
1	B	448/487 (91%)	0.68	54 (12%) 4 3	53, 90, 136, 186	0
All	All	900/974 (92%)	0.47	73 (8%) 12 10	40, 81, 126, 186	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	TYR	6.8
1	A	158	ARG	5.7
1	A	479	LEU	5.6
1	B	253	VAL	4.4
1	B	341	ASN	4.3
1	B	256	MET	3.9
1	B	168	LYS	3.9
1	B	493	VAL	3.9
1	B	468	CYS	3.7
1	B	213	PHE	3.4
1	B	34	LYS	3.3
1	B	160	LEU	3.2
1	A	226	PHE	3.2
1	B	495	SER	3.2
1	B	226	PHE	3.1
1	A	197	ASN	3.1
1	A	412	GLU	3.0
1	B	159	ASN	3.0
1	B	295	LEU	3.0
1	B	292	ASP	3.0
1	A	386	MET	3.0
1	A	382	GLU	2.9
1	B	166	THR	2.9
1	B	161	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	216	LEU	2.9
1	B	218	PRO	2.9
1	B	225	VAL	2.8
1	B	278	SER	2.8
1	A	277	ASP	2.8
1	B	466	LYS	2.7
1	B	189	PHE	2.7
1	A	280	ASN	2.7
1	B	251	LYS	2.7
1	B	217	ASP	2.7
1	B	412	GLU	2.7
1	A	193	ILE	2.6
1	B	158	ARG	2.6
1	B	232	ILE	2.6
1	A	406	LYS	2.6
1	B	165	GLU	2.6
1	B	113	PHE	2.6
1	B	482	LEU	2.5
1	B	56	GLY	2.5
1	B	38	ILE	2.5
1	B	118	ILE	2.4
1	B	241	PHE	2.4
1	B	215	PHE	2.4
1	B	210	LEU	2.4
1	B	162	ARG	2.4
1	A	161	ARG	2.4
1	A	464	SER	2.3
1	B	249	LEU	2.3
1	B	33	PHE	2.3
1	B	190	GLY	2.2
1	A	291	SER	2.2
1	B	290	LEU	2.2
1	A	255	ARG	2.2
1	B	269	VAL	2.2
1	B	384	ASN	2.2
1	B	492	LYS	2.2
1	A	109	GLY	2.1
1	B	277	ASP	2.1
1	B	480	GLY	2.1
1	B	36	LEU	2.1
1	B	481	GLY	2.1
1	B	209	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLU	2.1
1	B	65	HIS	2.1
1	B	156	LEU	2.1
1	A	279	GLN	2.0
1	A	295	LEU	2.0
1	B	276	ILE	2.0
1	A	290	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

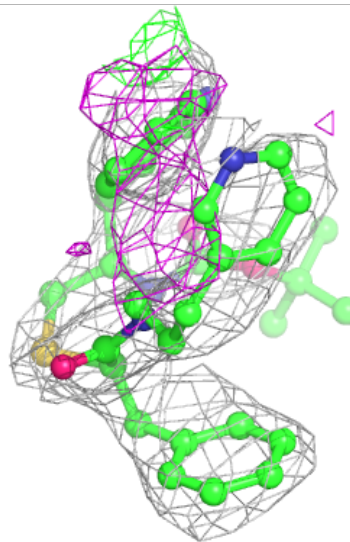
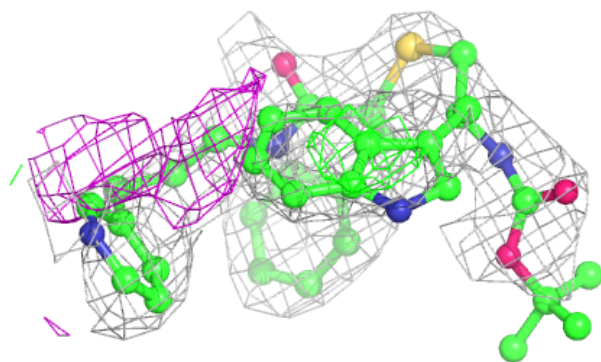
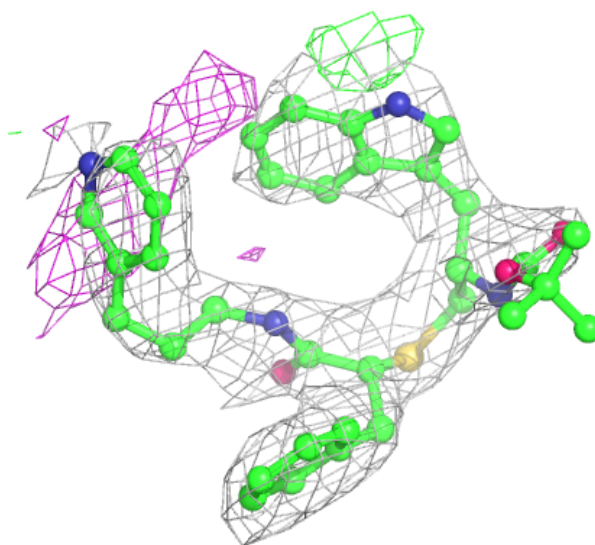
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	X6V	B	602	41/41	0.85	0.27	54,85,125,136	0
3	X6V	A	602	41/41	0.87	0.25	40,58,89,98	0
2	HEM	B	601	43/43	0.97	0.23	48,52,68,81	0
2	HEM	A	601	43/43	0.98	0.23	33,35,59,66	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 X6V B 602:**

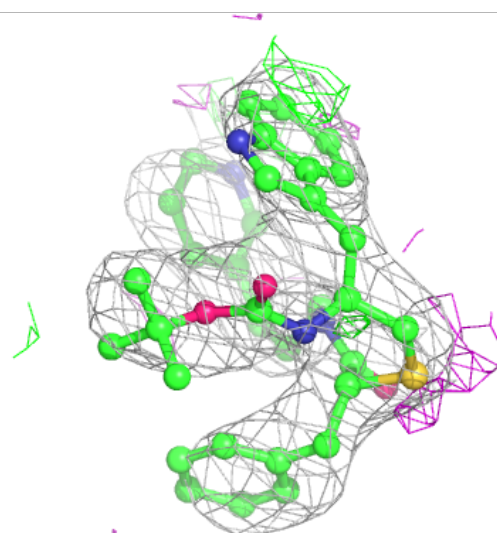
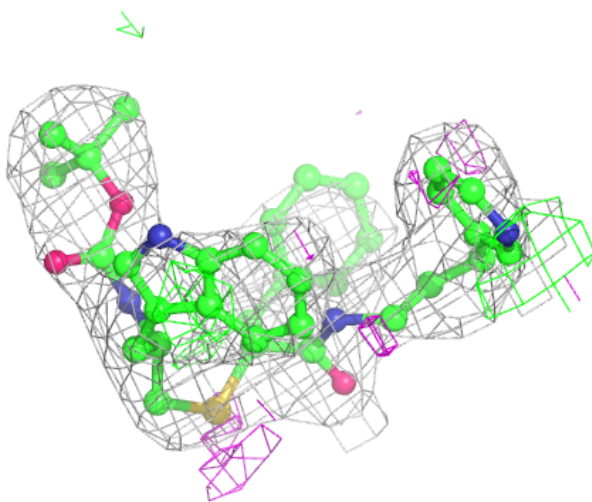
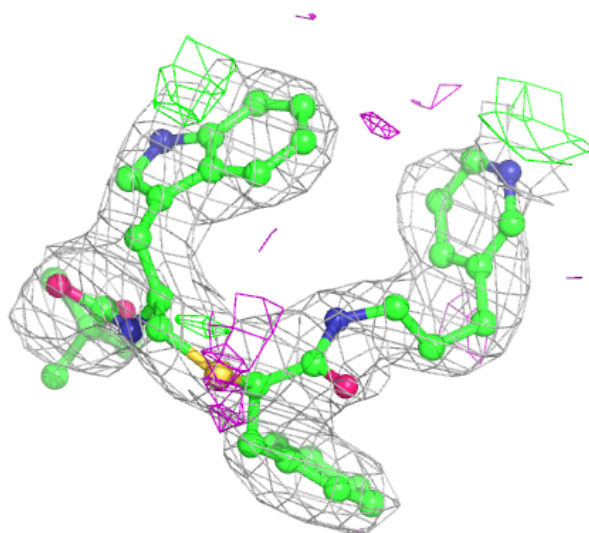
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





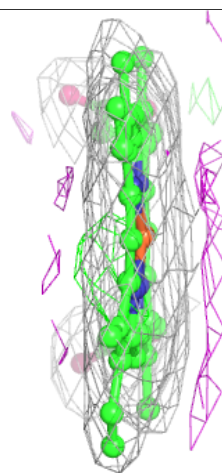
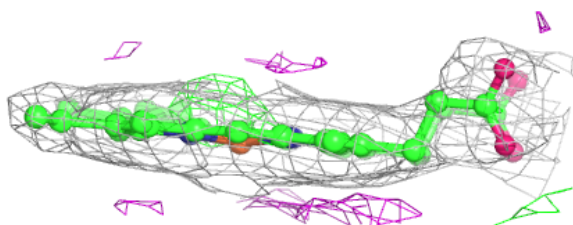
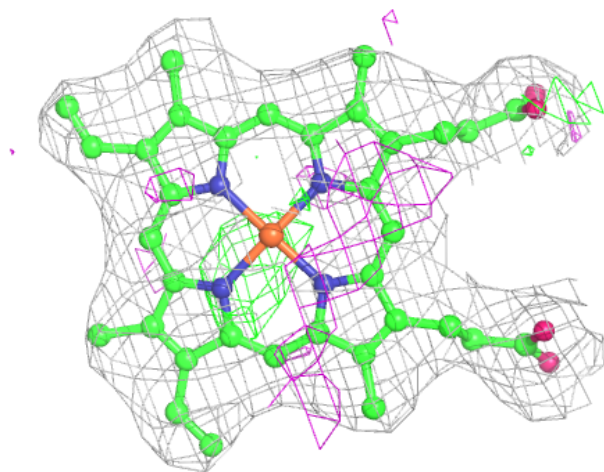
**Electron density around X6V A 602:**

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



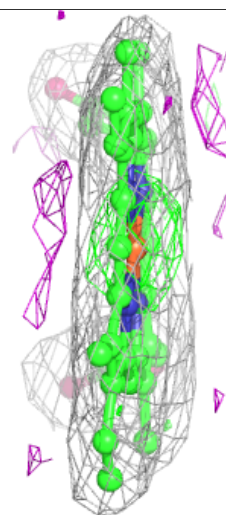
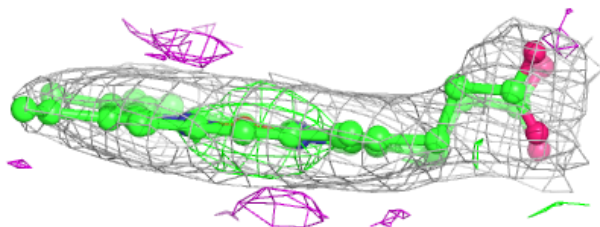
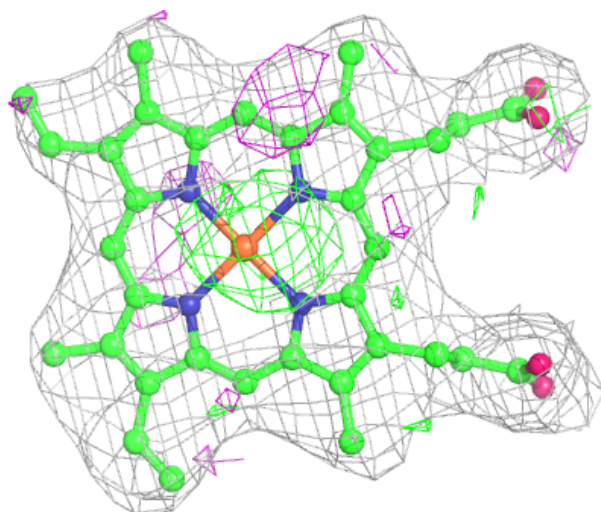
**Electron density around HEM B 601:**

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



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.