Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 09:17 AM EDT

PDB ID	:	6E8Q
Title	:	S. CEREVISIAE CYP51 COMPLEXED WITH Posaconazole
Authors	:	Tyndall, J.D.; Keniya, M.V.; Sabherwal, M.; Monk, B.C.
Deposited on	:	2018-07-30
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

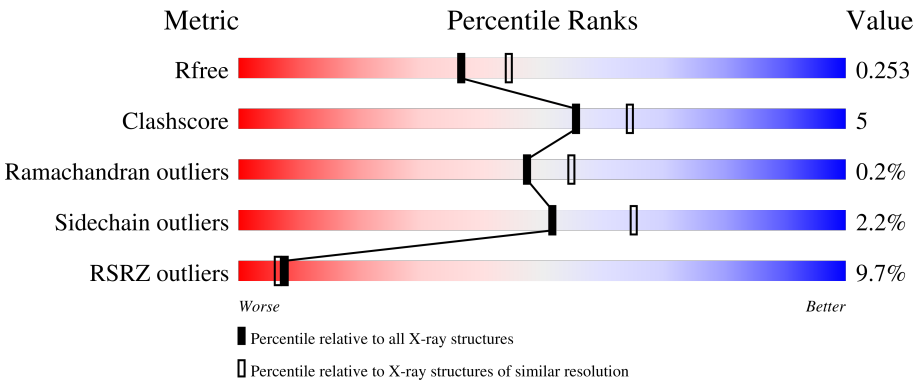
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	539	9% 84% 13%

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
5	LMT	A	604	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4509 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.

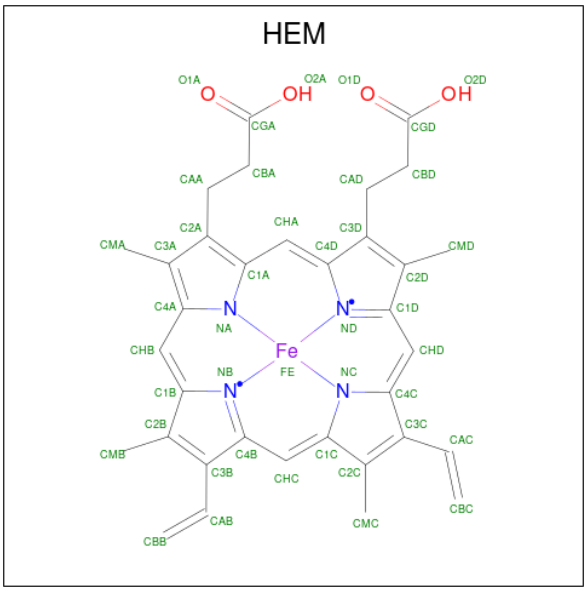
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4263	2760	721	761	21	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

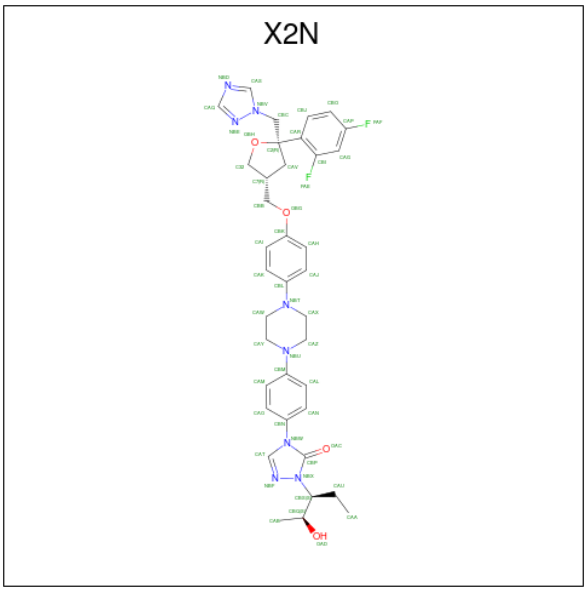
Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP A6ZSR0
A	532	GLY	-	expression tag	UNP A6ZSR0
A	533	ARG	-	expression tag	UNP A6ZSR0
A	534	HIS	-	expression tag	UNP A6ZSR0
A	535	HIS	-	expression tag	UNP A6ZSR0
A	536	HIS	-	expression tag	UNP A6ZSR0
A	537	HIS	-	expression tag	UNP A6ZSR0
A	538	HIS	-	expression tag	UNP A6ZSR0
A	539	HIS	-	expression tag	UNP A6ZSR0

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



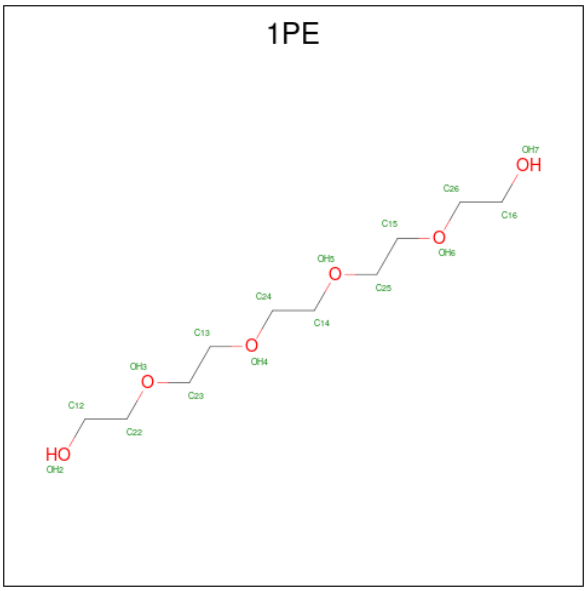
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is POSACONAZOLE (three-letter code: X2N) (formula: $C_{37}H_{42}F_2N_8O_4$) (labeled as "Ligand of Interest" by depositor).



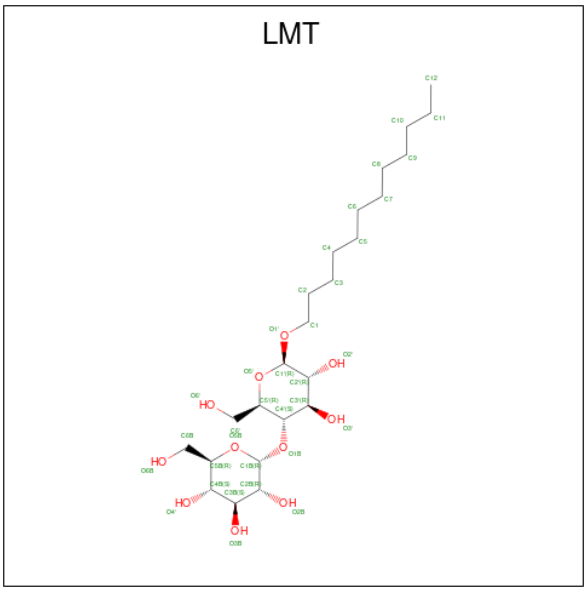
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	51	37	2	8	4	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	16	10	6	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	35	24	11	0	0

- Molecule 6 is water.

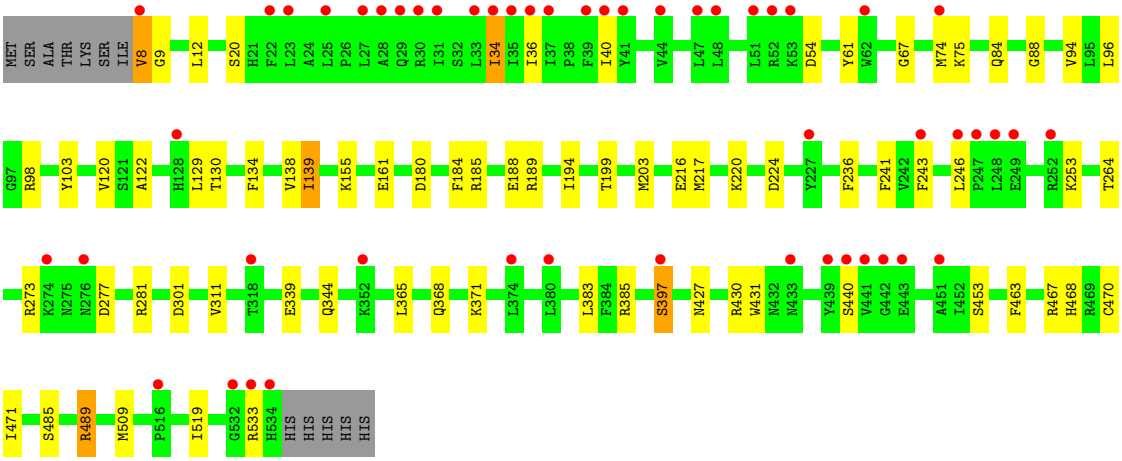
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	101	101	101	0	0

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: Lanosterol 14-alpha demethylase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.35Å 66.56Å 80.77Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	34.25 – 2.20 34.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.25-2.20) 96.8 (34.25-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.210 , 0.253 0.211 , 0.253	Depositor DCC
R_{free} test set	1994 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4509	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, X2N, LMT, 1PE

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	0.41	0/4381	0.55	2/5935 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	489	ARG	NE-CZ-NH1	5.32	122.96	120.30

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	4263	0	4248	43	0
2	A	43	0	30	3	0
3	A	51	0	42	1	0
4	A	16	0	22	2	0
5	A	35	0	46	1	0
6	A	101	0	0	0	0
All	All	4509	0	4388	45	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 5.

All (45) 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:264:THR:HG23	4:A:603:1PE:H222	1.58	0.82
1:A:161:GLU:HG2	5:A:604:LMT:H12	1.67	0.76
1:A:67:GLY:HA3	1:A:94:VAL:HG23	1.76	0.68
1:A:440:SER:HB3	1:A:453:SER:HB2	1.77	0.67
1:A:368:GLN:HG2	1:A:431:TRP:HB2	1.82	0.61
1:A:217:MET:HE3	1:A:220:LYS:HG3	1.83	0.61
1:A:243:PHE:HB3	1:A:246:LEU:HD13	1.84	0.60
1:A:74:MET:O	1:A:75:LYS:HD2	2.04	0.58
1:A:509:MET:HA	1:A:509:MET:HE3	1.89	0.55
1:A:138:VAL:HG23	1:A:139:ILE:HG13	1.89	0.53
1:A:371:LYS:HE2	1:A:431:TRP:CZ3	2.44	0.52
1:A:339:GLU:HG2	1:A:365:LEU:HD13	1.91	0.51
1:A:463:PHE:HB3	1:A:470:CYS:HB3	1.92	0.51
1:A:383:LEU:HD22	2:A:601:HEM:HBA2	1.92	0.51
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.92	0.50
1:A:180:ASP:HA	1:A:185:ARG:HH11	1.77	0.49
1:A:199:THR:O	1:A:203:MET:HG3	2.14	0.48
1:A:8:VAL:HG13	1:A:9:GLY:H	1.80	0.47
1:A:96:LEU:O	1:A:98:ARG:NH1	2.49	0.46
1:A:371:LYS:HE2	1:A:431:TRP:CE3	2.51	0.46
1:A:129:LEU:HD22	1:A:241:PHE:CZ	2.52	0.45
1:A:311:VAL:HG13	2:A:601:HEM:HAC	1.99	0.45
1:A:130:THR:HB	1:A:134:PHE:CE2	2.53	0.44
1:A:344:GLN:OE1	1:A:489:ARG:HD2	2.18	0.44
1:A:134:PHE:CD2	1:A:139:ILE:HD12	2.53	0.44
1:A:216:GLU:HB3	4:A:603:1PE:H242	2.00	0.44
1:A:61:TYR:CD2	1:A:67:GLY:HA2	2.53	0.43
1:A:273:ARG:NH2	1:A:301:ASP:OD2	2.46	0.43
1:A:277:ASP:O	1:A:281:ARG:NH2	2.50	0.43
1:A:427:ASN:O	1:A:430:ARG:HG2	2.19	0.43
1:A:84:GLN:HA	1:A:88:GLY:O	2.19	0.42
1:A:34:ILE:HD12	1:A:34:ILE:HA	1.79	0.42
1:A:194:ILE:HD11	1:A:519:ILE:HD11	2.01	0.42
1:A:467:ARG:HG3	1:A:468:HIS:CD2	2.55	0.42
1:A:184:PHE:O	1:A:189:ARG:HD3	2.18	0.42
1:A:122:ALA:HB3	1:A:468:HIS:CE1	2.55	0.42
1:A:54:ASP:HA	1:A:397:SER:O	2.20	0.41
1:A:440:SER:HB3	1:A:453:SER:CB	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:SER:O	1:A:489:ARG:HD3	2.21	0.41
1:A:36:ILE:O	1:A:40:ILE:HG12	2.21	0.41
1:A:236:PHE:CE2	1:A:509:MET:HG2	2.56	0.41
3:A:602:X2N:OAC	3:A:602:X2N:HAO	2.20	0.40
1:A:61:TYR:CZ	1:A:94:VAL:HG21	2.55	0.40
1:A:155:LYS:HG3	1:A:471:ILE:HB	2.04	0.40
1:A:120:VAL:HB	1:A:385:ARG:HB3	2.04	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	525/539 (97%)	505 (96%)	19 (4%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE

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	462/473 (98%)	452 (98%)	10 (2%)	52 65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	12	LEU
1	A	20	SER
1	A	34	ILE
1	A	103	TYR
1	A	188	GLU
1	A	224	ASP
1	A	253	LYS
1	A	397	SER
1	A	533	ARG

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	601	3,1	41,50,50	1.53	7 (17%)	45,82,82	1.57	7 (15%)
3	X2N	A	602	2	51,57,57	1.81	7 (13%)	57,82,82	2.40	20 (35%)
4	1PE	A	603	-	15,15,15	0.68	0	14,14,14	0.53	0
5	LMT	A	604	-	36,36,36	0.66	1 (2%)	47,47,47	1.06	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	3,1	-	2/12/54/54	-
3	X2N	A	602	2	-	11/38/59/59	0/7/7/7
4	1PE	A	603	-	-	3/13/13/13	-
5	LMT	A	604	-	-	6/21/61/61	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	X2N	CAR-CBI	6.06	1.47	1.38
3	A	602	X2N	CBN-NBW	-5.45	1.36	1.44
3	A	602	X2N	CAT-NBF	4.94	1.37	1.30
2	A	601	HEM	C3C-CAC	4.10	1.56	1.47
3	A	602	X2N	CBP-NBW	-4.02	1.34	1.39
3	A	602	X2N	OAC-CBP	3.95	1.29	1.22
2	A	601	HEM	C3C-C2C	-3.44	1.35	1.40
2	A	601	HEM	FE-ND	3.37	2.13	1.96
3	A	602	X2N	NBE-NBV	3.30	1.40	1.35
5	A	604	LMT	O1'-C1'	2.88	1.45	1.40
2	A	601	HEM	CAB-C3B	2.81	1.55	1.47
3	A	602	X2N	NBX-NBF	2.78	1.41	1.37
2	A	601	HEM	CMD-C2D	2.36	1.55	1.50
2	A	601	HEM	CMB-C2B	2.33	1.55	1.50
2	A	601	HEM	C4A-NA	2.01	1.40	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	X2N	CAS-NBD-CAQ	7.54	110.83	102.34
3	A	602	X2N	CAG-CBI-CAR	-5.86	117.65	124.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	X2N	NBD-CAS-NBV	-5.64	105.42	112.24
3	A	602	X2N	CBS-NBX-CBP	4.58	134.25	125.09
3	A	602	X2N	CBI-CAG-CAP	4.50	121.35	116.62
5	A	604	LMT	C1-O1'-C1'	3.91	120.33	113.84
3	A	602	X2N	CAX-CAZ-NBU	-3.66	103.60	110.70
2	A	601	HEM	CMC-C2C-C3C	3.46	131.15	124.68
3	A	602	X2N	CAW-CAY-NBU	-3.39	104.11	110.70
3	A	602	X2N	FAE-CBI-CAR	3.35	123.01	118.98
5	A	604	LMT	O5'-C1'-O1'	3.31	117.81	109.97
2	A	601	HEM	C4D-ND-C1D	3.23	108.41	105.07
2	A	601	HEM	C4B-CHC-C1C	3.21	126.80	122.56
3	A	602	X2N	C2-CAR-CBI	-3.08	120.09	122.78
3	A	602	X2N	CAN-CBN-NBW	3.08	123.61	119.63
3	A	602	X2N	CBJ-CAR-CBI	3.03	119.87	116.10
2	A	601	HEM	CHD-C1D-ND	2.91	127.60	124.43
3	A	602	X2N	CAL-CAN-CBN	2.90	124.14	120.32
3	A	602	X2N	CAT-NBF-NBX	2.89	106.79	103.66
2	A	601	HEM	C1B-NB-C4B	2.89	108.06	105.07
2	A	601	HEM	CMA-C3A-C4A	-2.80	124.16	128.46
3	A	602	X2N	CAO-CBN-CAN	-2.70	113.66	119.16
3	A	602	X2N	CBS-NBX-NBF	-2.70	118.59	121.46
2	A	601	HEM	C4A-C3A-C2A	2.67	108.86	107.00
3	A	602	X2N	CBB-OBG-CBK	2.63	123.51	117.93
3	A	602	X2N	CAM-CBM-NBU	-2.58	117.83	121.38
3	A	602	X2N	CAM-CAO-CBN	2.57	123.70	120.32
3	A	602	X2N	CAO-CBN-NBW	2.36	122.68	119.63
3	A	602	X2N	NBW-CAT-NBF	-2.13	107.13	111.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	X2N	C2-CBC-NBV-CAS
3	A	602	X2N	CAB-CBQ-CBS-CAU
3	A	602	X2N	CAB-CBQ-CBS-NBX
3	A	602	X2N	OAD-CBQ-CBS-CAU
3	A	602	X2N	OAD-CBQ-CBS-NBX
5	A	604	LMT	C2'-C1'-O1'-C1
5	A	604	LMT	O5'-C1'-O1'-C1
5	A	604	LMT	C4'-C5'-C6'-O6'
5	A	604	LMT	O5'-C5'-C6'-O6'
5	A	604	LMT	O1'-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	602	X2N	CAN-CBN-NBW-CAT
4	A	603	1PE	OH7-C16-C26-OH6
4	A	603	1PE	OH4-C13-C23-OH3
3	A	602	X2N	CAO-CBN-NBW-CAT
3	A	602	X2N	CAN-CBN-NBW-CBP
5	A	604	LMT	C11-C10-C9-C8
3	A	602	X2N	CAH-CBK-OBG-CBB
3	A	602	X2N	CAI-CBK-OBG-CBB
2	A	601	HEM	CAA-CBA-CGA-O2A
4	A	603	1PE	C15-C25-OH5-C14
3	A	602	X2N	CAO-CBN-NBW-CBP
2	A	601	HEM	CAA-CBA-CGA-O1A

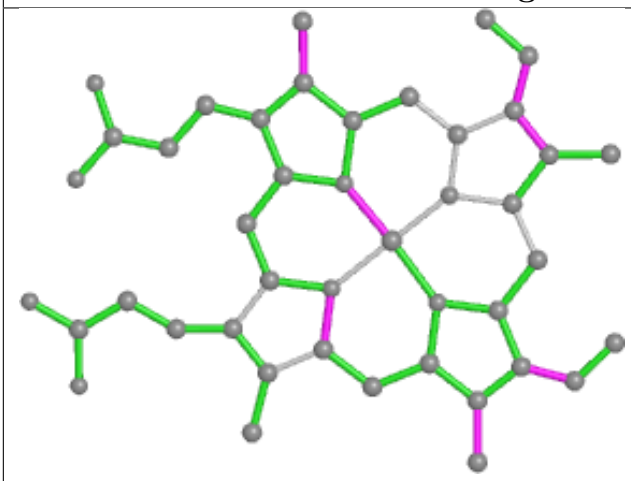
There are no ring outliers.

4 monomers are involved in 7 short contacts:

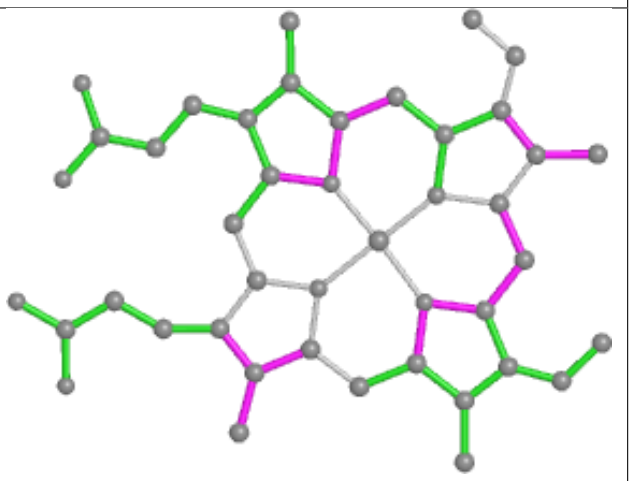
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	3	0
3	A	602	X2N	1	0
4	A	603	1PE	2	0
5	A	604	LMT	1	0

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 then 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.

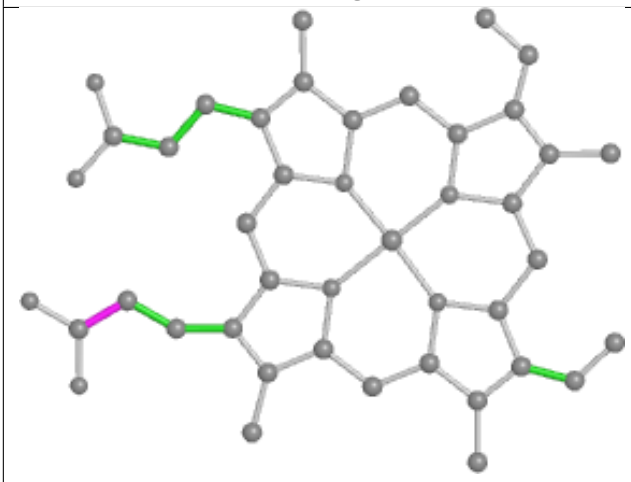
Ligand HEM A 601



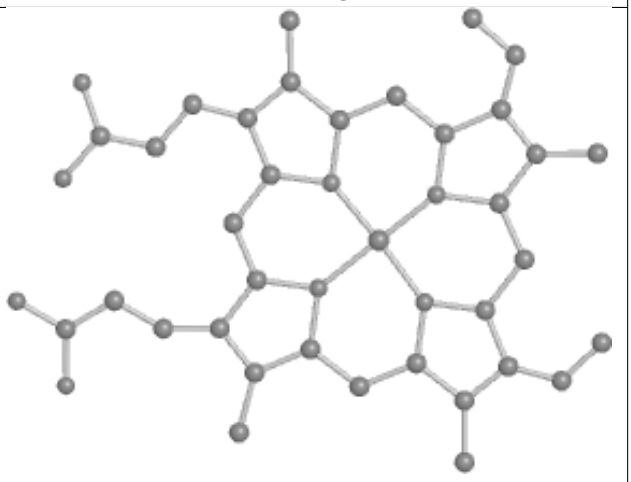
Bond lengths



Bond angles

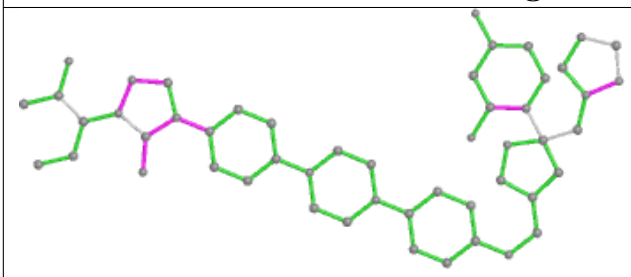


Torsions

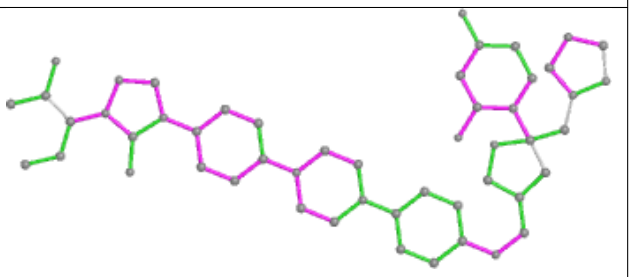


Rings

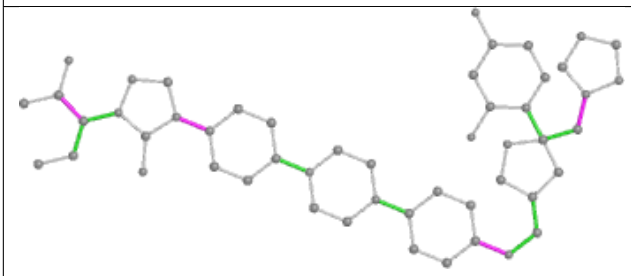
Ligand X2N A 602



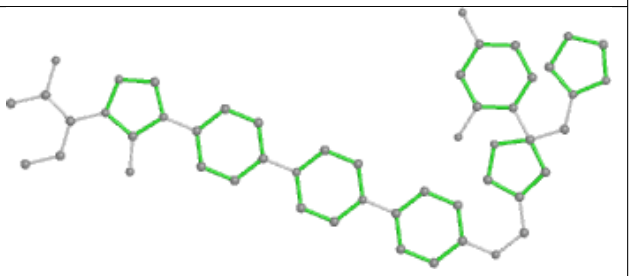
Bond lengths



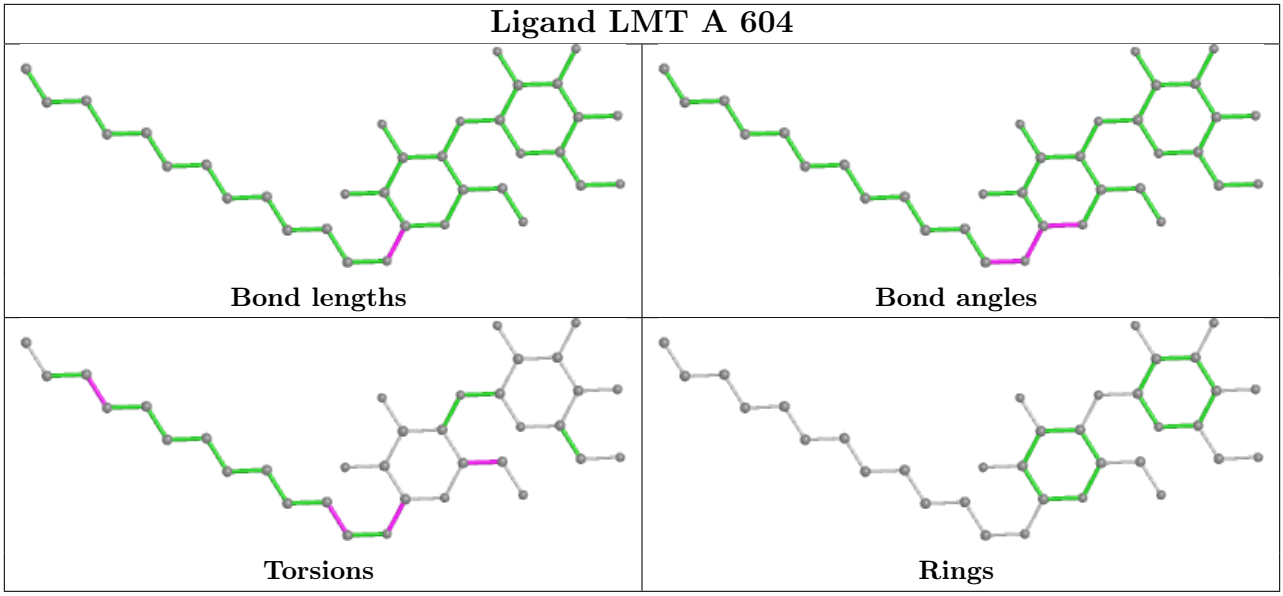
Bond angles



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 (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	527/539 (97%)	0.42	51 (9%) 7 6	21, 36, 62, 75	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	6.7
1	A	439	TYR	6.5
1	A	31	ILE	6.4
1	A	22	PHE	6.0
1	A	34	ILE	5.2
1	A	248	LEU	5.0
1	A	30	ARG	4.9
1	A	33	LEU	4.7
1	A	53	LYS	4.5
1	A	534	HIS	4.5
1	A	28	ALA	4.3
1	A	274	LYS	4.3
1	A	51	LEU	4.2
1	A	441	VAL	4.1
1	A	39	PHE	4.1
1	A	48	LEU	4.0
1	A	27	LEU	3.9
1	A	532	GLY	3.7
1	A	443	GLU	3.5
1	A	252	ARG	3.4
1	A	276	ASN	3.4
1	A	47	LEU	3.3
1	A	23	LEU	3.2
1	A	52	ARG	3.2
1	A	35	ILE	3.2
1	A	25	LEU	3.0
1	A	41	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	3.0
1	A	352	LYS	2.9
1	A	433	ASN	2.9
1	A	8	VAL	2.9
1	A	29	GLN	2.9
1	A	40	ILE	2.8
1	A	516	PRO	2.8
1	A	44	VAL	2.8
1	A	243	PHE	2.7
1	A	37	ILE	2.6
1	A	318	THR	2.5
1	A	36	ILE	2.5
1	A	74	MET	2.3
1	A	533	ARG	2.2
1	A	249	GLU	2.2
1	A	62	TRP	2.2
1	A	128	HIS	2.2
1	A	451	ALA	2.2
1	A	397	SER	2.2
1	A	227	TYR	2.1
1	A	374	LEU	2.1
1	A	380	LEU	2.1
1	A	440	SER	2.1
1	A	442	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

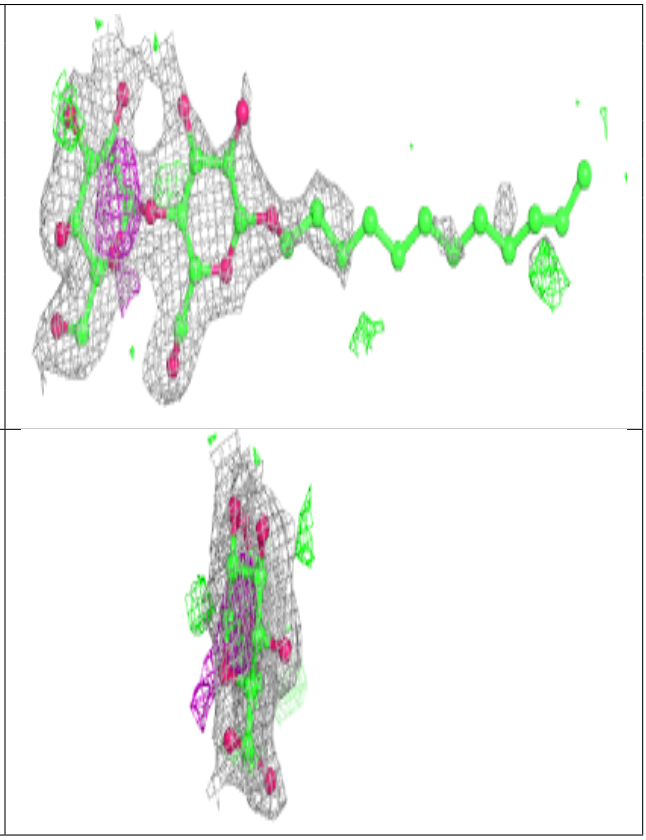
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LMT	A	604	35/35	0.72	0.44	43,64,81,83	0
4	1PE	A	603	16/16	0.85	0.17	33,43,51,53	0
3	X2N	A	602	51/51	0.92	0.19	20,35,53,56	0
2	HEM	A	601	43/43	0.99	0.20	20,23,28,32	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.

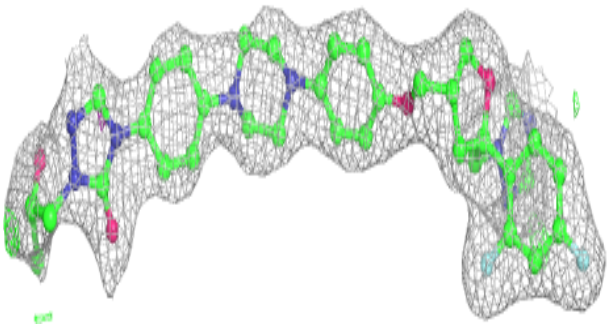
Electron density around LMT A 604:

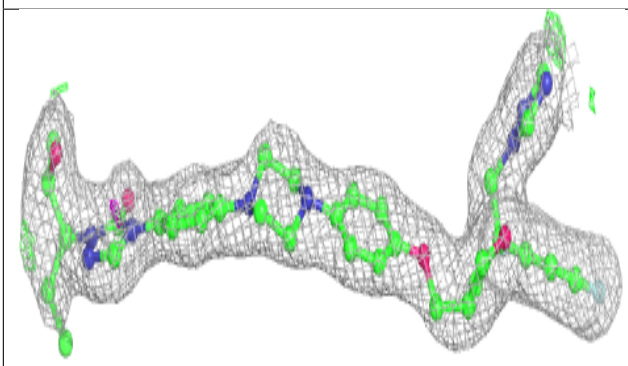
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

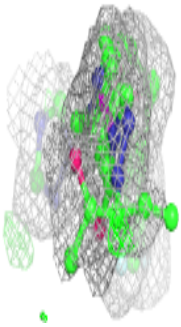


Electron density around X2N A 602:

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

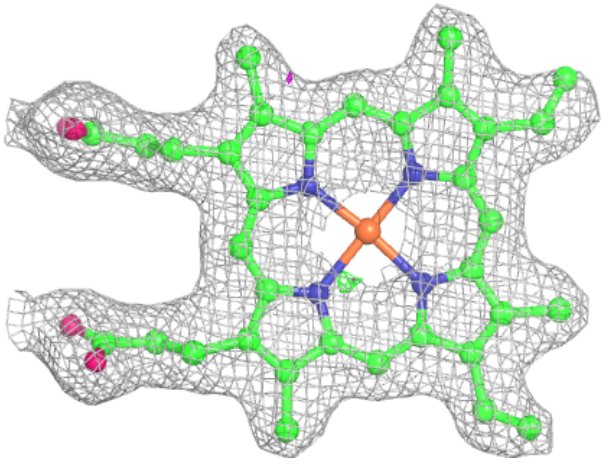


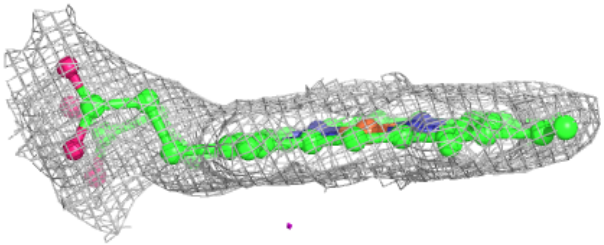


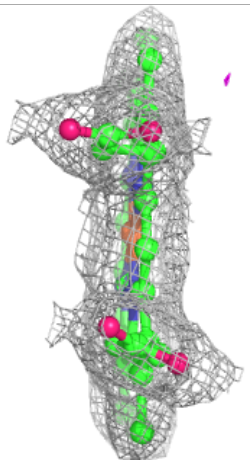


Electron density around HEM A 601:

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.