Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 10:04 PM EDT

PDB ID	:	4NKW
Title	:	Human steroidogenic cytochrome P450 17A1 mutant A105L with substrate pregnenolone
Authors	:	Scott, E.E.; Petrunak, E.P.
Deposited on	:	2013-11-13
Resolution	:	2.50 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:

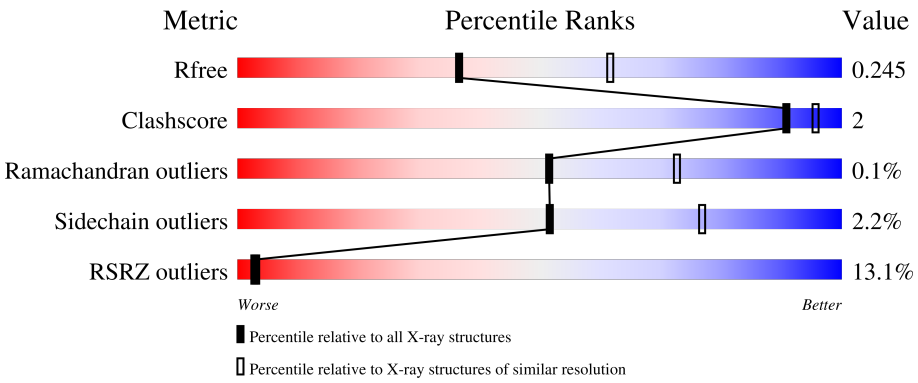
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	494	9% 89% 5% 6%
1	B	494	9% 90% • 6%
1	C	494	18% 88% 7% 5%
1	D	494	14% 88% 6% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30612 atoms, of which 15409 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	464	7487	2379	3784	640	669	15	0	0	0
1	B	464	7494	2379	3791	640	669	15	0	0	0
1	C	467	7520	2389	3797	644	675	15	0	0	0
1	D	467	7512	2389	3789	644	675	15	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	105	LEU	ALA	engineered mutation	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	expression tag	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	105	LEU	ALA	engineered mutation	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	expression tag	UNP P05093

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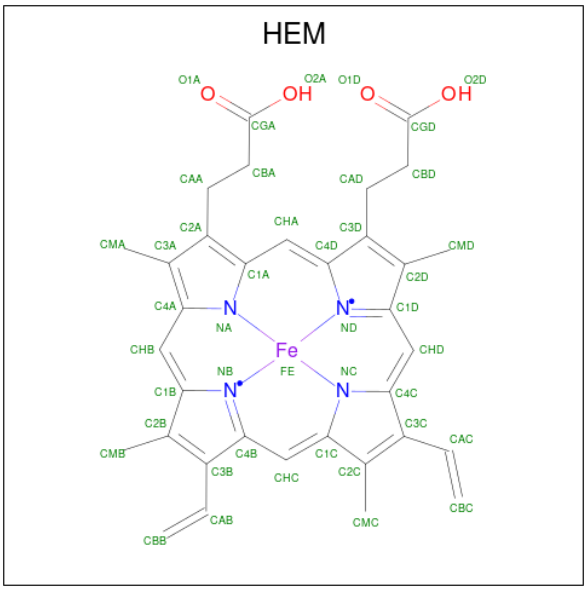
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	105	LEU	ALA	engineered mutation	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	105	LEU	ALA	engineered mutation	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- 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	H	N	O		
2	A	1	73	34	1	30	4	4	0	0

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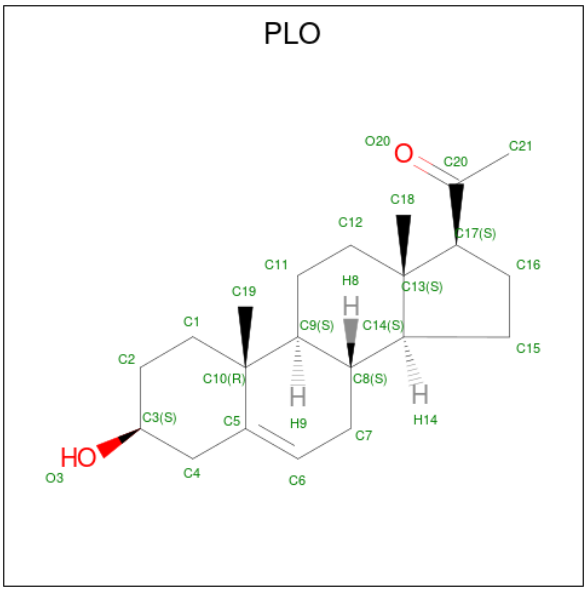
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
2	C	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
2	D	1	73	34	1	30	4	4	0	0

- Molecule 3 is (3BETA)-3-HYDROXYPREGN-5-EN-20-ONE (three-letter code: PLO) (formula: $C_{21}H_{32}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	55	21	32	2	0	0
			Total	C	H	O		
3	B	1	55	21	32	2	0	0
			Total	C	H	O		
3	C	1	55	21	32	2	0	0
			Total	C	H	O		
3	D	1	55	21	32	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	29	29	29	0	0
			Total	O		
4	B	20	20	20	0	0

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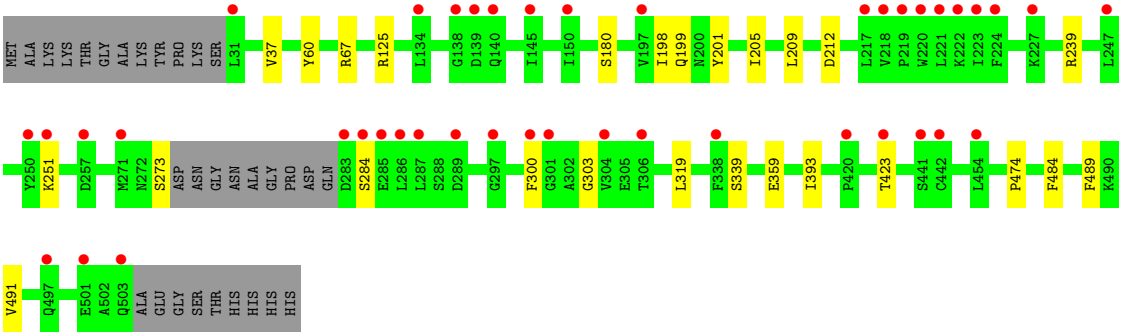
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	17	17	17	0	0
			Total	O		
4	D	21	21	21	0	0

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.

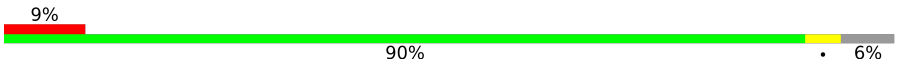
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

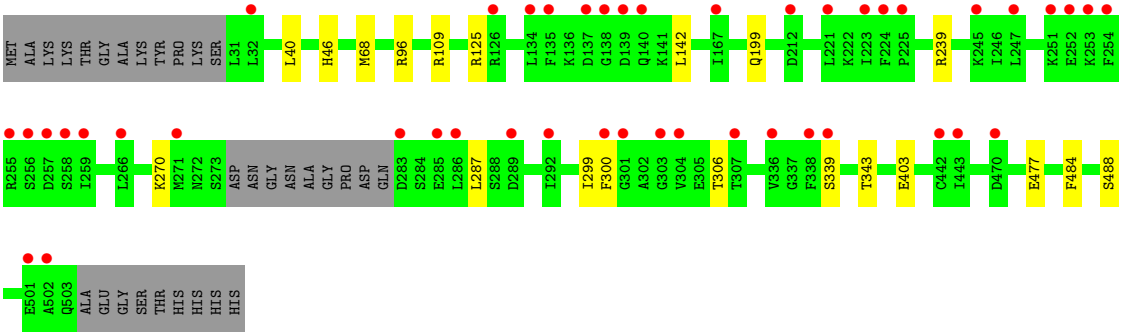
Chain A:



• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

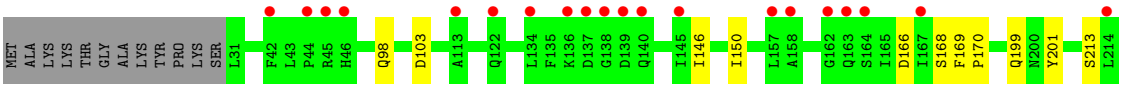
Chain B:

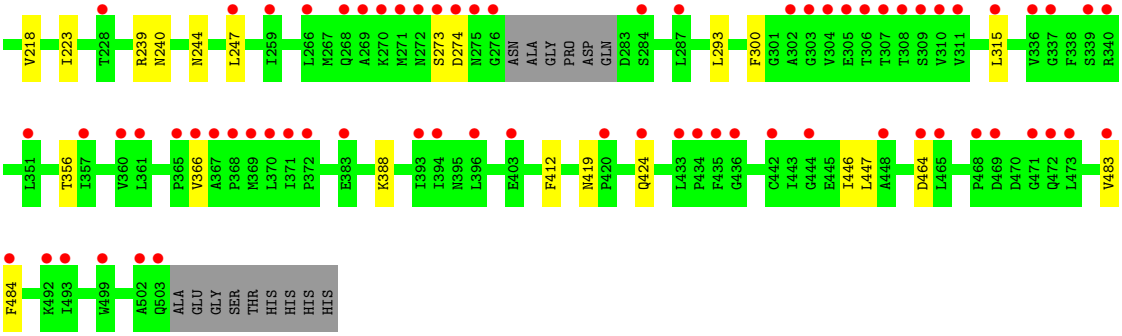




• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

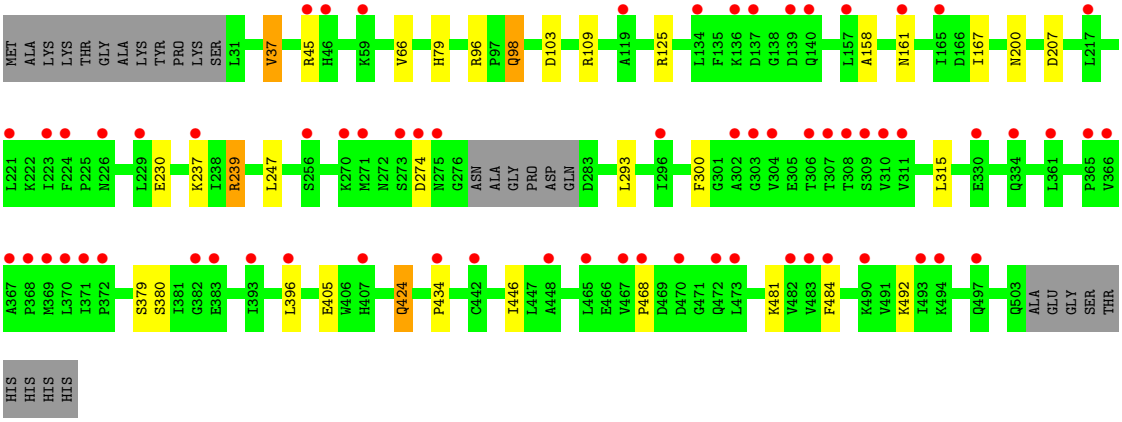
Chain C:





- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.07Å 152.63Å 173.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 2.50 39.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.11-2.50) 99.2 (39.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.245 0.191 , 0.245	Depositor DCC
R_{free} test set	3978 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30612	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3453e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PLO, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/3783	0.55	0/5121
1	B	0.40	0/3783	0.53	0/5121
1	C	0.38	0/3803	0.56	0/5148
1	D	0.39	0/3803	0.53	0/5148
All	All	0.39	0/15172	0.54	0/20538

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 (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	3703	3784	3781	14	0
1	B	3703	3791	3781	8	0
1	C	3723	3797	3794	12	0
1	D	3723	3789	3794	19	0
2	A	43	30	30	2	0
2	B	43	30	30	4	0
2	C	43	30	30	1	0
2	D	43	30	30	3	0
3	A	23	32	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	32	32	1	0
3	C	23	32	32	0	0
3	D	23	32	32	0	0
4	A	29	0	0	2	0
4	B	20	0	0	1	0
4	C	17	0	0	0	0
4	D	21	0	0	1	0
All	All	15203	15409	15398	53	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 2.

All (53) 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:D:96:ARG:O	1:D:109:ARG:NH2	2.31	0.62
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.80	0.62
1:B:199:GLN:NE2	4:B:716:HOH:O	2.24	0.61
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.82	0.60
2:B:600:HEM:HHD	2:B:600:HEM:HBC2	1.83	0.59
1:C:388:LYS:NZ	1:D:274:ASP:OD1	2.35	0.59
1:B:125:ARG:NH1	2:B:600:HEM:O1D	2.37	0.57
2:D:600:HEM:HBB2	2:D:600:HEM:HHC	1.86	0.56
1:A:37:VAL:CG2	1:D:66:VAL:HG22	2.40	0.52
1:A:37:VAL:HG22	1:D:66:VAL:HG22	1.93	0.51
1:C:166:ASP:OD1	1:C:168:SER:OG	2.21	0.50
1:D:247:LEU:HB2	1:D:293:LEU:HD21	1.93	0.50
1:B:299:ILE:HG23	2:B:600:HEM:HBC1	1.92	0.49
1:C:240:ASN:O	1:C:244:ASN:ND2	2.45	0.49
1:A:201:TYR:OH	4:A:727:HOH:O	2.20	0.49
1:D:379:SER:OG	1:D:380:SER:N	2.46	0.49
1:A:319:LEU:HD11	1:A:491:VAL:HG12	1.95	0.49
1:D:207:ASP:HA	1:D:481:LYS:HE2	1.93	0.49
1:D:98:GLN:NE2	1:D:103:ASP:OD2	2.47	0.48
1:C:218:VAL:CG1	1:C:223:ILE:HD11	2.45	0.47
1:C:446:ILE:HG22	1:C:447:LEU:N	2.31	0.45
1:C:356:THR:HG23	1:C:412:PHE:HZ	1.82	0.45
2:B:600:HEM:HBB2	2:B:600:HEM:HHC	1.97	0.45
1:C:146:ILE:O	1:C:150:ILE:HG12	2.16	0.45
1:A:60:TYR:CD2	1:D:37:VAL:HG21	2.53	0.44
1:A:125:ARG:NH1	2:A:600:HEM:O1D	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:HB2	1:C:293:LEU:HD21	1.99	0.44
1:C:98:GLN:NE2	1:C:103:ASP:OD2	2.50	0.44
1:C:419:ASN:ND2	1:C:424:GLN:HG2	2.33	0.44
1:A:251:LYS:NZ	4:A:720:HOH:O	2.51	0.44
1:B:96:ARG:O	1:B:109:ARG:NH1	2.50	0.44
1:B:477:GLU:OE1	1:D:237:LYS:NZ	2.44	0.44
1:D:468:PRO:HA	1:D:492:LYS:HB2	2.00	0.44
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.53	0.43
1:B:306:THR:HG21	3:B:601:PLO:H213	2.00	0.43
1:A:303:GLY:HA2	2:A:600:HEM:HMC2	2.01	0.43
1:A:359:GLU:OE1	1:A:359:GLU:HA	2.19	0.42
1:C:169:PHE:N	1:C:170:PRO:HD2	2.34	0.42
1:D:79:HIS:NE2	1:D:405:GLU:OE2	2.52	0.42
1:B:40:LEU:HD21	1:B:68:MET:HE2	2.01	0.42
1:D:239:ARG:NH2	4:D:718:HOH:O	2.53	0.42
1:C:366:VAL:HG13	1:C:483:VAL:HG13	2.01	0.42
1:A:273:SER:O	1:A:284:SER:OG	2.37	0.41
1:D:167:ILE:HD11	1:D:315:LEU:CD1	2.50	0.41
1:D:98:GLN:HG2	1:D:109:ARG:HD2	2.02	0.41
1:D:158:ALA:O	1:D:161:ASN:HB2	2.20	0.41
1:A:198:ILE:HA	1:A:201:TYR:CE2	2.56	0.41
1:A:205:ILE:O	1:A:209:LEU:HB2	2.21	0.41
1:B:270:LYS:HA	1:B:287:LEU:HD13	2.03	0.41
1:D:396:LEU:HD21	1:D:434:PRO:HA	2.02	0.41
1:A:393:ILE:HD12	1:A:393:ILE:N	2.36	0.40
1:D:125:ARG:NH1	2:D:600:HEM:O1D	2.54	0.40
1:D:45:ARG:HA	1:D:45:ARG:HD3	1.83	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	460/494 (93%)	440 (96%)	19 (4%)	1 (0%)	47	68
1	B	460/494 (93%)	442 (96%)	18 (4%)	0	100	100
1	C	463/494 (94%)	442 (96%)	21 (4%)	0	100	100
1	D	463/494 (94%)	439 (95%)	23 (5%)	1 (0%)	47	68
All	All	1846/1976 (93%)	1763 (96%)	81 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASP
1	D	424	GLN

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	415/437 (95%)	407 (98%)	8 (2%)	57	80
1	B	415/437 (95%)	406 (98%)	9 (2%)	52	77
1	C	417/437 (95%)	407 (98%)	10 (2%)	49	74
1	D	417/437 (95%)	408 (98%)	9 (2%)	52	77
All	All	1664/1748 (95%)	1628 (98%)	36 (2%)	52	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	180	SER
1	A	199	GLN
1	A	239	ARG
1	A	300	PHE
1	A	339	SER
1	A	423	THR
1	A	484	PHE
1	B	46	HIS

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	239	ARG
1	B	300	PHE
1	B	339	SER
1	B	343	THR
1	B	403	GLU
1	B	484	PHE
1	B	488	SER
1	C	199	GLN
1	C	201	TYR
1	C	213	SER
1	C	239	ARG
1	C	273	SER
1	C	274	ASP
1	C	300	PHE
1	C	315	LEU
1	C	464	ASP
1	C	484	PHE
1	D	37	VAL
1	D	98	GLN
1	D	200	ASN
1	D	230	GLU
1	D	239	ARG
1	D	300	PHE
1	D	424	GLN
1	D	446	ILE
1	D	484	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	B	50	HIS
1	C	50	HIS
1	C	291	HIS
1	D	46	HIS
1	D	50	HIS

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)

8 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	B	600	1	41,50,50	1.97	6 (14%)	45,82,82	1.88	10 (22%)
2	HEM	A	600	1	41,50,50	1.89	7 (17%)	45,82,82	1.56	9 (20%)
3	PLO	A	601	-	26,26,26	2.17	10 (38%)	42,42,42	2.41	13 (30%)
3	PLO	D	601	-	26,26,26	2.14	9 (34%)	42,42,42	2.30	14 (33%)
2	HEM	D	600	1	41,50,50	1.88	6 (14%)	45,82,82	1.80	9 (20%)
3	PLO	C	601	-	26,26,26	2.20	9 (34%)	42,42,42	2.11	9 (21%)
2	HEM	C	600	1	41,50,50	1.82	6 (14%)	45,82,82	1.81	12 (26%)
3	PLO	B	601	-	26,26,26	2.28	11 (42%)	42,42,42	2.21	12 (28%)

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	B	600	1	-	2/12/54/54	-
2	HEM	A	600	1	-	1/12/54/54	-
3	PLO	A	601	-	-	0/4/62/62	0/4/4/4
3	PLO	D	601	-	-	0/4/62/62	0/4/4/4
2	HEM	D	600	1	-	1/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLO	C	601	-	-	0/4/62/62	0/4/4/4
2	HEM	C	600	1	-	1/12/54/54	-
3	PLO	B	601	-	-	0/4/62/62	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3D-C2D	7.84	1.53	1.36
2	A	600	HEM	C3D-C2D	7.46	1.52	1.36
2	D	600	HEM	C3D-C2D	7.30	1.52	1.36
2	C	600	HEM	C3D-C2D	7.17	1.52	1.36
3	B	601	PLO	C1-C10	-5.71	1.43	1.54
3	C	601	PLO	C1-C10	-5.43	1.43	1.54
3	A	601	PLO	C1-C10	-5.30	1.44	1.54
3	D	601	PLO	C1-C10	-5.28	1.44	1.54
2	B	600	HEM	C3C-C2C	-4.98	1.33	1.40
2	D	600	HEM	C3C-C2C	-4.26	1.34	1.40
3	A	601	PLO	C4-C5	4.00	1.60	1.51
2	A	600	HEM	C3C-CAC	3.98	1.56	1.47
2	C	600	HEM	C3C-CAC	3.98	1.56	1.47
3	C	601	PLO	C4-C5	3.88	1.60	1.51
2	B	600	HEM	C3C-CAC	3.74	1.55	1.47
2	D	600	HEM	C3C-CAC	3.70	1.55	1.47
3	B	601	PLO	C4-C5	3.68	1.59	1.51
2	A	600	HEM	C3C-C2C	-3.65	1.35	1.40
3	D	601	PLO	C4-C5	3.60	1.59	1.51
3	A	601	PLO	C6-C5	3.55	1.40	1.33
2	C	600	HEM	C3C-C2C	-3.54	1.35	1.40
3	B	601	PLO	C7-C8	-3.48	1.47	1.53
3	D	601	PLO	C7-C8	-3.48	1.47	1.53
3	A	601	PLO	C13-C14	-3.41	1.48	1.55
3	C	601	PLO	C7-C8	-3.36	1.47	1.53
3	C	601	PLO	C6-C5	3.35	1.40	1.33
3	D	601	PLO	C6-C5	3.27	1.40	1.33
2	B	600	HEM	FE-NB	3.08	2.12	1.96
2	D	600	HEM	CAB-C3B	3.07	1.55	1.47
3	B	601	PLO	C13-C14	-3.03	1.49	1.55
3	A	601	PLO	C7-C8	-3.02	1.48	1.53
3	B	601	PLO	C6-C5	2.99	1.39	1.33
3	B	601	PLO	C8-C14	2.98	1.59	1.53
3	D	601	PLO	C13-C14	-2.97	1.49	1.55
3	C	601	PLO	C13-C14	-2.82	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	CAB-C3B	2.80	1.55	1.47
2	A	600	HEM	CAB-C3B	2.80	1.55	1.47
3	D	601	PLO	C10-C5	2.79	1.58	1.52
3	C	601	PLO	C10-C5	2.78	1.58	1.52
2	A	600	HEM	FE-ND	2.74	2.10	1.96
3	B	601	PLO	C15-C14	-2.72	1.48	1.54
2	C	600	HEM	CAB-C3B	2.61	1.54	1.47
3	D	601	PLO	C15-C14	-2.55	1.49	1.54
3	A	601	PLO	C10-C5	2.49	1.57	1.52
3	B	601	PLO	C10-C5	2.45	1.57	1.52
3	C	601	PLO	C15-C14	-2.38	1.49	1.54
3	A	601	PLO	C13-C17	-2.38	1.52	1.56
3	B	601	PLO	C13-C17	-2.37	1.52	1.56
3	B	601	PLO	C4-C3	2.36	1.56	1.52
2	D	600	HEM	FE-NB	2.34	2.08	1.96
2	A	600	HEM	FE-NB	2.28	2.08	1.96
3	C	601	PLO	C4-C3	2.27	1.56	1.52
3	A	601	PLO	C8-C14	2.27	1.57	1.53
3	A	601	PLO	C15-C14	-2.26	1.49	1.54
2	C	600	HEM	FE-ND	2.19	2.07	1.96
3	D	601	PLO	C8-C14	2.18	1.57	1.53
3	B	601	PLO	C11-C9	-2.13	1.50	1.53
2	D	600	HEM	CAA-C2A	2.13	1.55	1.52
3	C	601	PLO	C8-C14	2.13	1.57	1.53
2	B	600	HEM	CAA-C2A	2.12	1.55	1.52
3	D	601	PLO	C8-C9	-2.08	1.49	1.53
2	A	600	HEM	CMB-C2B	2.03	1.55	1.50
3	A	601	PLO	C4-C3	2.00	1.55	1.52
2	C	600	HEM	CAA-C2A	2.00	1.55	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	PLO	C3-C4-C5	-7.92	98.58	112.03
3	A	601	PLO	C3-C4-C5	-7.15	99.90	112.03
3	B	601	PLO	C3-C4-C5	-6.60	100.82	112.03
3	D	601	PLO	C3-C4-C5	-6.55	100.91	112.03
3	A	601	PLO	C16-C17-C13	-6.25	98.64	104.21
2	B	600	HEM	C4D-ND-C1D	6.06	111.33	105.07
3	B	601	PLO	C16-C17-C13	-6.04	98.83	104.21
2	D	600	HEM	C4D-ND-C1D	5.93	111.20	105.07
2	C	600	HEM	C4D-ND-C1D	5.61	110.87	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	C4D-ND-C1D	4.63	109.86	105.07
3	D	601	PLO	C7-C8-C9	4.45	115.11	109.71
3	A	601	PLO	C1-C2-C3	4.26	115.93	110.47
3	A	601	PLO	C14-C8-C9	-4.24	103.41	109.09
3	D	601	PLO	C7-C8-C14	-4.21	104.80	110.91
3	B	601	PLO	C7-C8-C9	4.08	114.66	109.71
3	C	601	PLO	C7-C8-C14	-4.06	105.02	110.91
3	C	601	PLO	C7-C8-C9	3.98	114.54	109.71
3	D	601	PLO	C16-C17-C13	-3.90	100.73	104.21
3	B	601	PLO	C14-C8-C9	-3.80	104.01	109.09
3	D	601	PLO	C14-C8-C9	-3.79	104.01	109.09
3	A	601	PLO	C7-C8-C14	-3.68	105.57	110.91
3	C	601	PLO	C14-C8-C9	-3.68	104.17	109.09
2	B	600	HEM	C4C-CHD-C1D	3.63	127.34	122.56
3	D	601	PLO	C13-C17-C20	3.59	120.04	114.98
2	C	600	HEM	CHB-C1B-NB	3.57	128.79	124.38
2	D	600	HEM	C4B-CHC-C1C	3.56	127.25	122.56
2	B	600	HEM	C3B-C2B-C1B	3.41	109.02	106.49
3	A	601	PLO	C12-C13-C17	-3.38	111.96	116.10
3	C	601	PLO	C16-C17-C13	-3.38	101.20	104.21
2	A	600	HEM	CAA-CBA-CGA	-3.29	104.52	113.76
3	D	601	PLO	C21-C20-C17	3.21	122.22	117.56
3	D	601	PLO	C15-C14-C8	-3.20	113.81	119.08
3	A	601	PLO	C12-C11-C9	3.18	118.63	113.11
3	C	601	PLO	C15-C14-C8	-3.13	113.93	119.08
3	B	601	PLO	C11-C12-C13	-3.11	107.45	112.78
3	D	601	PLO	C4-C5-C10	3.09	120.53	116.42
2	B	600	HEM	C4B-CHC-C1C	3.06	126.59	122.56
3	D	601	PLO	C1-C2-C3	3.03	114.36	110.47
3	B	601	PLO	C21-C20-C17	3.00	121.93	117.56
3	A	601	PLO	C13-C17-C20	2.98	119.18	114.98
2	A	600	HEM	C4B-CHC-C1C	2.98	126.49	122.56
3	A	601	PLO	C7-C8-C9	2.97	113.31	109.71
3	B	601	PLO	C12-C13-C17	-2.96	112.48	116.10
3	A	601	PLO	C19-C10-C5	-2.96	103.56	108.34
3	B	601	PLO	C7-C8-C14	-2.91	106.69	110.91
2	C	600	HEM	C4C-CHD-C1D	2.90	126.38	122.56
2	D	600	HEM	CMA-C3A-C4A	-2.89	124.03	128.46
2	B	600	HEM	CHD-C1D-ND	2.79	127.46	124.43
2	C	600	HEM	CHC-C4B-C3B	2.78	128.82	124.57
3	B	601	PLO	C11-C9-C8	-2.75	107.80	111.75
2	D	600	HEM	CMD-C2D-C1D	2.74	129.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	C1B-NB-C4B	2.72	107.88	105.07
2	A	600	HEM	CMC-C2C-C3C	2.69	129.71	124.68
2	D	600	HEM	CHA-C4D-ND	2.66	127.67	124.38
2	C	600	HEM	CMC-C2C-C3C	2.65	129.63	124.68
3	A	601	PLO	C2-C3-C4	2.62	113.90	110.31
3	C	601	PLO	C16-C15-C14	-2.61	99.95	105.13
2	D	600	HEM	C4C-CHD-C1D	2.61	126.00	122.56
3	D	601	PLO	C16-C15-C14	-2.61	99.97	105.13
2	C	600	HEM	C4B-CHC-C1C	2.60	125.99	122.56
2	C	600	HEM	C3B-C2B-C1B	2.59	108.41	106.49
3	A	601	PLO	C15-C14-C8	-2.51	114.95	119.08
3	C	601	PLO	C11-C12-C13	-2.47	108.54	112.78
2	D	600	HEM	C3B-C2B-C1B	2.47	108.32	106.49
3	B	601	PLO	C4-C5-C10	2.46	119.69	116.42
2	B	600	HEM	CHA-C4D-ND	2.46	127.42	124.38
3	D	601	PLO	C12-C11-C9	2.46	117.38	113.11
3	B	601	PLO	C16-C15-C14	-2.46	100.27	105.13
3	D	601	PLO	C18-C13-C12	-2.45	106.72	110.59
2	C	600	HEM	CHA-C4D-ND	2.45	127.40	124.38
3	B	601	PLO	C15-C14-C8	-2.44	115.07	119.08
2	D	600	HEM	CHC-C4B-C3B	2.42	128.27	124.57
2	A	600	HEM	C4C-CHD-C1D	2.40	125.72	122.56
2	B	600	HEM	C3C-C4C-NC	-2.39	106.42	110.94
2	C	600	HEM	C1B-NB-C4B	2.38	107.53	105.07
2	B	600	HEM	CHB-C1B-NB	2.37	127.31	124.38
2	A	600	HEM	O2D-CGD-CBD	2.24	121.23	114.03
2	C	600	HEM	CAA-CBA-CGA	-2.24	107.49	113.76
2	C	600	HEM	CAB-C3B-C2B	-2.22	121.28	128.60
2	B	600	HEM	CAB-C3B-C2B	-2.20	121.35	128.60
3	C	601	PLO	C4-C5-C10	2.19	119.33	116.42
3	A	601	PLO	C16-C15-C14	-2.18	100.82	105.13
2	B	600	HEM	O2A-CGA-CBA	2.17	120.99	114.03
2	A	600	HEM	CMB-C2B-C1B	-2.15	121.77	125.04
2	D	600	HEM	CAB-C3B-C2B	-2.14	121.57	128.60
3	D	601	PLO	C1-C10-C5	2.08	112.57	108.75
2	C	600	HEM	CMD-C2D-C1D	2.07	128.20	125.04
2	A	600	HEM	CAD-C3D-C4D	2.01	128.17	124.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C3A-C2A-CAA-CBA
2	C	600	HEM	C4B-C3B-CAB-CBB
2	D	600	HEM	C4B-C3B-CAB-CBB
2	A	600	HEM	CAD-CBD-CGD-O2D

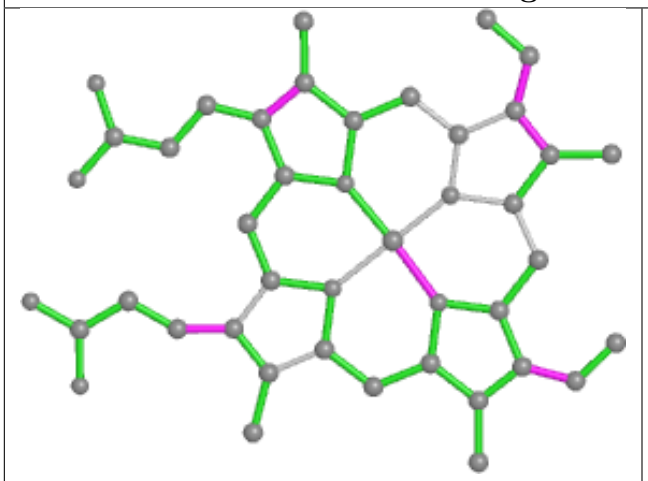
There are no ring outliers.

5 monomers are involved in 11 short contacts:

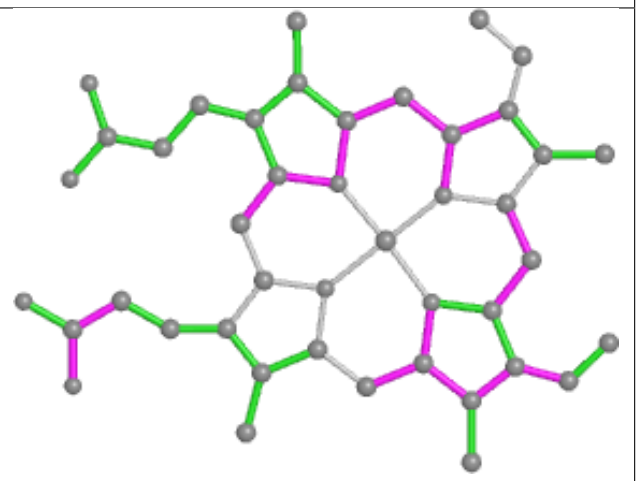
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	4	0
2	A	600	HEM	2	0
2	D	600	HEM	3	0
2	C	600	HEM	1	0
3	B	601	PLO	1	0

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.

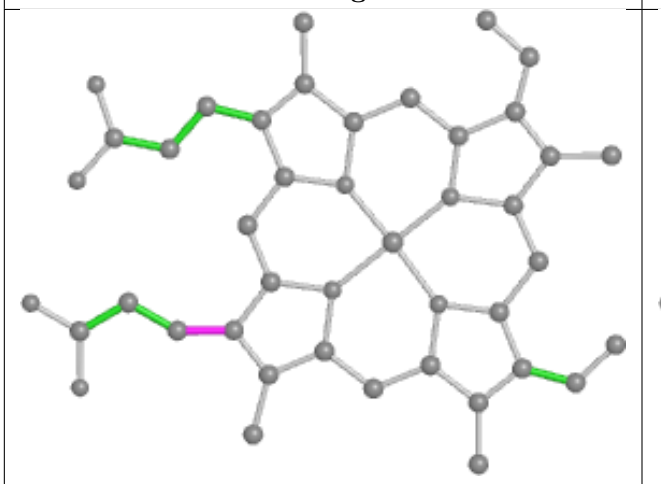
Ligand HEM B 600



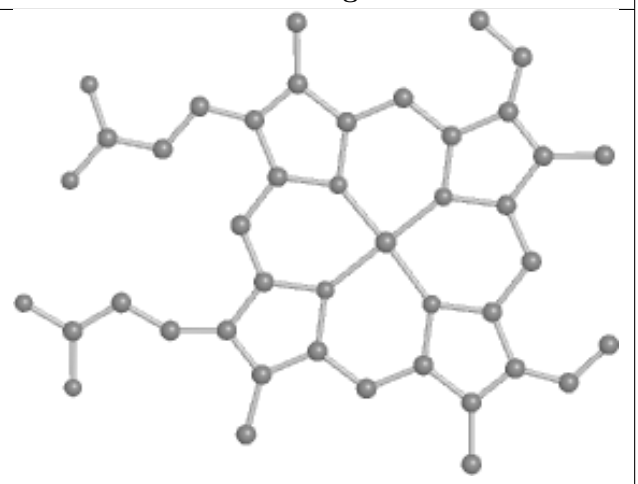
Bond lengths



Bond angles

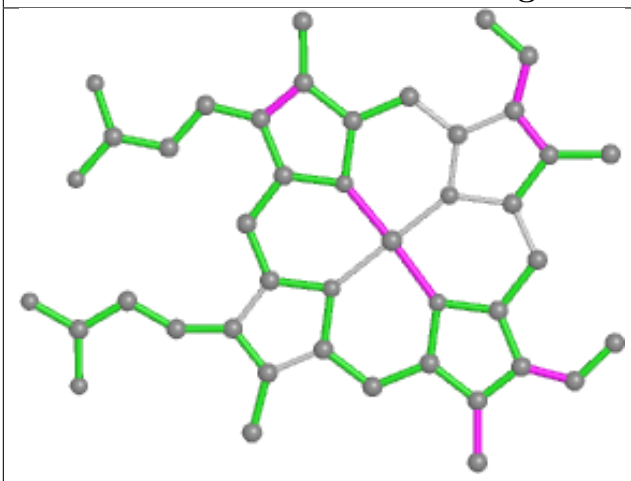


Torsions

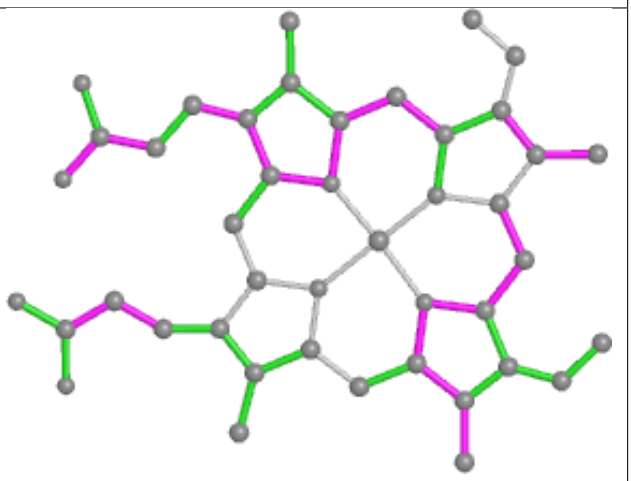


Rings

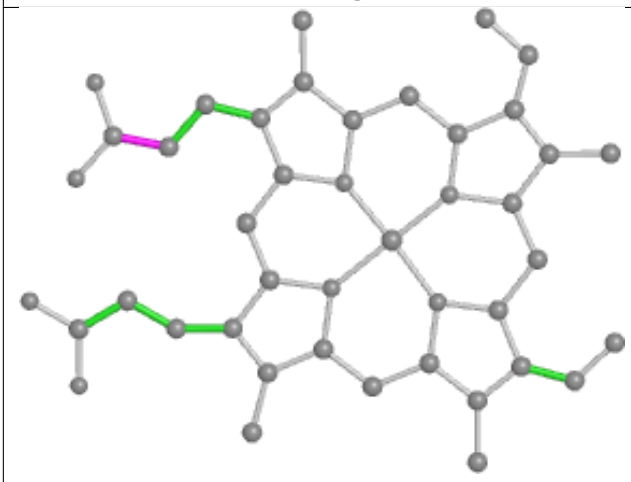
Ligand HEM A 600



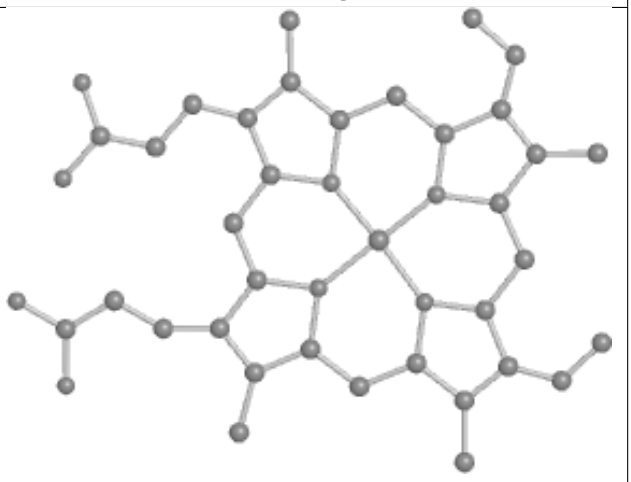
Bond lengths



Bond angles

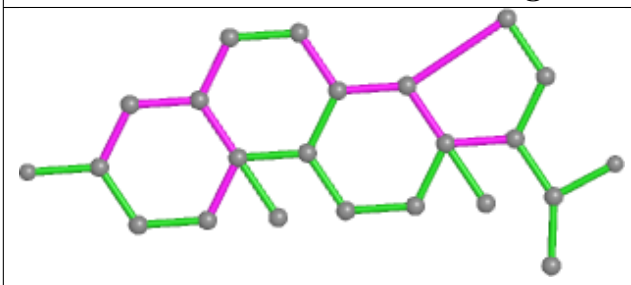


Torsions

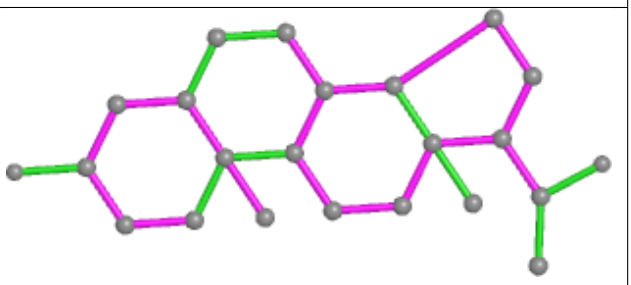


Rings

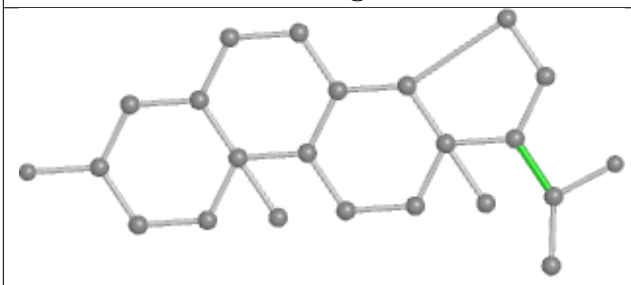
Ligand PLO A 601



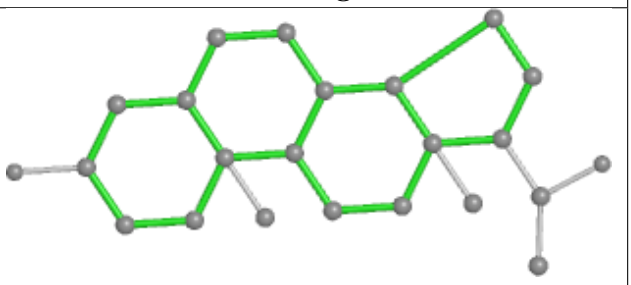
Bond lengths



Bond angles

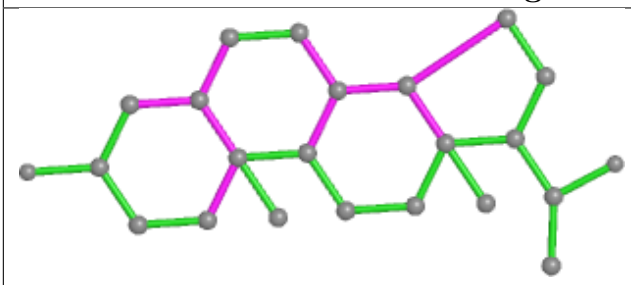


Torsions

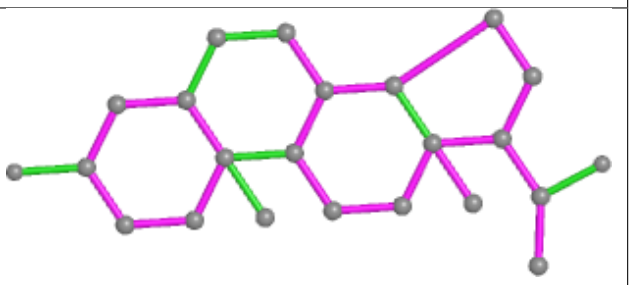


Rings

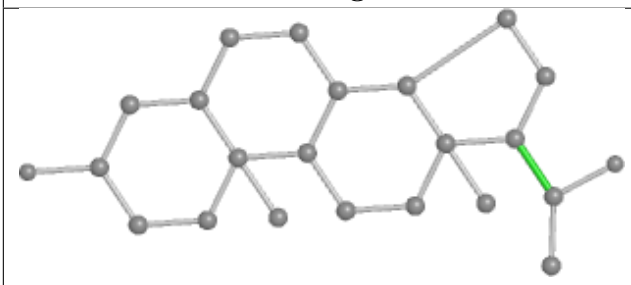
Ligand PLO D 601



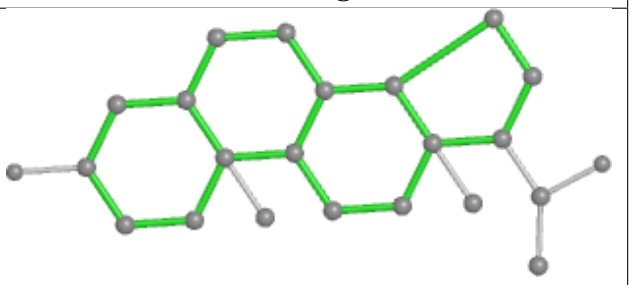
Bond lengths



Bond angles

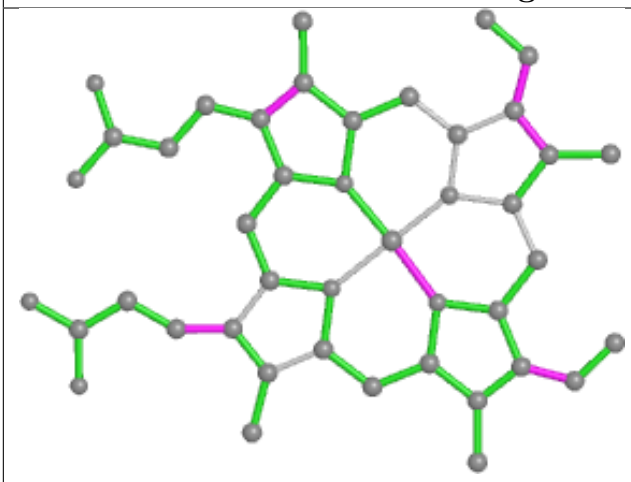


Torsions

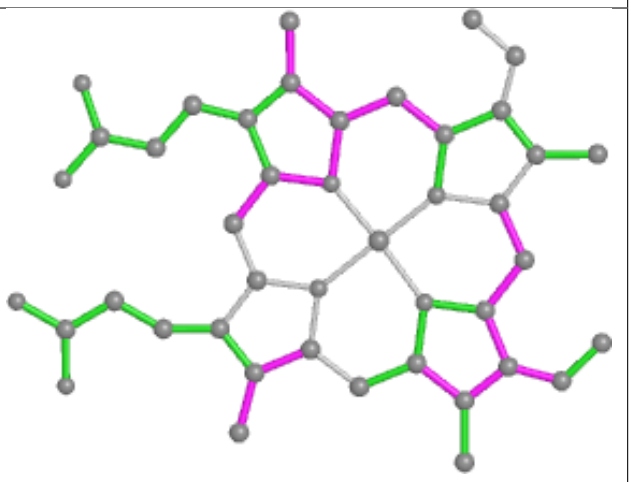


Rings

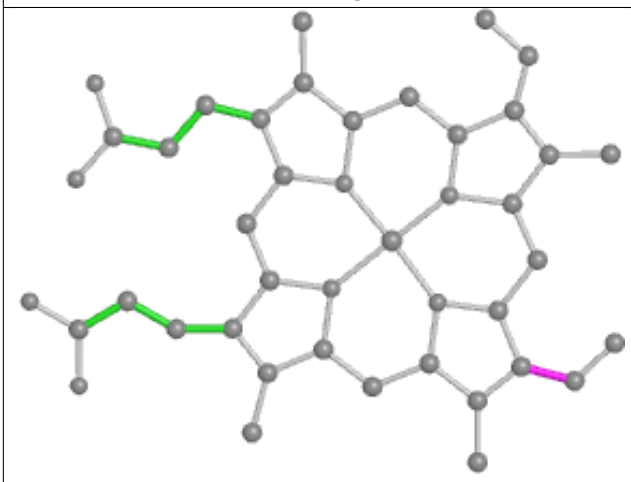
Ligand HEM D 600



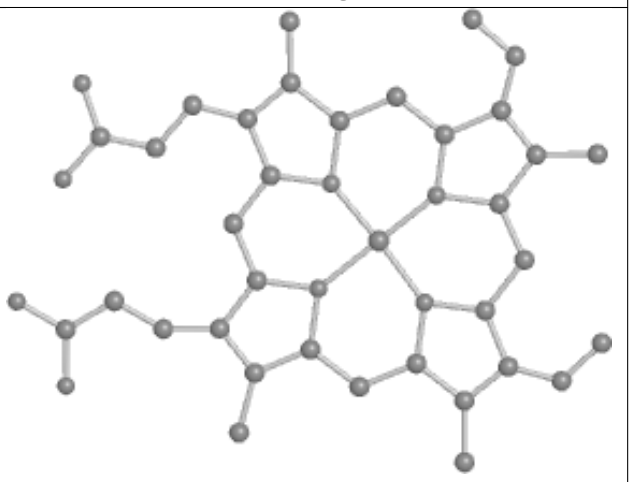
Bond lengths



Bond angles

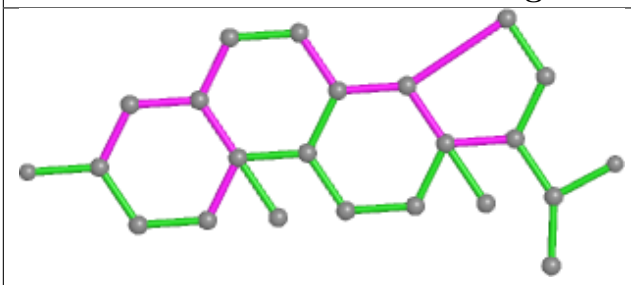


Torsions

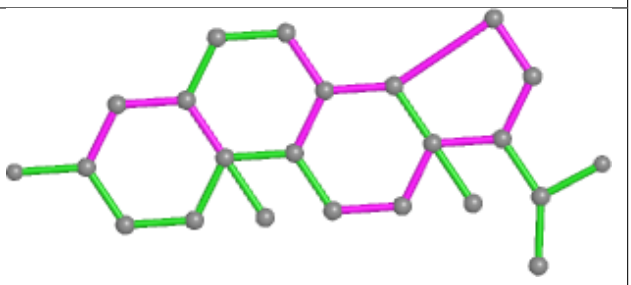


Rings

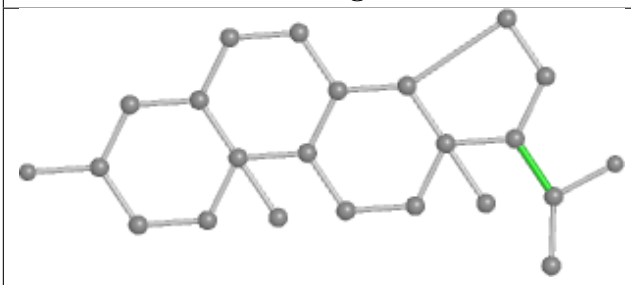
Ligand PLO C 601



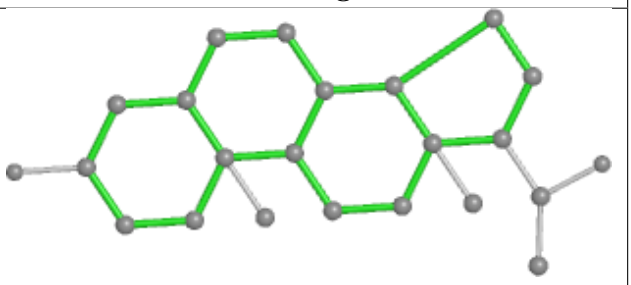
Bond lengths



Bond angles

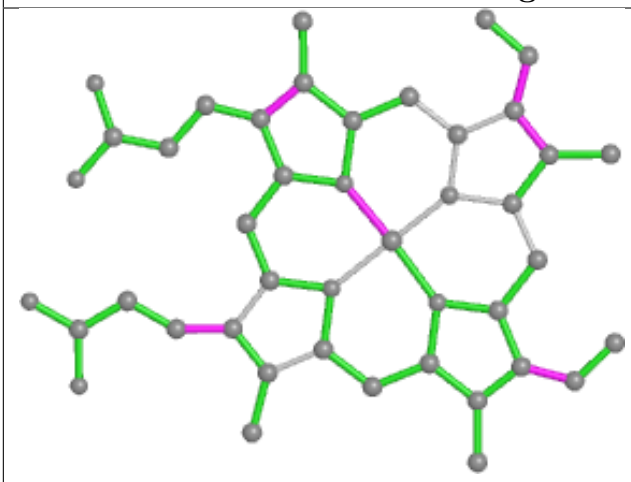


Torsions

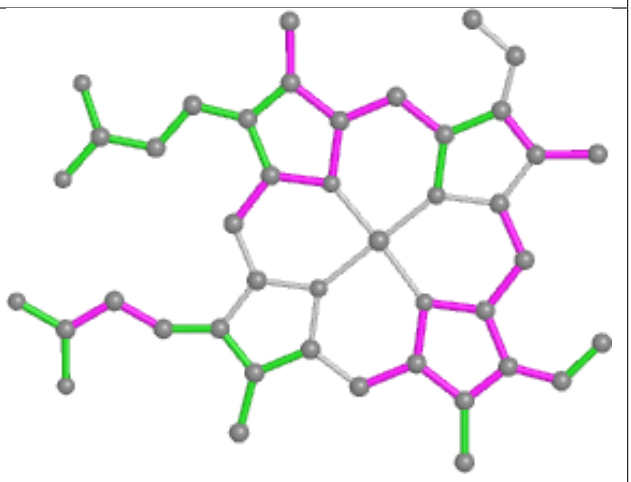


Rings

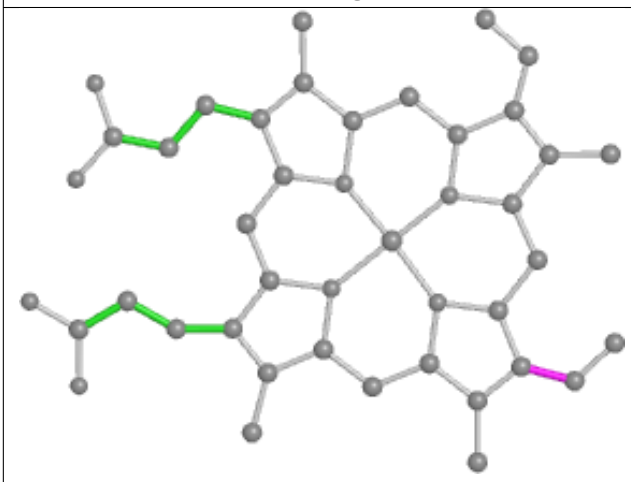
Ligand HEM C 600



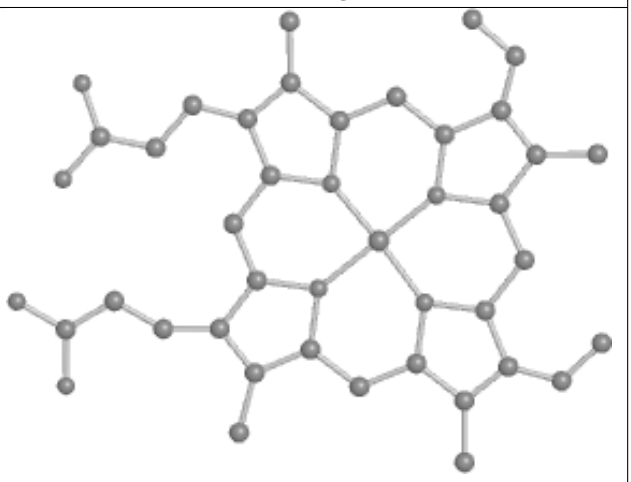
Bond lengths



Bond angles

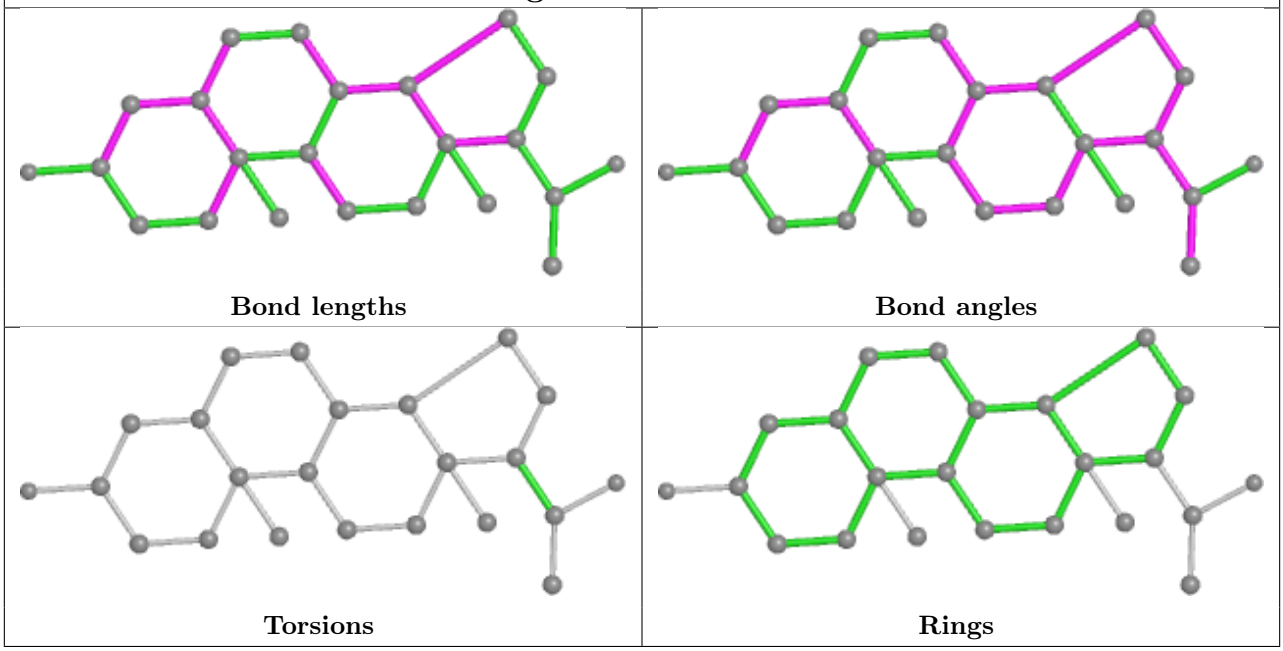


Torsions



Rings

Ligand PLO B 601



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	464/494 (93%)	0.69	42 (9%)	9	9	38, 59, 93, 123	0
1	B	464/494 (93%)	0.64	45 (9%)	7	7	39, 59, 92, 123	0
1	C	467/494 (94%)	1.01	90 (19%)	1	1	37, 64, 98, 114	0
1	D	467/494 (94%)	0.84	67 (14%)	2	2	40, 64, 95, 125	0
All	All	1862/1976 (94%)	0.80	244 (13%)	3	3	37, 62, 96, 125	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	8.4
1	C	473	LEU	6.7
1	A	223	ILE	6.5
1	A	220	TRP	6.3
1	A	217	LEU	5.9
1	C	45	ARG	5.7
1	C	274	ASP	5.6
1	A	286	LEU	5.4
1	A	139	ASP	5.1
1	C	493	ILE	5.0
1	A	271	MET	4.9
1	C	46	HIS	4.8
1	C	469	ASP	4.8
1	D	136	LYS	4.7
1	C	336	VAL	4.7
1	A	140	GLN	4.7
1	B	251	LYS	4.7
1	B	247	LEU	4.7
1	C	157	LEU	4.6
1	C	139	ASP	4.6
1	D	383	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	139	ASP	4.5
1	C	442	CYS	4.5
1	C	136	LYS	4.4
1	B	283	ASP	4.4
1	C	306	THR	4.4
1	A	251	LYS	4.3
1	D	273	SER	4.3
1	C	471	GLY	4.2
1	A	31	LEU	4.2
1	B	252	GLU	4.1
1	B	286	LEU	4.1
1	D	45	ARG	4.1
1	D	367	ALA	4.0
1	D	306	THR	4.0
1	C	434	PRO	4.0
1	D	274	ASP	4.0
1	C	273	SER	3.9
1	D	221	LEU	3.9
1	A	284	SER	3.9
1	C	137	ASP	3.8
1	B	501	GLU	3.8
1	C	340	ARG	3.8
1	C	367	ALA	3.8
1	B	134	LEU	3.8
1	D	307	THR	3.8
1	B	258	SER	3.8
1	D	223	ILE	3.8
1	C	42	PHE	3.8
1	D	493	ILE	3.8
1	D	442	CYS	3.8
1	A	247	LEU	3.8
1	D	140	GLN	3.7
1	A	219	PRO	3.7
1	C	302	ALA	3.7
1	B	253	LYS	3.6
1	C	259	ILE	3.6
1	B	502	ALA	3.6
1	D	369	MET	3.6
1	A	285	GLU	3.6
1	B	140	GLN	3.6
1	D	275	ASN	3.6
1	B	135	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	308	THR	3.5
1	C	435	PHE	3.5
1	D	473	LEU	3.5
1	A	420	PRO	3.5
1	A	283	ASP	3.5
1	C	465	LEU	3.4
1	D	137	ASP	3.4
1	A	221	LEU	3.4
1	D	309	SER	3.4
1	D	368	PRO	3.4
1	C	284	SER	3.3
1	C	503	GLN	3.3
1	C	337	GLY	3.3
1	C	134	LEU	3.3
1	C	366	VAL	3.3
1	D	366	VAL	3.3
1	B	212	ASP	3.2
1	C	492	LYS	3.2
1	A	287	LEU	3.2
1	C	272	ASN	3.2
1	C	499	TRP	3.2
1	D	224	PHE	3.2
1	B	138	GLY	3.2
1	C	365	PRO	3.2
1	B	301	GLY	3.1
1	A	501	GLU	3.1
1	C	310	VAL	3.1
1	D	434	PRO	3.1
1	D	497	GLN	3.1
1	D	310	VAL	3.1
1	C	163	GLN	3.0
1	A	250	TYR	3.0
1	A	289	ASP	3.0
1	B	255	ARG	3.0
1	A	134	LEU	3.0
1	C	214	LEU	3.0
1	C	368	PRO	3.0
1	B	442	CYS	3.0
1	D	119	ALA	2.9
1	B	336	VAL	2.9
1	D	472	GLN	2.9
1	D	134	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	137	ASP	2.9
1	D	468	PRO	2.9
1	D	46	HIS	2.9
1	B	470	ASP	2.8
1	C	307	THR	2.8
1	A	218	VAL	2.8
1	B	224	PHE	2.8
1	C	468	PRO	2.8
1	B	221	LEU	2.8
1	D	217	LEU	2.8
1	B	271	MET	2.8
1	C	369	MET	2.8
1	A	300	PHE	2.7
1	D	484	PHE	2.7
1	C	304	VAL	2.7
1	A	301	GLY	2.7
1	A	224	PHE	2.7
1	C	158	ALA	2.7
1	C	266	LEU	2.7
1	D	334	GLN	2.7
1	D	494	LYS	2.7
1	C	270	LYS	2.7
1	D	302	ALA	2.7
1	B	300	PHE	2.7
1	A	138	GLY	2.7
1	C	444	GLY	2.7
1	B	32	LEU	2.7
1	A	304	VAL	2.6
1	C	309	SER	2.6
1	C	361	LEU	2.6
1	C	275	ASN	2.6
1	C	311	VAL	2.6
1	C	360	VAL	2.6
1	C	424	GLN	2.6
1	D	270	LYS	2.6
1	B	304	VAL	2.6
1	C	351	LEU	2.5
1	D	271	MET	2.5
1	B	285	GLU	2.5
1	A	497	GLN	2.5
1	B	266	LEU	2.5
1	A	442	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	338	PHE	2.5
1	D	393	ILE	2.5
1	C	308	THR	2.5
1	C	287	LEU	2.5
1	D	161	ASN	2.5
1	D	465	LEU	2.5
1	A	297	GLY	2.5
1	C	247	LEU	2.5
1	D	303	GLY	2.5
1	A	423	THR	2.5
1	D	370	LEU	2.4
1	D	396	LEU	2.4
1	D	304	VAL	2.4
1	D	365	PRO	2.4
1	C	483	VAL	2.4
1	C	276	GLY	2.4
1	D	226	ASN	2.4
1	B	307	THR	2.4
1	D	448	ALA	2.4
1	D	361	LEU	2.4
1	D	165	ILE	2.4
1	C	164	SER	2.4
1	B	259	ILE	2.4
1	C	140	GLN	2.4
1	D	311	VAL	2.4
1	D	483	VAL	2.4
1	C	371	ILE	2.4
1	B	303	GLY	2.3
1	C	372	PRO	2.3
1	C	383	GLU	2.3
1	C	502	ALA	2.3
1	C	113	ALA	2.3
1	C	167	ILE	2.3
1	C	448	ALA	2.3
1	B	225	PRO	2.3
1	B	338	PHE	2.3
1	C	472	GLN	2.3
1	C	403	GLU	2.3
1	C	357	ILE	2.3
1	B	289	ASP	2.3
1	C	396	LEU	2.3
1	D	157	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	44	PRO	2.3
1	A	197	VAL	2.3
1	C	484	PHE	2.3
1	B	245	LYS	2.2
1	D	470	ASP	2.2
1	B	292	ILE	2.2
1	D	371	ILE	2.2
1	C	228	THR	2.2
1	C	271	MET	2.2
1	D	482	VAL	2.2
1	B	223	ILE	2.2
1	D	407	HIS	2.2
1	A	503	GLN	2.2
1	B	257	ASP	2.2
1	C	436	GLY	2.2
1	D	59	LYS	2.2
1	B	126	ARG	2.2
1	B	339	SER	2.2
1	A	306	THR	2.2
1	B	443	ILE	2.2
1	D	296	ILE	2.2
1	A	257	ASP	2.2
1	D	382	GLY	2.1
1	C	464	ASP	2.1
1	C	303	GLY	2.1
1	C	305	GLU	2.1
1	A	454	LEU	2.1
1	C	315	LEU	2.1
1	A	227	LYS	2.1
1	A	145	ILE	2.1
1	C	420	PRO	2.1
1	B	256	SER	2.1
1	A	222	LYS	2.1
1	C	138	GLY	2.1
1	C	269	ALA	2.1
1	B	254	PHE	2.1
1	A	441	SER	2.1
1	A	150	ILE	2.1
1	C	145	ILE	2.1
1	C	433	LEU	2.1
1	C	122	GLN	2.1
1	D	372	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	394	ILE	2.1
1	C	268	GLN	2.1
1	D	490	LYS	2.1
1	C	339	SER	2.0
1	D	256	SER	2.0
1	D	330	GLU	2.0
1	D	467	VAL	2.0
1	B	167	ILE	2.0
1	C	162	GLY	2.0
1	D	229	LEU	2.0
1	D	237	LYS	2.0
1	C	370	LEU	2.0
1	C	393	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

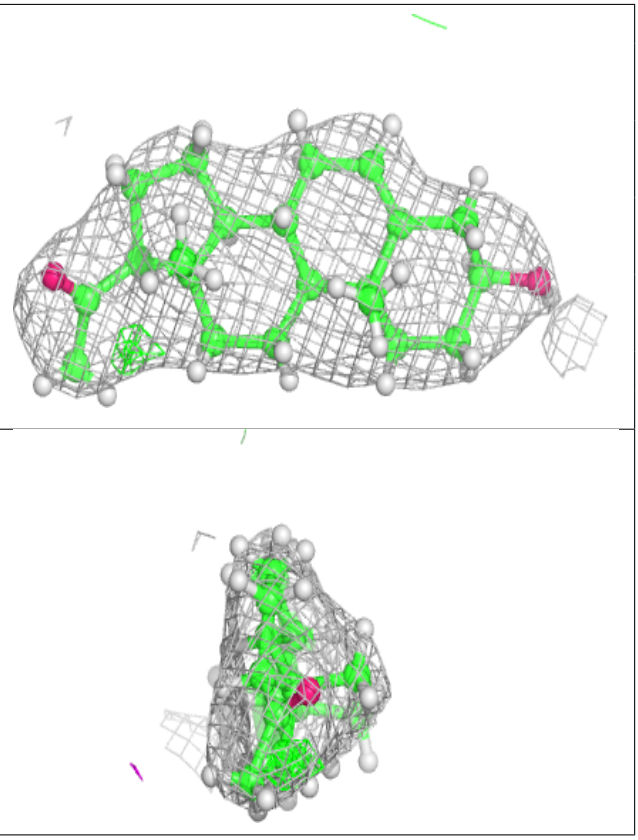
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PLO	A	601	23/23	0.94	0.28	44,60,72,72	0
3	PLO	B	601	23/23	0.94	0.22	43,56,72,73	0
3	PLO	D	601	23/23	0.94	0.27	47,60,75,78	0
3	PLO	C	601	23/23	0.96	0.31	49,62,73,75	0
2	HEM	D	600	43/43	0.96	0.33	35,47,59,70	0
2	HEM	C	600	43/43	0.97	0.35	33,48,67,77	0
2	HEM	A	600	43/43	0.97	0.28	33,48,70,74	0
2	HEM	B	600	43/43	0.97	0.30	39,51,68,69	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.

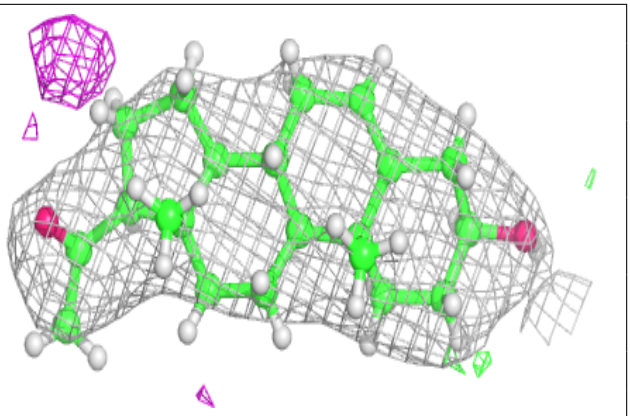
Electron density around PLO A 601:

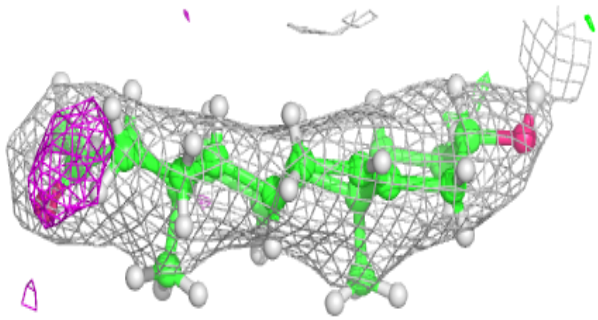
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

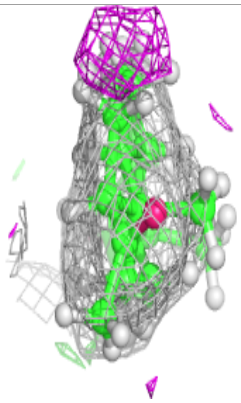


Electron density around PLO B 601:

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

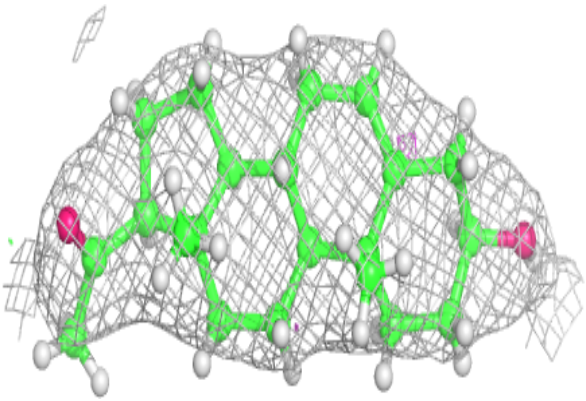


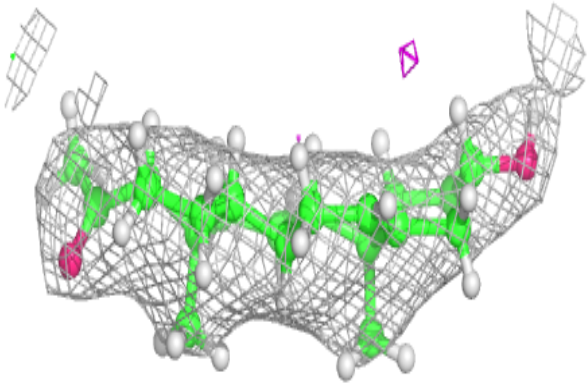


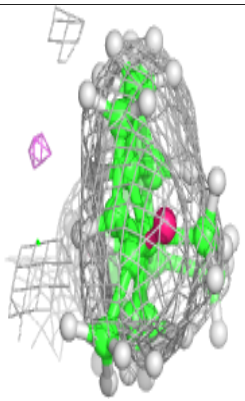


Electron density around PLO D 601:

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

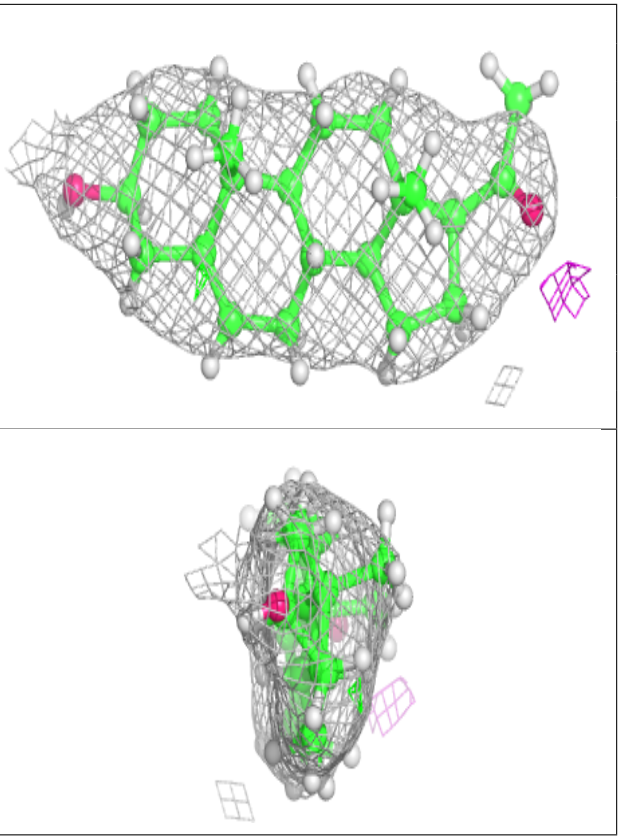


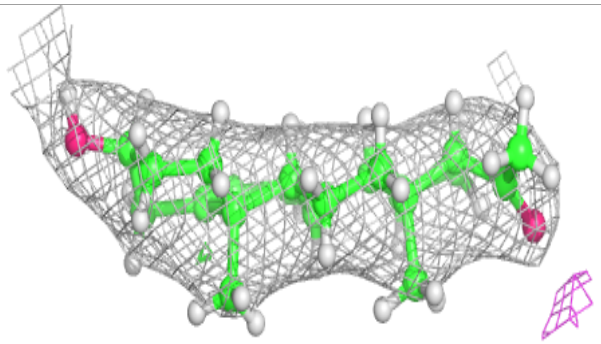




Electron density around PLO C 601:

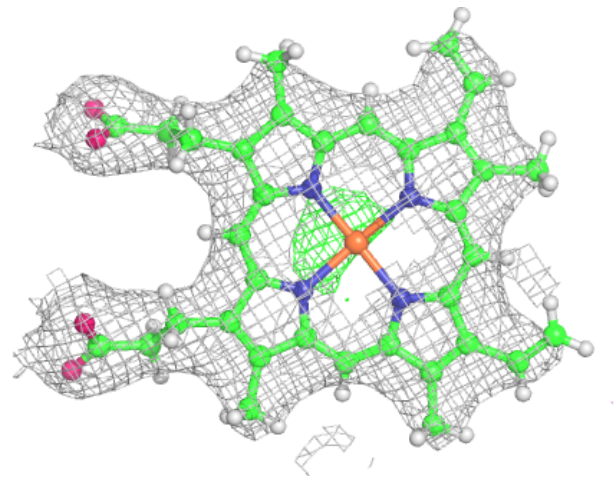
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

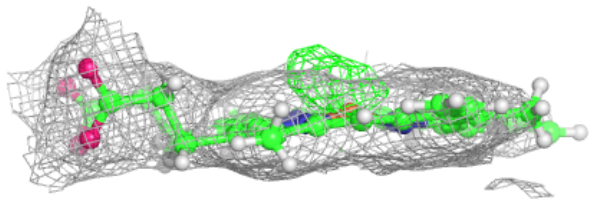


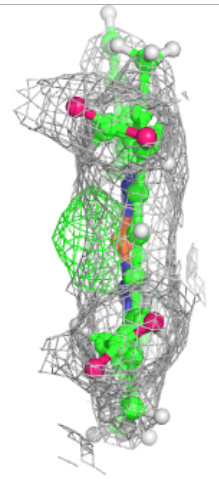


Electron density around HEM D 600:

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

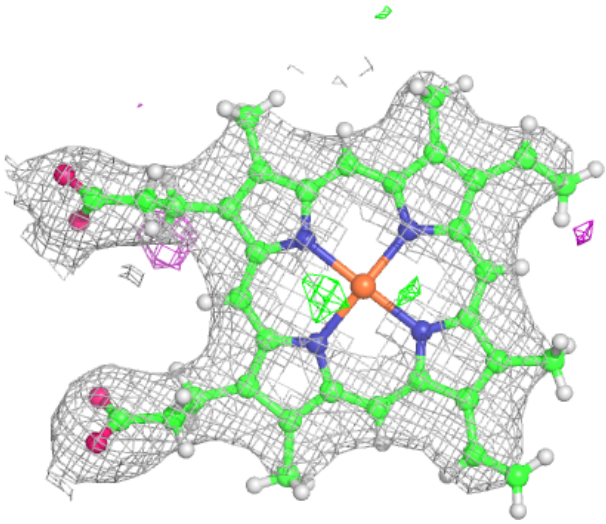


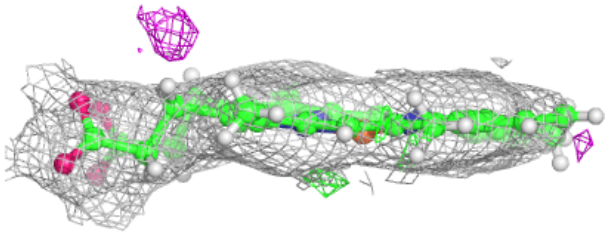


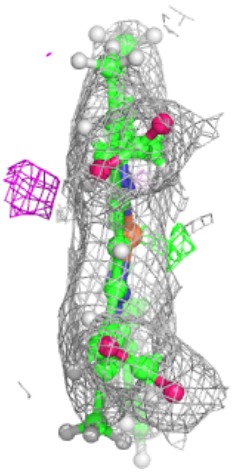


Electron density around HEM C 600:

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

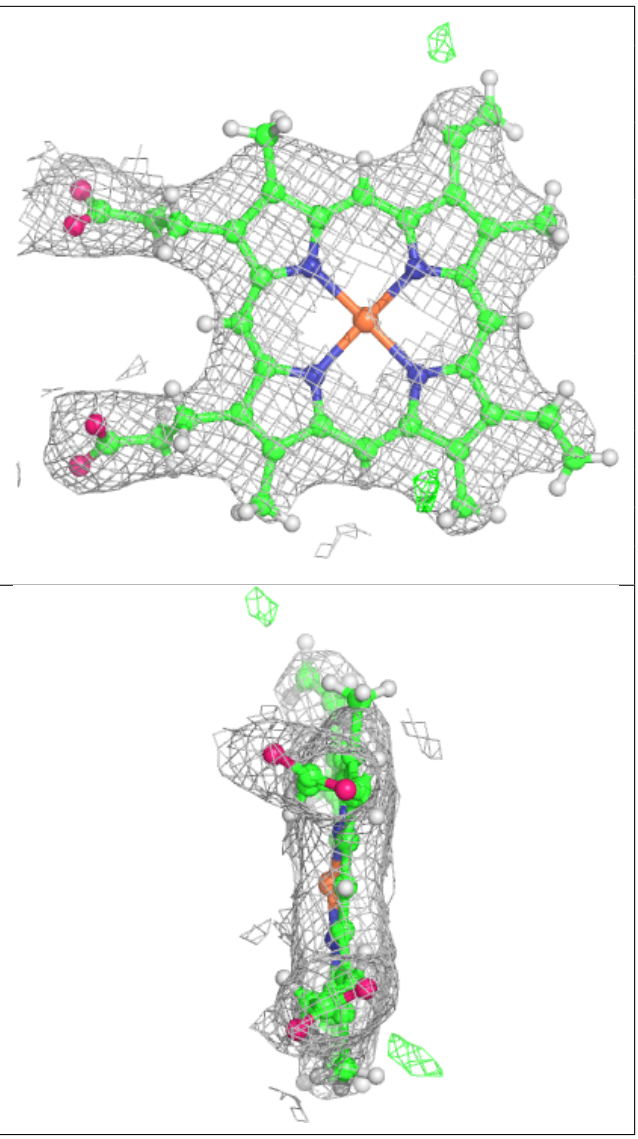


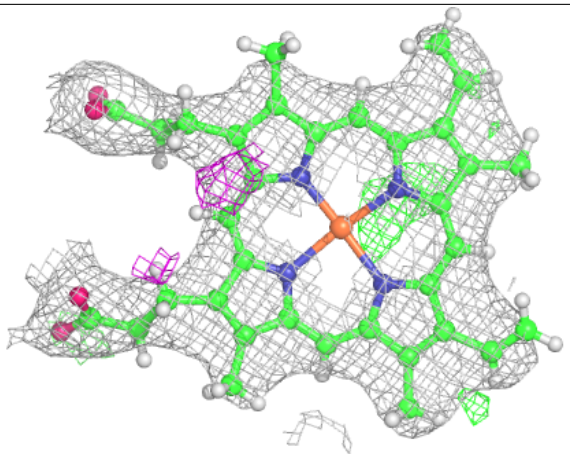
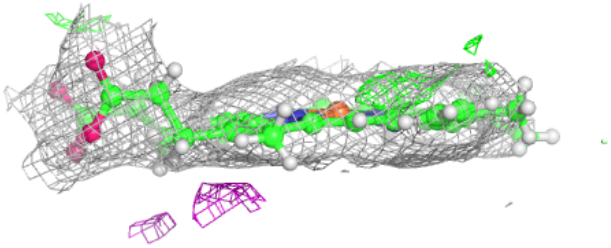
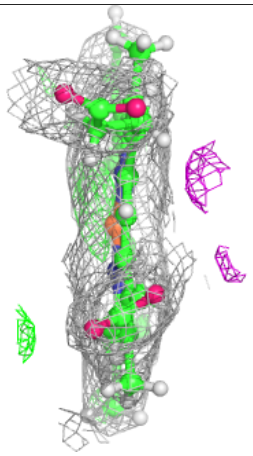




Electron density around HEM A 600:

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



Electron density around HEM B 600: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.