



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2021 – 04:07 PM EST

PDB ID : 7KVQ  
Title : Human CYP3A4 bound to an inhibitor  
Authors : Sevrioukova, I.  
Deposited on : 2020-11-28  
Resolution : 2.75 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

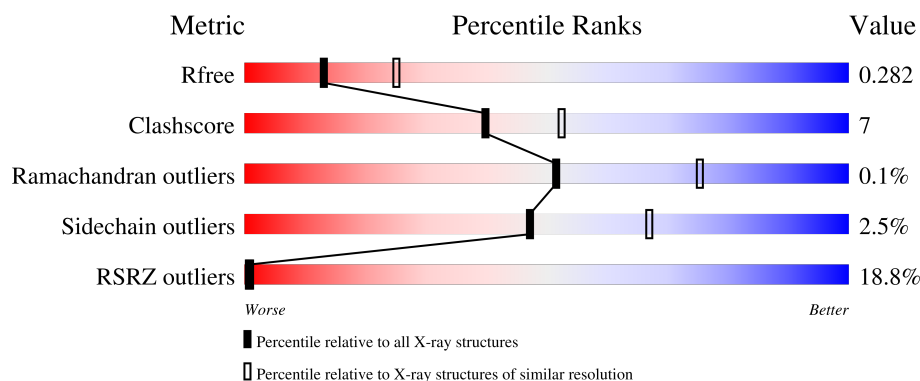
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	
1	B	487	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	X7D	B	602	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7468 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	454	Total	C	N	O	S	0	2	0
			3669	2390	605	649	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:

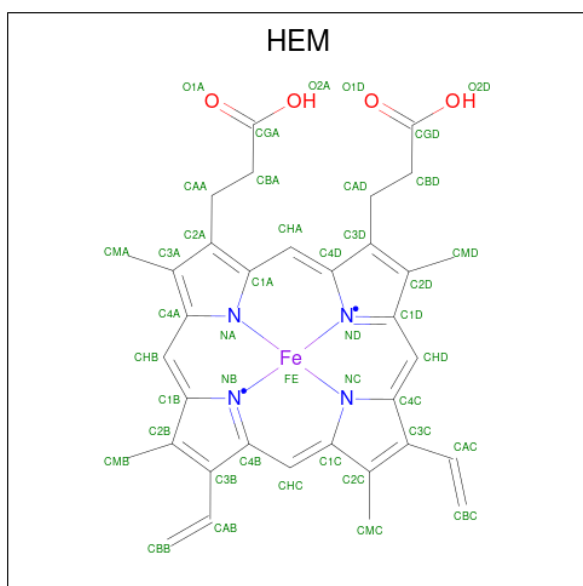
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	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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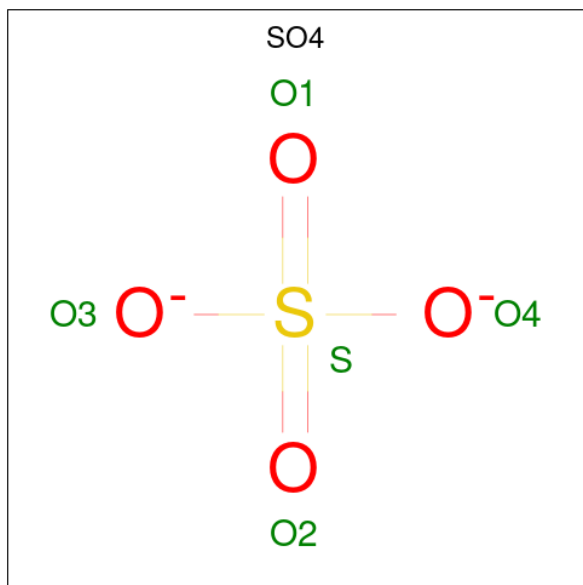
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	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:  $C_{34}H_{32}FeN_4O_4$ ).



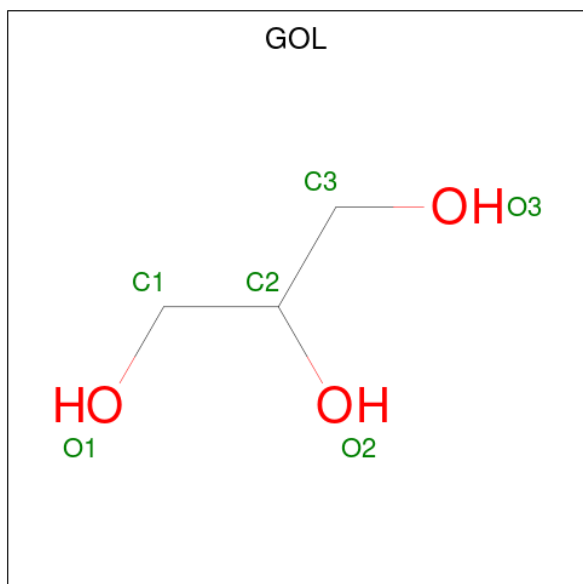
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



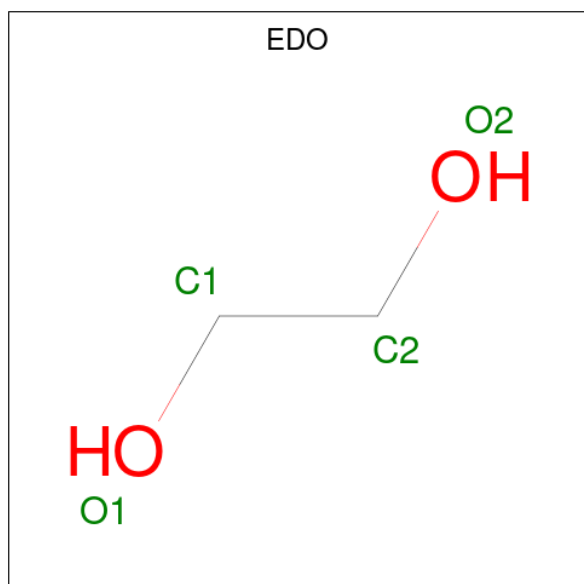
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S		
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



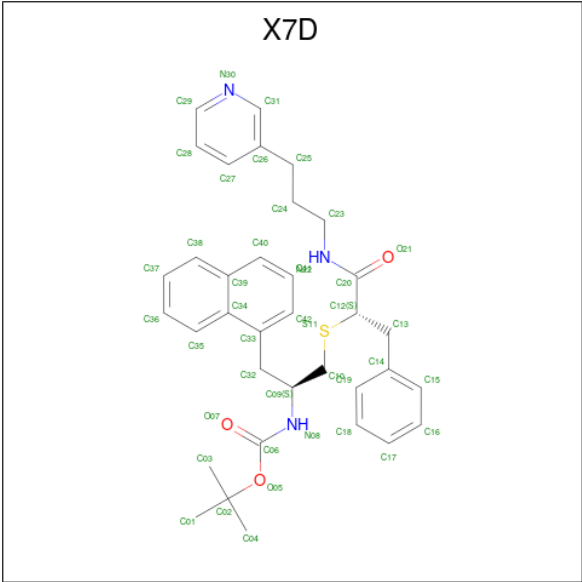
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is tert-butyl [(2S)-1-(naphthalen-1-yl)-3-[[[(2S)-1-oxo-3-phenyl-1-{[3-(pyridin-3-yl)propyl]amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (three-letter code: X7D) (formula: C<sub>35</sub>H<sub>41</sub>N<sub>3</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).

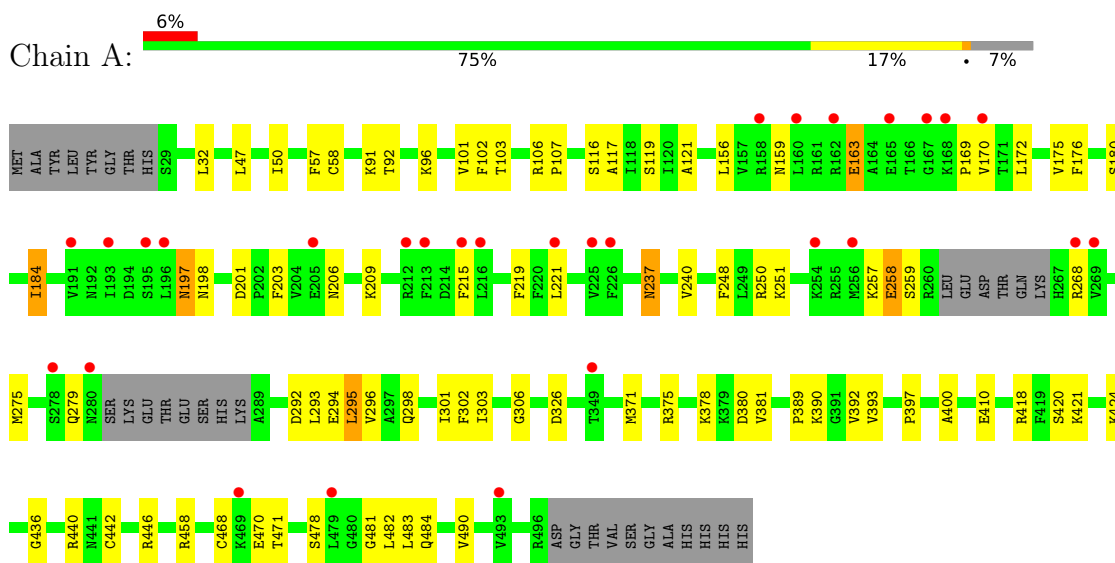


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			42	35	3	3	1		
6	B	1	Total	C	N	O	S	0	0
			42	35	3	3	1		

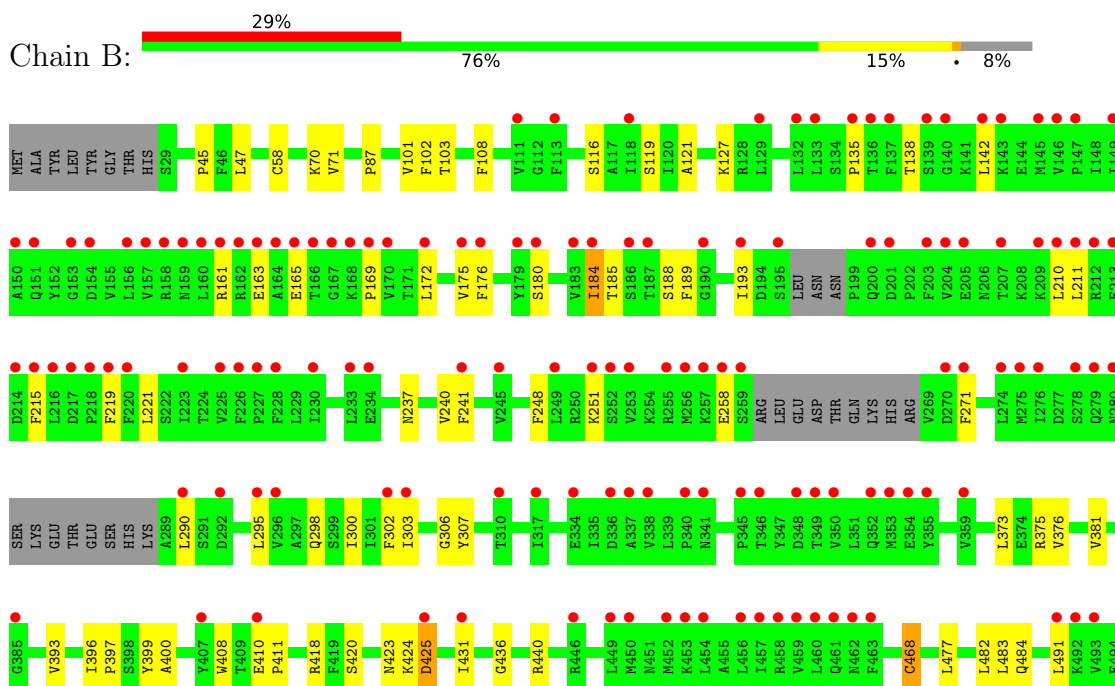
### 3 Residue-property plots

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



S495
R496
ASP
GLY
THR
VAL
SER
GLY
ALA
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.86Å 97.36Å 93.23Å 90.00° 124.32° 90.00°	Depositor
Resolution (Å)	63.54 – 2.75 63.54 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (63.54-2.75) 96.0 (63.54-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.250 , 0.280 0.253 , 0.282	Depositor DCC
$R_{free}$ test set	1371 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, X7D, EDO, HEM, SO4

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	0.27	0/3764	0.41	0/5089
1	B	0.25	0/3696	0.38	0/4997
All	All	0.26	0/7460	0.40	0/10086

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3669	0	3765	58	0
1	B	3606	0	3695	48	0
2	A	43	0	30	7	0
2	B	43	0	30	5	0
3	A	5	0	0	0	0
4	A	6	0	8	0	0
5	A	12	0	18	1	0
6	A	42	0	0	4	0
6	B	42	0	0	4	0
All	All	7468	0	7546	110	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 7.

All (110) 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:106:ARG:HB3	6:A:607:X7D:C03	1.78	1.13
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.67	0.76
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.68	0.76
1:A:172:LEU:HB3	1:A:176:PHE:CE2	2.29	0.67
1:B:410:GLU:O	1:B:418:ARG:NH2	2.28	0.67
1:A:248:PHE:HA	1:A:251:LYS:HE2	1.78	0.66
1:B:248:PHE:HA	1:B:251:LYS:HE2	1.80	0.64
1:A:446[A]:ARG:HE	1:B:425:ASP:HB3	1.64	0.63
1:A:410:GLU:O	1:A:418:ARG:NH2	2.30	0.62
1:A:482:LEU:HD23	1:A:482:LEU:H	1.68	0.58
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.87	0.57
1:B:219:PHE:HE2	1:B:240:VAL:HG12	1.69	0.56
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.87	0.55
1:A:257:LYS:NZ	1:A:292:ASP:OD1	2.40	0.55
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.88	0.55
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.89	0.54
1:B:482:LEU:HD11	1:B:484:GLN:CD	2.28	0.54
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.89	0.54
1:A:206:ASN:HA	1:A:209:LYS:HE2	1.90	0.53
1:B:169:PRO:HG3	1:B:468:CYS:SG	2.49	0.52
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.91	0.52
1:B:103:THR:O	1:B:440:ARG:NH1	2.41	0.52
1:A:258:GLU:OE1	1:A:259:SER:N	2.41	0.51
1:A:169:PRO:HG2	1:A:470:GLU:OE2	2.11	0.51
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.93	0.51
1:A:159:ASN:ND2	1:A:197:ASN:OD1	2.39	0.50
1:B:408:TRP:HB2	1:B:411:PRO:HB3	1.94	0.50
1:A:184:ILE:HG21	1:A:303:ILE:HA	1.93	0.50
1:B:108:PHE:HE2	1:B:240:VAL:HG21	1.77	0.50
1:A:219:PHE:HE2	1:A:240:VAL:HG12	1.77	0.50
1:A:116:SER:O	1:A:298:GLN:NE2	2.44	0.49
1:B:373:LEU:HB2	1:B:396:ILE:HB	1.94	0.49
1:A:103:THR:O	1:A:440:ARG:NH1	2.43	0.49
1:B:420:SER:HG	1:B:423:ASN:HD22	1.58	0.49
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.95	0.49
1:A:397:PRO:HB2	1:A:400:ALA:HB3	1.95	0.48
1:B:376:VAL:HG22	1:B:393:VAL:HG22	1.96	0.48
1:B:241:PHE:CE2	6:B:602:X7D:C15	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLY:HA3	2:B:601:HEM:HBA1	1.94	0.48
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.48	0.48
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.94	0.48
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.96	0.47
1:A:478:SER:N	1:A:484:GLN:O	2.41	0.47
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.96	0.47
1:B:175:VAL:HG13	1:B:176:PHE:N	2.29	0.47
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.49	0.47
1:B:121:ALA:O	1:B:440:ARG:NH2	2.46	0.47
1:A:275:MET:HB3	1:A:295:LEU:HD12	1.97	0.47
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.28	0.47
1:A:279:GLN:NE2	1:A:292:ASP:OD1	2.47	0.46
1:A:169:PRO:HG2	1:A:470:GLU:CD	2.35	0.46
1:B:161:ARG:O	1:B:165:GLU:HG3	2.15	0.46
1:B:180:SER:HB3	1:B:307:TYR:HA	1.96	0.46
1:A:197:ASN:HA	1:A:198:ASN:HB3	1.97	0.46
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.98	0.46
1:B:70:LYS:HG3	1:B:71:VAL:HG23	1.97	0.46
2:A:601:HEM:C1D	6:A:607:X7D:C31	2.99	0.46
1:A:106:ARG:HG3	1:A:393:VAL:HG21	1.98	0.45
1:B:420:SER:O	1:B:424:LYS:N	2.49	0.45
1:A:172:LEU:HB3	1:A:176:PHE:CD2	2.51	0.45
1:A:389:PRO:HD2	1:A:392:VAL:HG21	1.98	0.45
1:A:468:CYS:HB3	1:A:470:GLU:HG2	1.98	0.45
1:B:185:THR:HA	1:B:189:PHE:HD2	1.81	0.45
1:B:210:LEU:HD21	1:B:300:ILE:HG23	1.99	0.45
1:B:211:LEU:HB3	6:B:602:X7D:C18	2.47	0.45
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.98	0.45
1:A:92:THR:HA	1:A:96:LYS:HB2	1.99	0.45
1:B:425:ASP:N	1:B:425:ASP:OD1	2.40	0.45
1:B:420:SER:OG	1:B:423:ASN:ND2	2.40	0.45
1:A:237:ASN:ND2	1:A:237:ASN:O	2.42	0.44
1:A:106:ARG:HG2	1:A:107:PRO:HD2	2.00	0.44
1:A:380:ASP:OD1	1:A:390:LYS:N	2.50	0.44
1:A:117:ALA:O	1:A:121:ALA:N	2.45	0.44
1:A:301:ILE:HD13	6:A:607:X7D:C16	2.48	0.44
1:A:119:SER:HB2	6:A:607:X7D:C42	2.48	0.43
1:B:172:LEU:O	1:B:176:PHE:HB2	2.18	0.43
1:B:87:PRO:HG3	1:B:431:ILE:HD11	2.00	0.43
1:B:482:LEU:HD11	1:B:484:GLN:NE2	2.34	0.43
1:A:156:LEU:CD1	1:A:175:VAL:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:SD	1:A:483:LEU:HB2	2.58	0.43
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.53	0.43
1:A:294:GLU:O	1:A:298:GLN:HG2	2.19	0.43
1:A:184:ILE:HG13	1:A:306:GLY:HA3	1.99	0.43
1:A:32:LEU:HD11	1:A:389:PRO:HG2	2.01	0.43
1:B:211:LEU:HD12	6:B:602:X7D:C19	2.48	0.42
1:B:420:SER:HG	1:B:423:ASN:ND2	2.17	0.42
1:A:442:CYS:HB2	2:A:601:HEM:C4A	2.54	0.42
1:B:116:SER:O	1:B:298:GLN:NE2	2.46	0.42
1:A:180:SER:HB3	1:A:306:GLY:O	2.19	0.42
1:A:326:ASP:OD1	1:A:326:ASP:N	2.52	0.42
1:B:119:SER:HB3	2:B:601:HEM:HAD1	2.00	0.42
1:A:101:VAL:HA	1:A:378:LYS:HG2	2.02	0.42
1:A:163:GLU:HB3	1:A:170:VAL:CG2	2.49	0.41
1:B:185:THR:HG21	1:B:193:ILE:HD12	2.02	0.41
1:A:57:PHE:HE2	1:A:481:GLY:HA2	1.86	0.41
1:B:477:LEU:HD13	1:B:483:LEU:HD11	2.01	0.41
1:A:91:LYS:HE2	1:A:96:LYS:HE3	2.03	0.41
1:B:45:PRO:O	1:B:47:LEU:N	2.50	0.41
1:A:471:THR:OG1	1:A:490:VAL:O	2.21	0.41
1:B:172:LEU:HA	1:B:175:VAL:HG12	2.01	0.41
1:B:188:SER:HA	1:B:271:PHE:HB3	2.03	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.82	0.41
1:A:58:CYS:SG	5:A:606:EDO:H12	2.60	0.41
1:B:175:VAL:CG1	1:B:176:PHE:N	2.84	0.41
1:B:211:LEU:HB3	6:B:602:X7D:C19	2.50	0.41
1:A:420:SER:O	1:A:424:LYS:N	2.49	0.40
1:B:135:PRO:HA	1:B:138:THR:HG23	2.03	0.40
1:A:172:LEU:HA	1:A:175:VAL:HG12	2.03	0.40
1:A:250:ARG:HA	1:A:296:VAL:HG11	2.03	0.40
1:A:201:ASP:OD2	1:A:203:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

## 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	450/487 (92%)	422 (94%)	27 (6%)	1 (0%)	47	69
1	B	441/487 (91%)	415 (94%)	26 (6%)	0	100	100
All	All	891/974 (92%)	837 (94%)	53 (6%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN

### 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	417/443 (94%)	408 (98%)	9 (2%)	52	70
1	B	410/443 (93%)	398 (97%)	12 (3%)	42	62
All	All	827/886 (93%)	806 (98%)	21 (2%)	47	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	A	184	ILE
1	A	215	PHE
1	A	221	LEU
1	A	237	ASN
1	A	258	GLU
1	A	268	ARG
1	A	295	LEU
1	A	458	ARG
1	B	127	LYS
1	B	142	LEU
1	B	163	GLU

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Mol	Chain	Res	Type
1	B	184	ILE
1	B	215	PHE
1	B	221	LEU
1	B	237	ASN
1	B	258	GLU
1	B	290	LEU
1	B	295	LEU
1	B	425	ASP
1	B	468	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

9 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	$\# Z  > 2$
4	GOL	A	603	-	5,5,5	0.39	0	5,5,5	0.21	0
5	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	601	1,6	27,50,50	1.88	4 (14%)	17,82,82	1.47	3 (17%)
5	EDO	A	606	-	3,3,3	0.46	0	2,2,2	0.29	0
6	X7D	A	607	2	44,45,45	1.76	8 (18%)	52,60,60	1.90	10 (19%)
5	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.30	0
3	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.05	0
6	X7D	B	602	2	44,45,45	1.66	8 (18%)	52,60,60	1.79	10 (19%)
2	HEM	B	601	1,6	27,50,50	1.90	5 (18%)	17,82,82	1.44	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
4	GOL	A	603	-	-	2/4/4/4	-
5	EDO	A	604	-	-	1/1/1/1	-
2	HEM	A	601	1,6	-	0/6/54/54	-
5	EDO	A	606	-	-	0/1/1/1	-
6	X7D	A	607	2	-	17/33/33/33	0/4/4/4
5	EDO	A	605	-	-	0/1/1/1	-
6	X7D	B	602	2	-	13/33/33/33	0/4/4/4
2	HEM	B	601	1,6	-	0/6/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	607	X7D	C10-S11	6.17	1.88	1.82
6	B	602	X7D	C10-S11	5.36	1.87	1.82
6	A	607	X7D	C12-S11	4.99	1.88	1.83
2	B	601	HEM	C3C-C2C	-4.63	1.33	1.40
2	A	601	HEM	C3C-C2C	-4.59	1.34	1.40
6	B	602	X7D	C12-S11	4.15	1.87	1.83
2	A	601	HEM	C3B-CAB	3.83	1.55	1.47
2	B	601	HEM	C3B-CAB	3.81	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.77	1.35	1.40
2	A	601	HEM	C3B-C2B	-3.70	1.35	1.40
2	A	601	HEM	C3C-CAC	3.69	1.55	1.47
2	B	601	HEM	C3C-CAC	3.67	1.55	1.47
6	B	602	X7D	C20-N22	2.95	1.40	1.33
6	A	607	X7D	C20-N22	2.93	1.40	1.33
6	B	602	X7D	C32-C09	2.72	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	607	X7D	C34-C39	-2.55	1.38	1.43
6	B	602	X7D	C34-C39	-2.50	1.38	1.43
6	B	602	X7D	C33-C34	2.46	1.48	1.42
6	A	607	X7D	C33-C34	2.36	1.47	1.42
6	B	602	X7D	O05-C06	2.19	1.39	1.34
6	A	607	X7D	C04-C02	2.16	1.57	1.51
6	B	602	X7D	C06-N08	2.12	1.39	1.34
6	A	607	X7D	C32-C09	2.11	1.58	1.53
6	A	607	X7D	C13-C14	2.06	1.56	1.51
2	B	601	HEM	CAA-C2A	2.02	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	607	X7D	O05-C06-N08	6.66	121.20	110.02
6	B	602	X7D	O05-C06-N08	6.05	120.19	110.02
6	A	607	X7D	C14-C13-C12	5.81	121.65	113.32
6	B	602	X7D	O07-C06-N08	-5.04	116.60	124.85
6	A	607	X7D	O07-C06-N08	-4.87	116.87	124.85
6	B	602	X7D	C14-C13-C12	4.63	119.95	113.32
6	A	607	X7D	C32-C33-C34	3.89	126.91	120.76
6	B	602	X7D	C32-C33-C34	3.63	126.50	120.76
6	A	607	X7D	O21-C20-N22	-2.97	116.62	122.99
2	A	601	HEM	CBD-CAD-C3D	-2.60	107.68	112.48
6	A	607	X7D	C40-C39-C38	-2.51	117.33	123.19
6	B	602	X7D	C42-C33-C34	-2.47	115.57	119.08
6	B	602	X7D	O21-C20-N22	-2.45	117.73	122.99
6	B	602	X7D	C40-C39-C38	-2.40	117.58	123.19
6	B	602	X7D	C23-N22-C20	2.39	126.85	122.59
6	A	607	X7D	O21-C20-C12	-2.30	118.28	121.61
2	A	601	HEM	CMB-C2B-C3B	2.23	128.84	124.68
6	A	607	X7D	C42-C33-C34	-2.22	115.93	119.08
2	B	601	HEM	CMB-C2B-C3B	2.19	128.77	124.68
6	B	602	X7D	C23-C24-C25	2.17	116.82	112.95
2	A	601	HEM	CAA-CBA-CGA	-2.08	109.19	112.67
6	A	607	X7D	C38-C39-C34	2.03	121.80	119.12
6	A	607	X7D	O05-C06-O07	-2.03	121.92	125.62
6	B	602	X7D	C09-N08-C06	2.02	125.42	122.30

There are no chirality outliers.

All (33) torsion outliers are listed below:

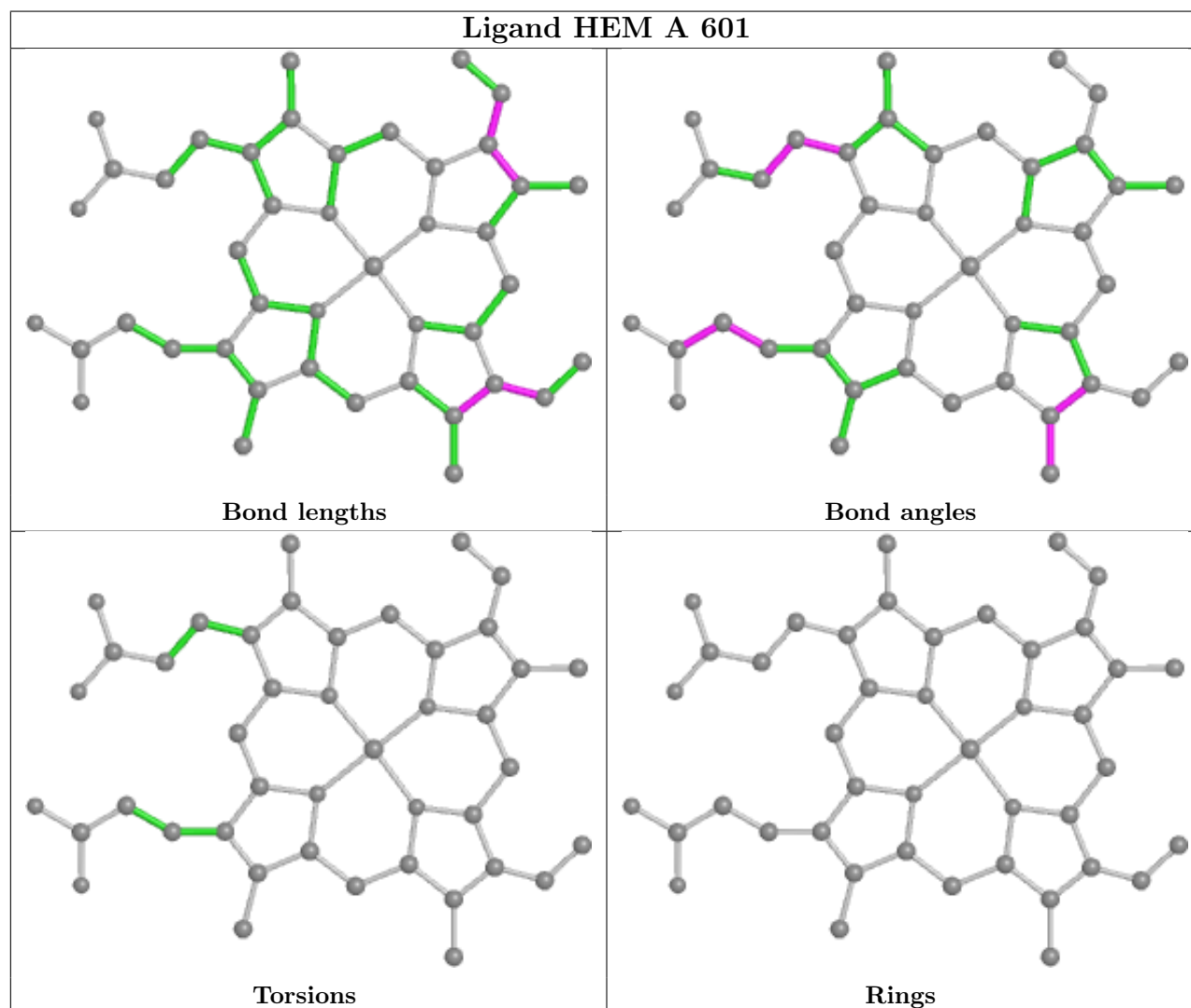
Mol	Chain	Res	Type	Atoms
6	A	607	X7D	O05-C06-N08-C09
6	A	607	X7D	C32-C09-C10-S11
6	A	607	X7D	C09-C32-C33-C34
6	A	607	X7D	C09-C32-C33-C42
6	B	602	X7D	O05-C06-N08-C09
6	B	602	X7D	C09-C32-C33-C34
6	B	602	X7D	C09-C32-C33-C42
6	A	607	X7D	O07-C06-N08-C09
6	B	602	X7D	O07-C06-N08-C09
6	A	607	X7D	N08-C06-O05-C02
6	B	602	X7D	C12-C13-C14-C15
6	A	607	X7D	C20-C12-C13-C14
6	B	602	X7D	C23-C24-C25-C26
6	A	607	X7D	C13-C12-C20-O21
6	A	607	X7D	C13-C12-C20-N22
6	B	602	X7D	C13-C12-C20-N22
4	A	603	GOL	O1-C1-C2-C3
6	A	607	X7D	O07-C06-O05-C02
6	A	607	X7D	C12-C13-C14-C15
6	A	607	X7D	C12-C13-C14-C19
6	B	602	X7D	C12-C13-C14-C19
5	A	604	EDO	O1-C1-C2-O2
6	A	607	X7D	N08-C09-C10-S11
6	B	602	X7D	C13-C12-C20-O21
6	B	602	X7D	C20-C12-C13-C14
6	A	607	X7D	C20-C12-S11-C10
6	A	607	X7D	C24-C25-C26-C31
6	B	602	X7D	C24-C25-C26-C31
6	A	607	X7D	C13-C12-S11-C10
6	B	602	X7D	C13-C12-S11-C10
4	A	603	GOL	O1-C1-C2-O2
6	A	607	X7D	C24-C25-C26-C27
6	B	602	X7D	C24-C25-C26-C27

There are no ring outliers.

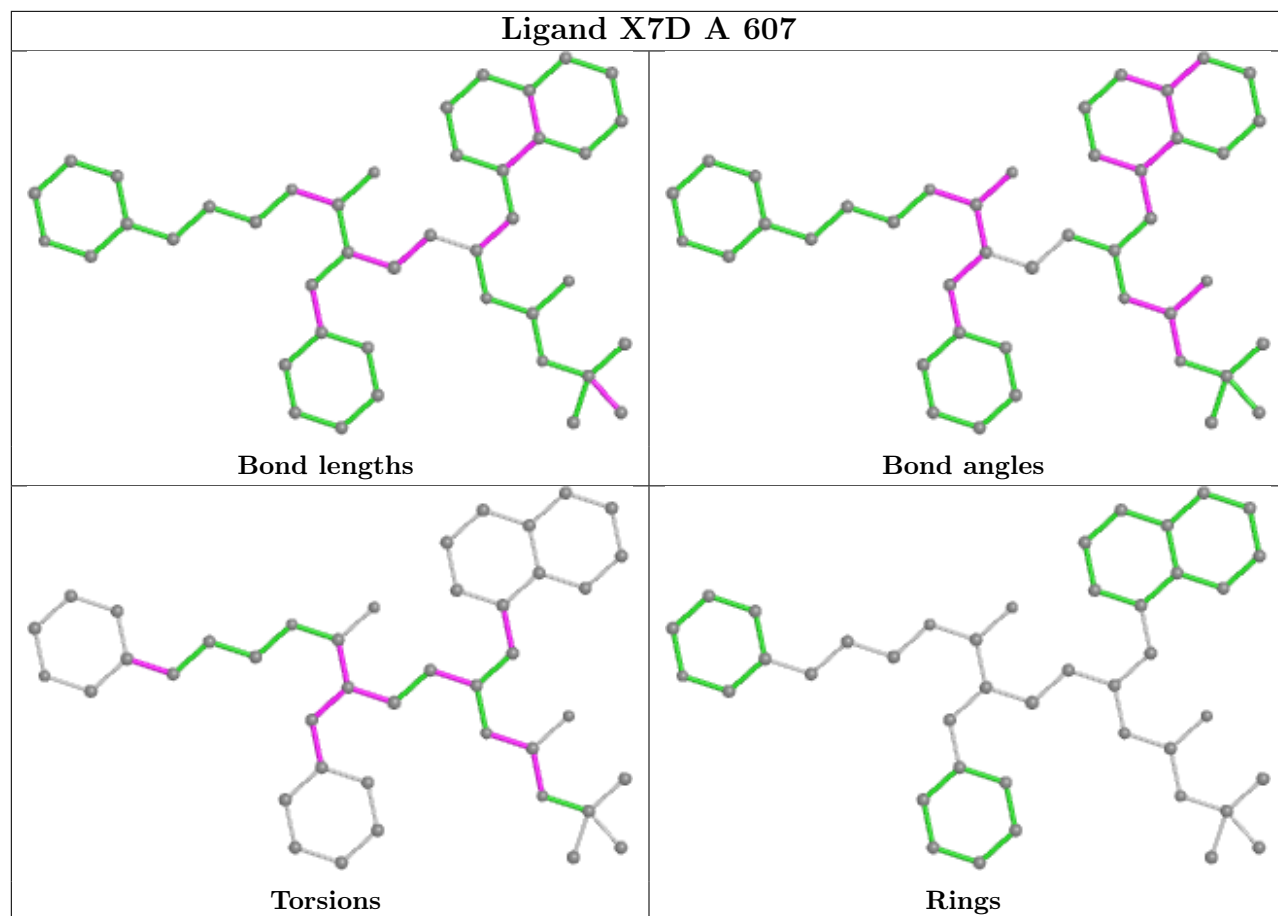
5 monomers are involved in 20 short contacts:

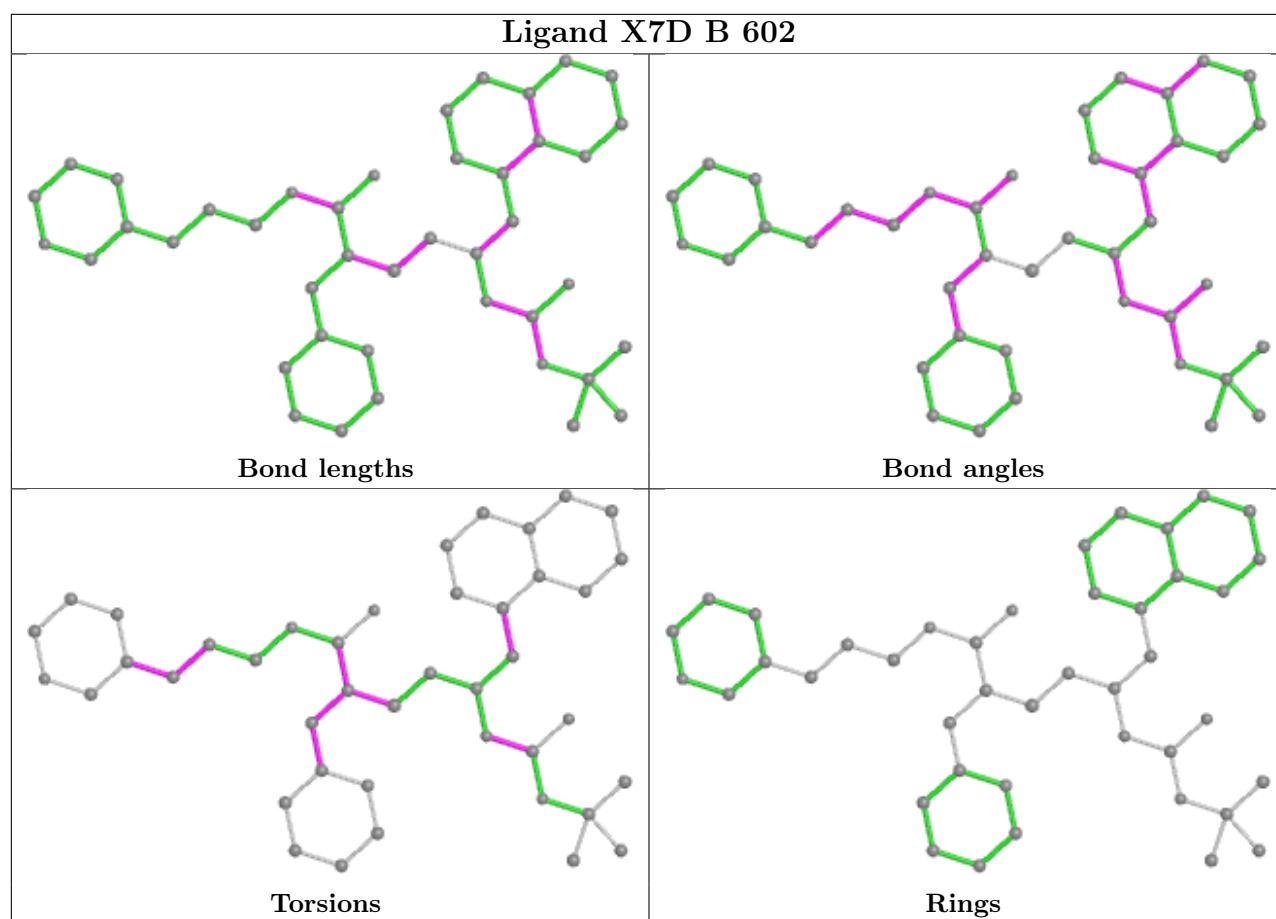
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	7	0
5	A	606	EDO	1	0
6	A	607	X7D	4	0
6	B	602	X7D	4	0
2	B	601	HEM	5	0

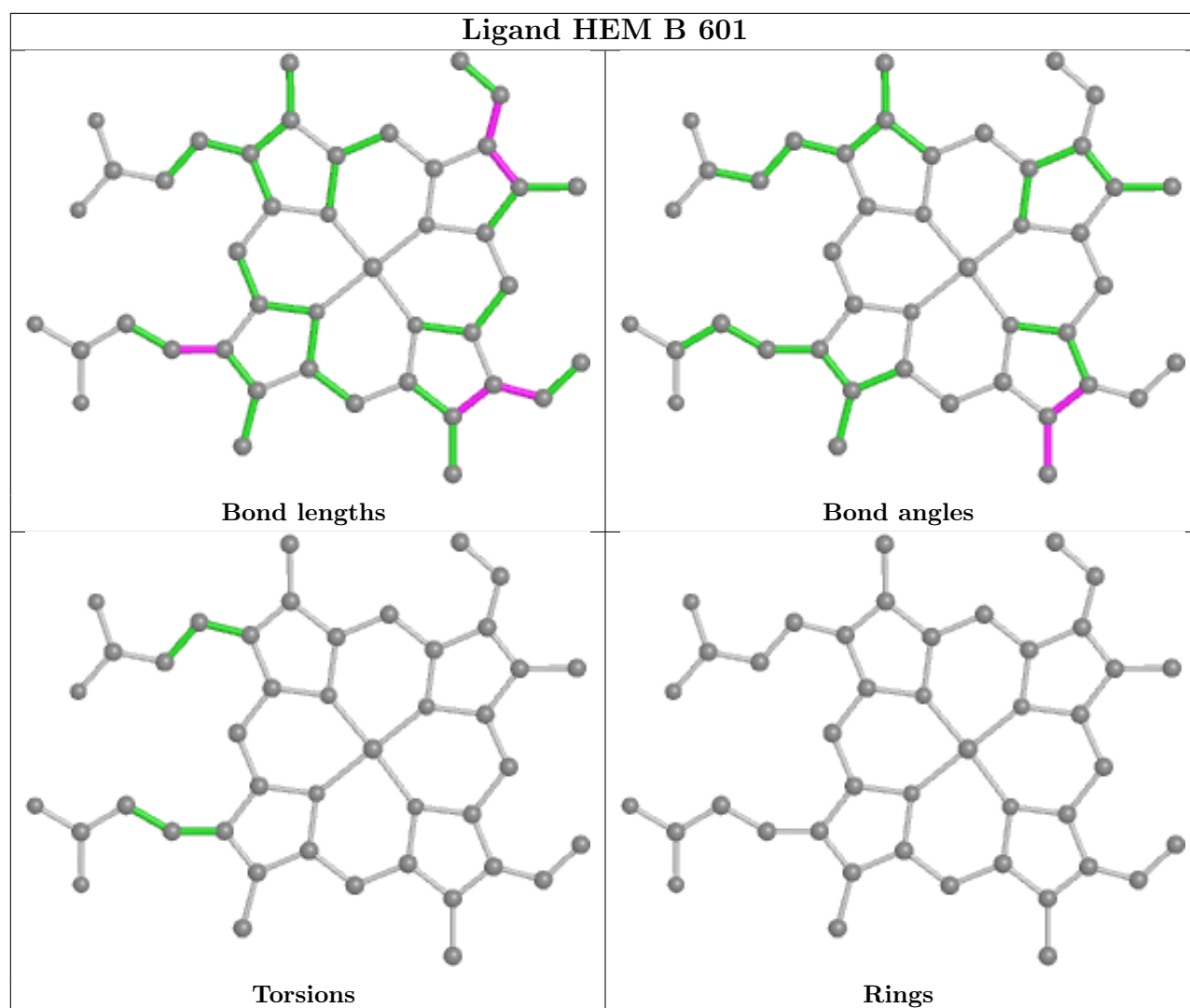
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 X7D A 607







## 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	454/487 (93%)	0.34	29 (6%)	19 23	52, 91, 168, 270	0
1	B	448/487 (91%)	1.84	141 (31%)	0 0	74, 160, 284, 463	0
All	All	902/974 (92%)	1.09	170 (18%)	1 1	52, 119, 248, 463	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLY	15.9
1	B	457	ILE	14.8
1	B	253	VAL	14.2
1	B	456	LEU	13.0
1	B	256	MET	11.9
1	B	190	GLY	11.7
1	B	258	GLU	11.3
1	B	147	PRO	11.2
1	B	249	LEU	10.5
1	B	257	LYS	10.3
1	B	210	LEU	10.1
1	B	179	TYR	9.9
1	B	216	LEU	9.7
1	B	164	ALA	9.6
1	B	156	LEU	9.3
1	B	146	VAL	9.3
1	B	154	ASP	9.1
1	B	160	LEU	8.5
1	B	493	VAL	8.1
1	B	195	SER	7.9
1	B	161	ARG	7.4
1	B	215	PHE	7.4
1	B	204	VAL	6.7
1	B	166	THR	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	157	VAL	6.5
1	B	184	ILE	6.4
1	B	150	ALA	6.3
1	B	345	PRO	6.3
1	B	341	ASN	6.3
1	B	292	ASP	6.2
1	B	167	GLY	6.1
1	B	337	ALA	6.1
1	B	334	GLU	6.0
1	B	172	LEU	5.9
1	B	175	VAL	5.9
1	B	209	LYS	5.9
1	B	241	PHE	5.8
1	B	280	ASN	5.8
1	B	145	MET	5.8
1	A	195	SER	5.7
1	A	168	LYS	5.7
1	B	295	LEU	5.6
1	B	176	PHE	5.6
1	B	460	LEU	5.5
1	B	278	SER	5.3
1	B	310	THR	5.2
1	B	143	LYS	5.1
1	B	452	MET	5.1
1	B	259	SER	5.0
1	B	495	SER	5.0
1	B	290	LEU	4.9
1	B	218	PRO	4.9
1	B	170	VAL	4.9
1	B	220	PHE	4.8
1	B	168	LYS	4.7
1	B	352[A]	GLN	4.7
1	B	303	ILE	4.7
1	B	133	LEU	4.6
1	B	118	ILE	4.6
1	B	349	THR	4.5
1	B	137	PHE	4.5
1	B	165	GLU	4.5
1	B	187	THR	4.3
1	A	216	LEU	4.3
1	B	183	VAL	4.2
1	B	271	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	159	ASN	4.2
1	B	338	VAL	4.2
1	B	212	ARG	4.1
1	B	113	PHE	4.1
1	B	276	ILE	4.1
1	B	158	ARG	4.0
1	B	142	LEU	4.0
1	B	491	LEU	4.0
1	B	496	ARG	4.0
1	B	186	SER	3.9
1	A	212	ARG	3.8
1	B	359	VAL	3.8
1	B	449	LEU	3.8
1	B	274	LEU	3.8
1	B	214	ASP	3.8
1	B	270	ASP	3.8
1	B	136	THR	3.7
1	A	213	PHE	3.7
1	A	479	LEU	3.7
1	B	201	ASP	3.7
1	B	149	ILE	3.7
1	B	230	ILE	3.7
1	B	226	PHE	3.6
1	B	459	VAL	3.6
1	B	340	PRO	3.6
1	A	256	MET	3.5
1	B	203	PHE	3.5
1	B	336	ASP	3.4
1	B	453	LYS	3.4
1	B	213	PHE	3.4
1	A	165	GLU	3.4
1	B	111	VAL	3.4
1	B	217	ASP	3.3
1	B	302	PHE	3.3
1	B	255	ARG	3.3
1	B	454	LEU	3.3
1	B	450	MET	3.2
1	B	211	LEU	3.2
1	B	348	ASP	3.2
1	A	226	PHE	3.1
1	B	346	THR	3.1
1	A	215	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	3.1
1	B	205	GLU	3.1
1	A	158	ARG	3.0
1	B	296	VAL	3.0
1	B	446	ARG	3.0
1	B	279	GLN	2.9
1	B	385	GLY	2.9
1	B	425	ASP	2.9
1	B	132	LEU	2.9
1	B	228	PHE	2.9
1	B	275	MET	2.9
1	A	269	VAL	2.9
1	B	431	ILE	2.8
1	B	355	TYR	2.8
1	B	317	ILE	2.7
1	B	219	PHE	2.7
1	B	251	LYS	2.7
1	B	252	SER	2.7
1	B	180	SER	2.6
1	B	461	GLN	2.6
1	B	139	SER	2.6
1	B	492	LYS	2.5
1	A	167	GLY	2.5
1	B	410	GLU	2.5
1	B	458	ARG	2.5
1	B	463	PHE	2.5
1	B	169	PRO	2.5
1	A	268	ARG	2.4
1	A	162	ARG	2.4
1	A	469	LYS	2.4
1	A	349	THR	2.4
1	B	207	THR	2.4
1	B	140	GLY	2.4
1	A	193	ILE	2.4
1	A	493	VAL	2.4
1	B	353	MET	2.4
1	A	170	VAL	2.3
1	A	196	LEU	2.3
1	B	354	GLU	2.3
1	B	223	ILE	2.3
1	B	233	LEU	2.3
1	B	245	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	LEU	2.3
1	B	225	VAL	2.3
1	B	350	VAL	2.3
1	B	462	ASN	2.2
1	A	160	LEU	2.2
1	B	163	GLU	2.2
1	B	234	GLU	2.2
1	A	280	ASN	2.2
1	A	191	VAL	2.1
1	B	151	GLN	2.1
1	B	162	ARG	2.1
1	B	407	TYR	2.1
1	B	135	PRO	2.1
1	B	129	LEU	2.1
1	B	200	GLN	2.1
1	B	227	PRO	2.1
1	A	205	GLU	2.1
1	A	278	SER	2.0
1	A	254	LYS	2.0
1	B	193	ILE	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(Å <sup>2</sup> )	Q<0.9
6	X7D	B	602	42/42	0.76	0.62	131,176,210,221	0
5	EDO	A	604	4/4	0.86	0.16	76,77,91,100	0
5	EDO	A	606	4/4	0.87	0.27	83,83,96,100	0

*Continued on next page...*

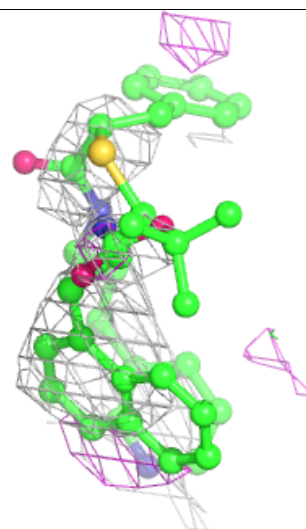
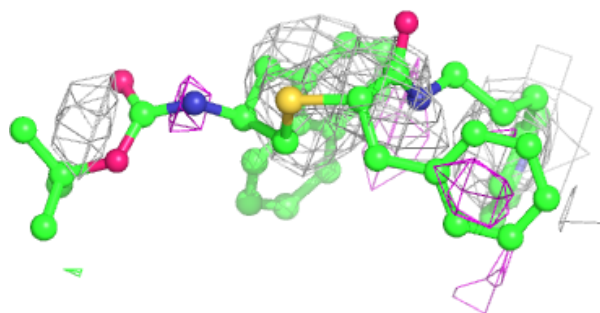
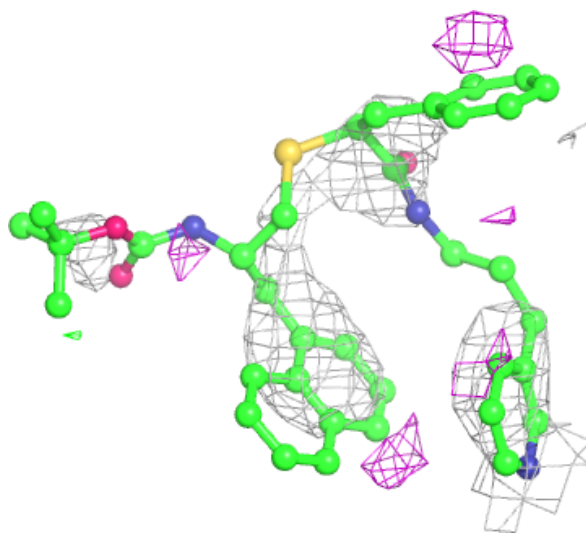
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	X7D	A	607	42/42	0.88	0.39	75,128,154,175	0
4	GOL	A	603	6/6	0.92	0.50	108,111,124,131	0
3	SO4	A	602	5/5	0.93	0.22	121,132,139,141	0
5	EDO	A	605	4/4	0.93	0.24	84,94,98,99	0
2	HEM	B	601	43/43	0.97	0.19	65,92,113,124	0
2	HEM	A	601	43/43	0.98	0.18	43,58,70,73	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.

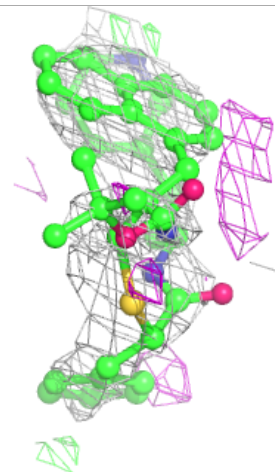
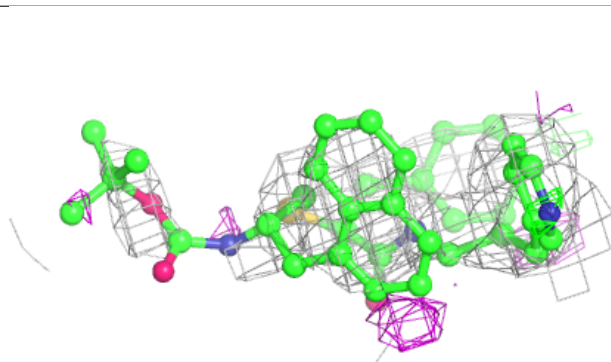
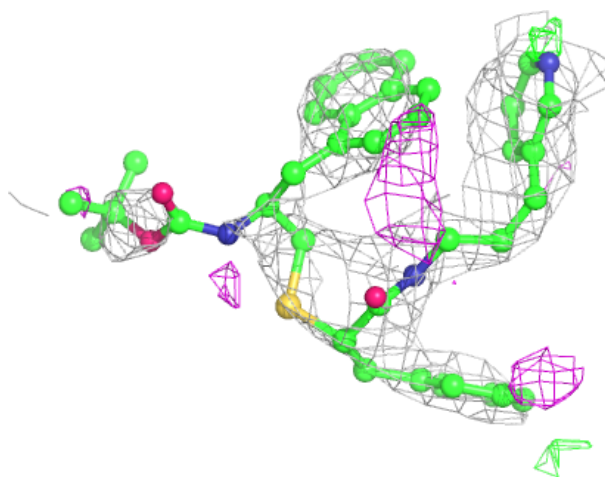
**Electron density around X7D B 602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



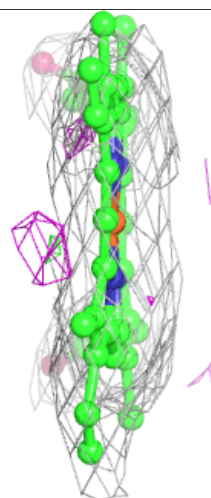
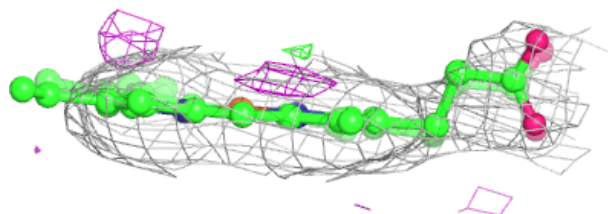
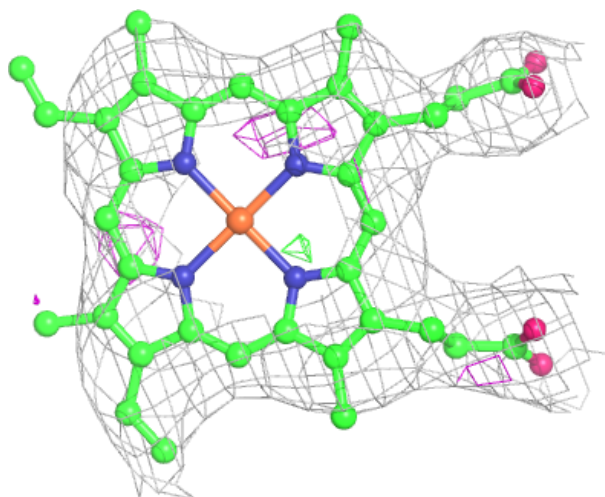
**Electron density around X7D A 607:**

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



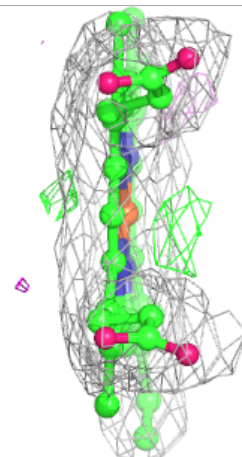
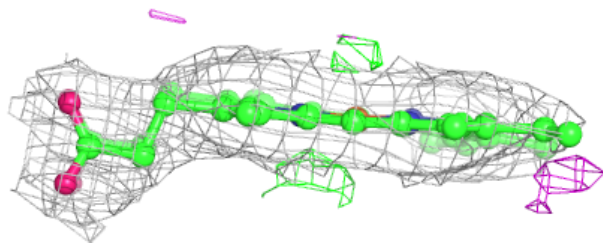
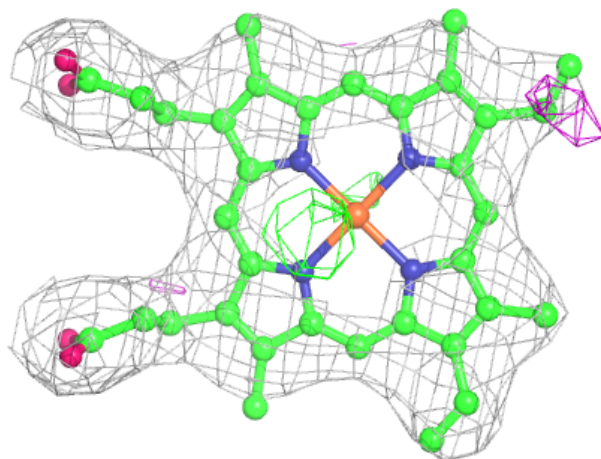
**Electron density around HEM B 601:**

$2mF_o-DF_c$  (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.