wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:36 AM EST

PDB ID	:	4PD4
Title	:	Structural analysis of atovaquone-inhibited cytochrome bc1 complex reveals the molecular basis of antimalarial drug action
Authors	:	Birth, D.; Kao, W.-C.; Hunte, C.
Deposited on	:	2014-04-17
Resolution	:	3.04 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

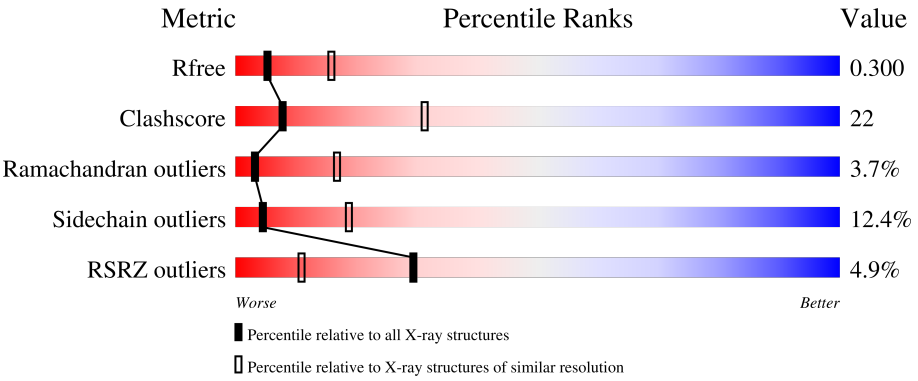
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	431	9% 49% 45% 6%
2	B	352	9% 55% 41%
3	C	385	48% 44% 8%
4	D	248	2% 48% 46% 5%
5	E	185	4% 49% 42% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	74	8% 59% 35% 5%
7	G	126	2% 52% 42% 6%
8	H	93	4% 62% 30% 5%
9	I	57	4% 58% 40%
10	J	127	2% 45% 42% 13%
11	K	107	7% 41% 48% 11%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 17646 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	115	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	72	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	10	0	0
			3090	2082	484	503	21			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	248	Total	C	N	O	S	5	0	0
			1961	1249	340	363	9			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	27	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	0	0	0
			465	310	77	78			

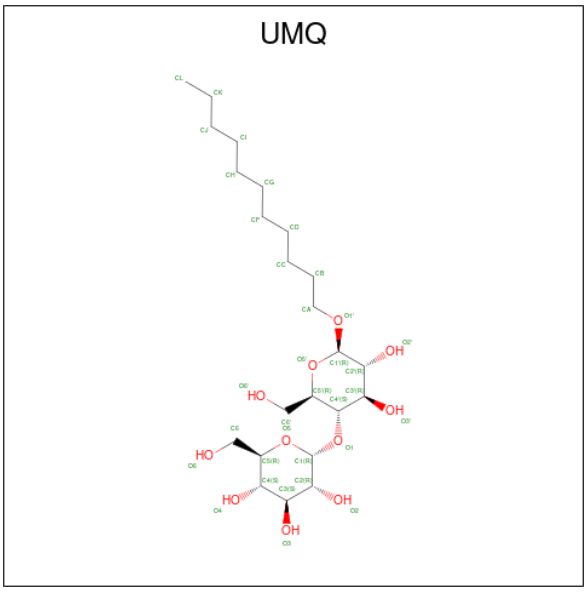
- Molecule 10 is a protein called Igh protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Ig kappa chain V-V region HP 124E1.

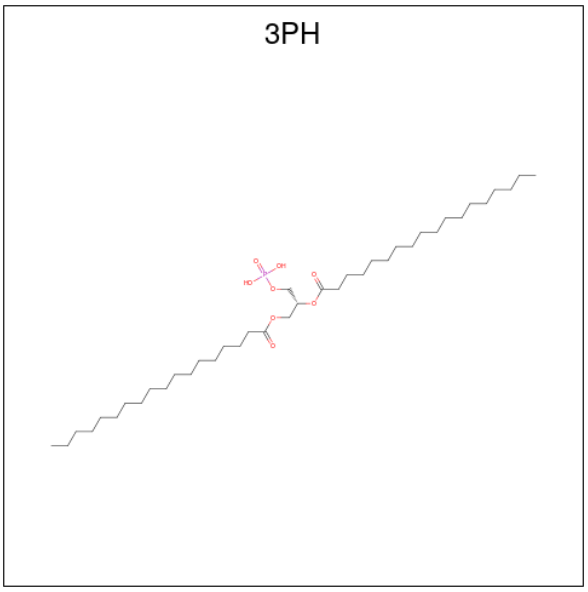
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 34 23 11	0	0

- Molecule 13 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



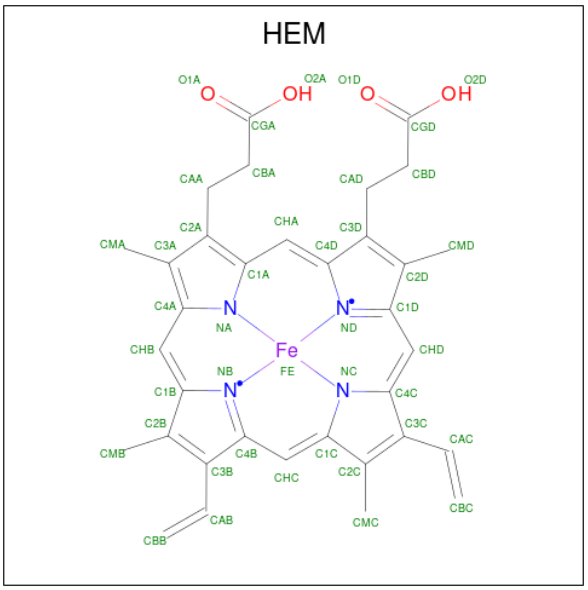
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O P 31 22 8 1	0	0
13	C	1	Total C O P 35 26 8 1	0	0

Continued on next page...

Continued from previous page...

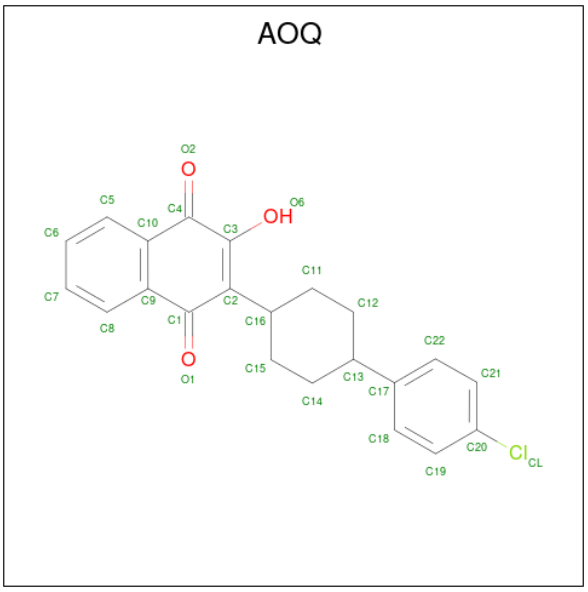
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	E	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



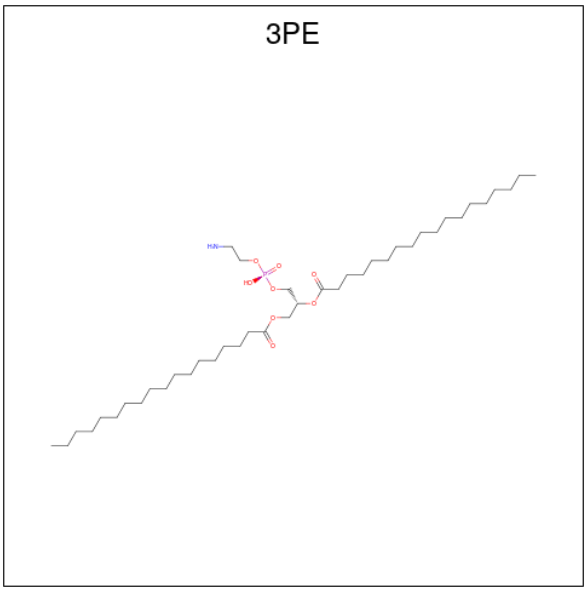
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (three-letter code: AOQ) (formula: $C_{22}H_{19}ClO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Cl	O	0	0
			26	22	1	3		

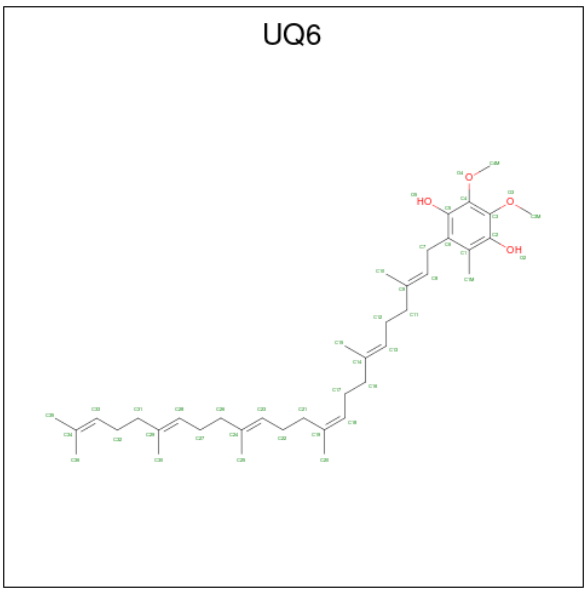
- Molecule 16 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			27	17	1	8	1		

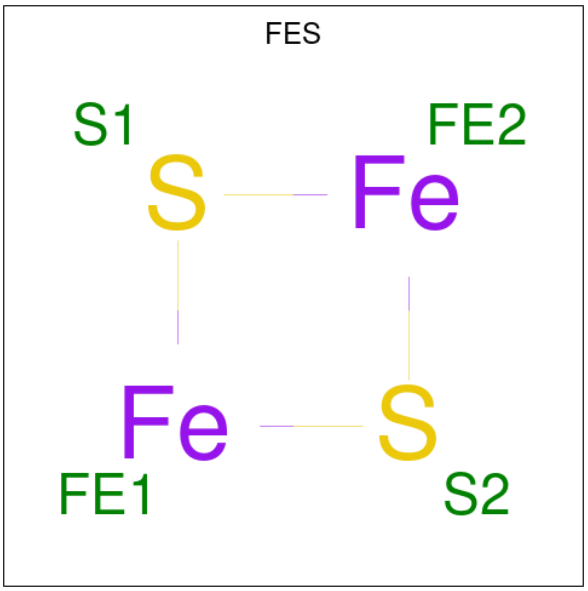
- Molecule 17 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6)

(formula: $C_{39}H_{60}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 43 39 4	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



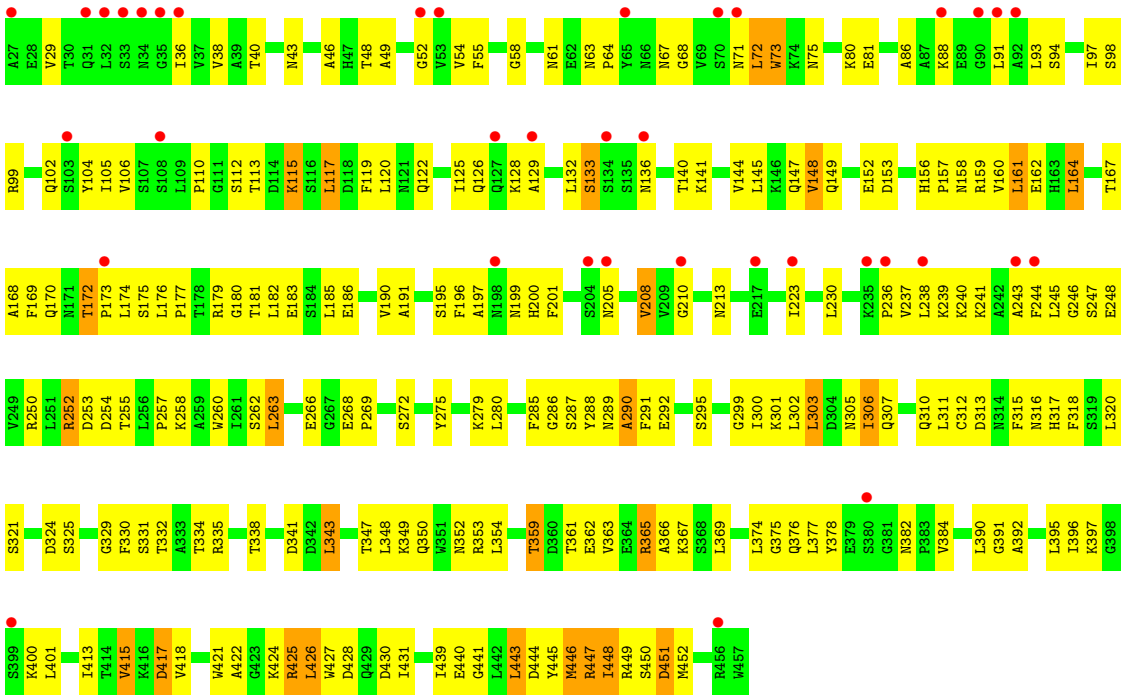
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	E	1	Total Fe S 4 2 2	0	0

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.

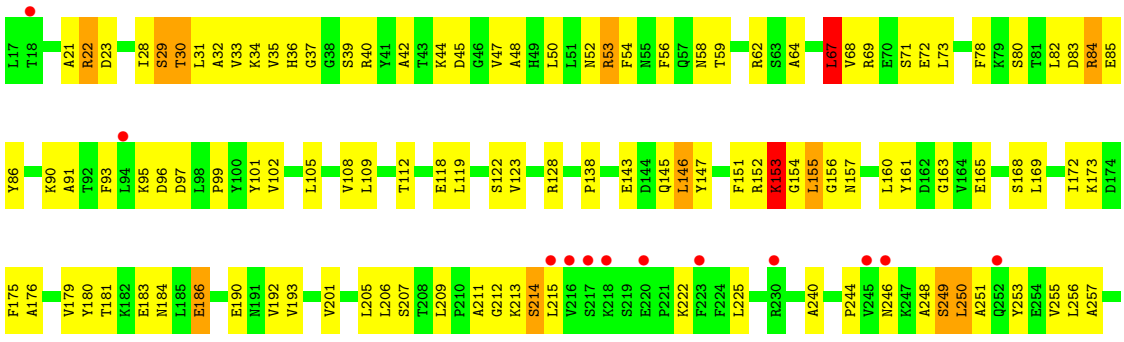
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

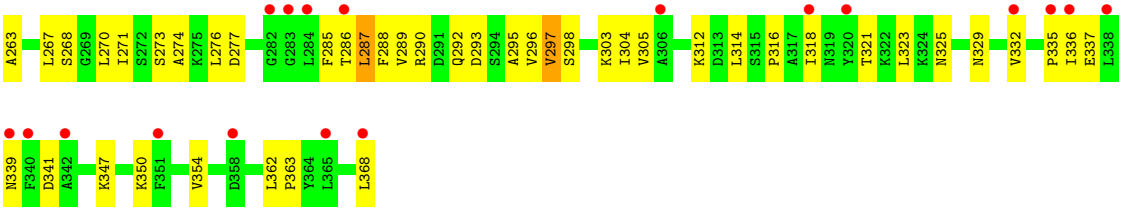
Chain A:



• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

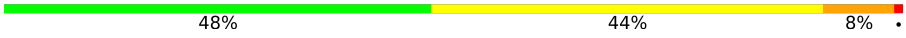
Chain B:

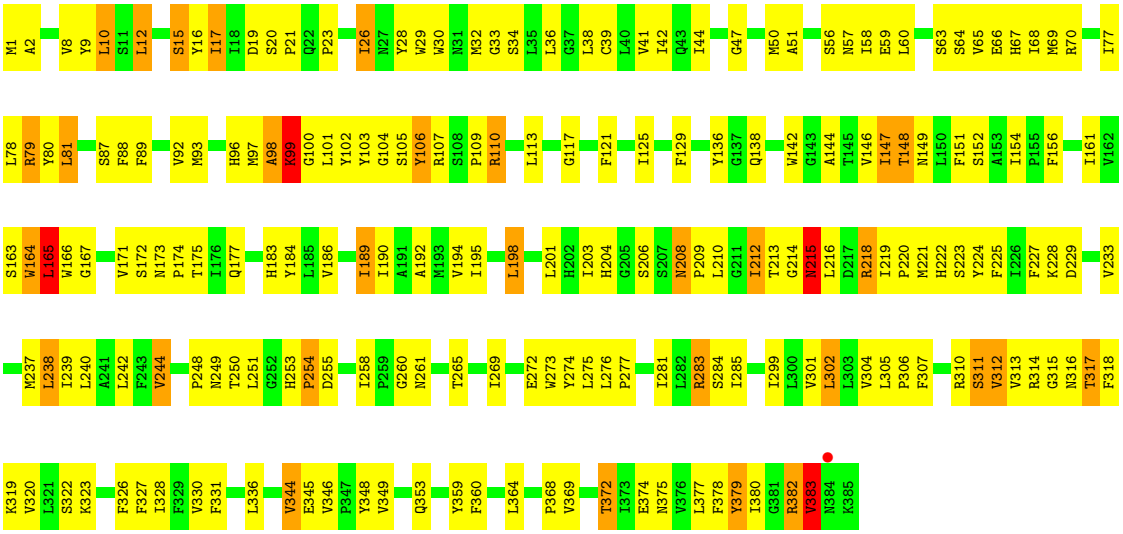




• Molecule 3: Cytochrome b

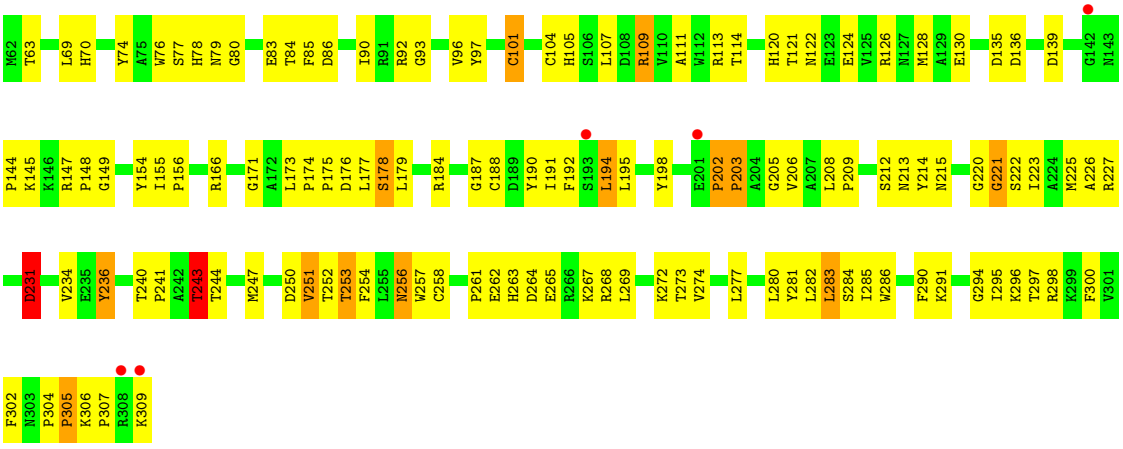
Chain C:





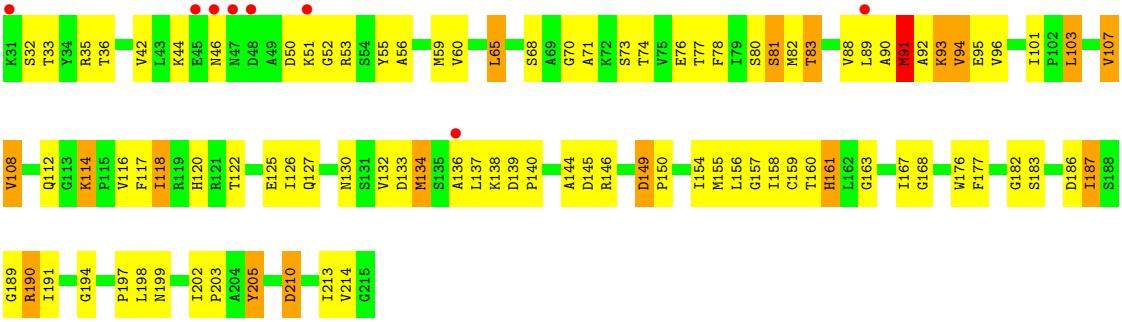
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:

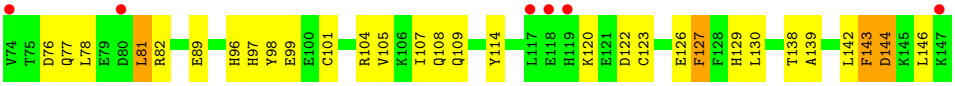


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

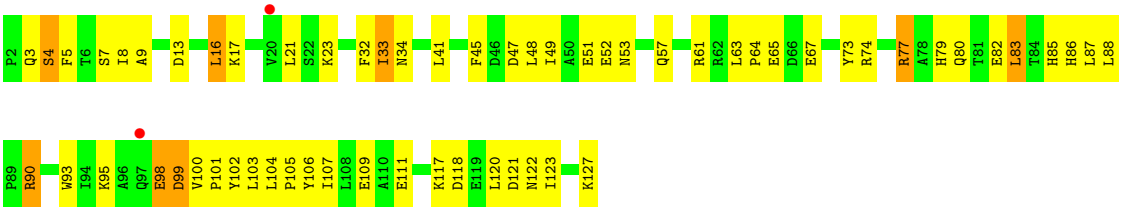
Chain E:



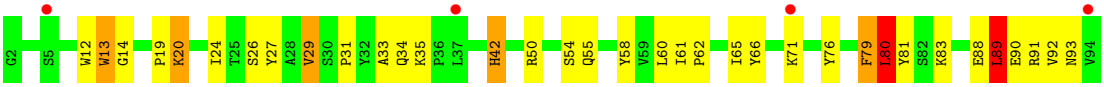
• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 7: Cytochrome b-c1 complex subunit 7

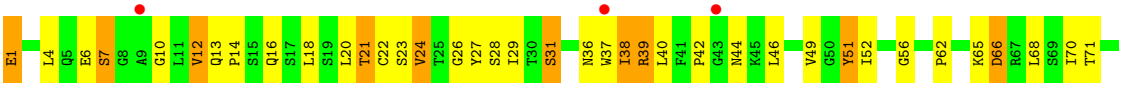


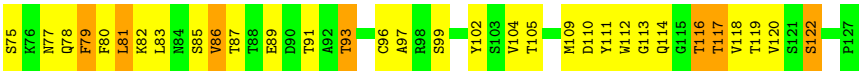
• Molecule 8: Cytochrome b-c1 complex subunit 8



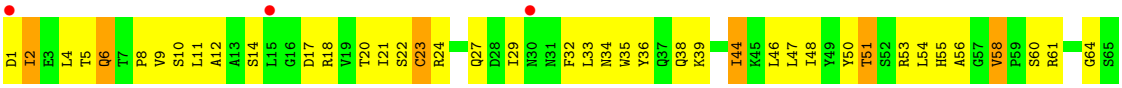
• Molecule 9: Cytochrome b-c1 complex subunit 9

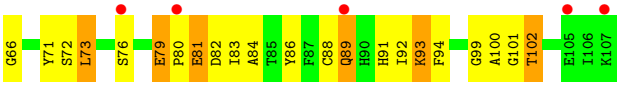
• Molecule 10: Igh protein





• Molecule 11: Ig kappa chain V-V region HP 124E1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	212.26Å 150.88Å 143.09Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	24.99 – 3.04 24.99 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.99-3.04) 98.6 (24.99-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.297 0.269 , 0.300	Depositor DCC
R_{free} test set	2008 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	97.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17646	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, FES, 3PE, HEM, UQ6, UMQ, AOQ

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	0.42	0/3405	0.62	0/4614
2	B	0.37	0/2781	0.58	1/3764 (0.0%)
3	C	0.70	0/3192	0.83	1/4354 (0.0%)
4	D	0.48	0/2022	0.69	0/2751
5	E	0.54	0/1444	0.74	0/1957
6	F	0.40	0/638	0.62	0/858
7	G	0.58	0/1040	0.80	0/1408
8	H	0.55	0/804	0.71	0/1088
9	I	0.43	0/479	0.59	0/646
10	J	0.48	0/1043	0.71	0/1422
11	K	0.38	0/863	0.59	0/1172
All	All	0.51	0/17711	0.69	2/24034 (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})
2	B	67	LEU	CA-CB-CG	5.30	127.50	115.30
3	C	110	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	3344	0	3321	152	0
2	B	2735	0	2774	108	0
3	C	3090	0	3129	167	0
4	D	1961	0	1890	101	0
5	E	1411	0	1386	66	0
6	F	624	0	581	23	0
7	G	1019	0	1034	52	0
8	H	773	0	736	34	0
9	I	465	0	459	18	0
10	J	1015	0	959	57	0
11	K	842	0	820	42	0
12	A	34	0	44	3	0
13	A	31	0	35	2	0
13	C	35	0	46	1	0
13	E	38	0	49	6	0
14	C	86	0	60	15	0
14	D	43	0	30	11	0
15	C	26	0	19	3	0
16	C	27	0	28	1	0
17	C	43	0	58	5	0
18	E	4	0	0	0	0
All	All	17646	0	17458	747	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 22.

The worst 5 of 747 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)
3:C:318:PHE:HD1	7:G:48:LEU:HD21	1.32	0.93
1:A:248:GLU:OE2	1:A:250:ARG:NH2	2.04	0.90
13:A:502:3PH:H321	13:A:502:3PH:H221	1.54	0.89
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.54	0.89
11:K:93:LYS:HD2	11:K:94:PHE:H	1.41	0.83

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	429/431 (100%)	349 (81%)	67 (16%)	13 (3%)	4 21
2	B	350/352 (99%)	284 (81%)	56 (16%)	10 (3%)	4 22
3	C	383/385 (100%)	318 (83%)	49 (13%)	16 (4%)	3 14
4	D	246/248 (99%)	199 (81%)	36 (15%)	11 (4%)	2 13
5	E	183/185 (99%)	142 (78%)	33 (18%)	8 (4%)	2 13
6	F	72/74 (97%)	60 (83%)	10 (14%)	2 (3%)	5 23
7	G	124/126 (98%)	102 (82%)	16 (13%)	6 (5%)	2 12
8	H	91/93 (98%)	61 (67%)	23 (25%)	7 (8%)	1 4
9	I	55/57 (96%)	41 (74%)	13 (24%)	1 (2%)	8 34
10	J	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	19 54
11	K	105/107 (98%)	76 (72%)	23 (22%)	6 (6%)	1 9
All	All	2163/2185 (99%)	1747 (81%)	335 (16%)	81 (4%)	3 17

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
2	B	153	LYS
3	C	99	LYS
3	C	164	TRP
3	C	165	LEU

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	370/370 (100%)	324 (88%)	46 (12%)	4	19
2	B	301/301 (100%)	272 (90%)	29 (10%)	8	29
3	C	338/338 (100%)	295 (87%)	43 (13%)	4	18
4	D	206/206 (100%)	181 (88%)	25 (12%)	5	20
5	E	151/151 (100%)	127 (84%)	24 (16%)	2	11
6	F	67/67 (100%)	59 (88%)	8 (12%)	5	20
7	G	110/110 (100%)	99 (90%)	11 (10%)	7	27
8	H	77/77 (100%)	69 (90%)	8 (10%)	7	25
9	I	47/47 (100%)	41 (87%)	6 (13%)	4	18
10	J	112/112 (100%)	94 (84%)	18 (16%)	2	11
11	K	93/93 (100%)	78 (84%)	15 (16%)	2	11
All	All	1872/1872 (100%)	1639 (88%)	233 (12%)	4	19

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	380	ILE
11	K	23	CYS
5	E	50	ASP
11	K	6	GLN
9	I	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	89	GLN
11	K	38	GLN
5	E	127	GLN
4	D	79	ASN
7	G	79	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
13	3PH	A	502	-	30,30,47	1.23	2 (6%)	34,35,52	1.14	3 (8%)
14	HEM	C	4002	3	41,50,50	1.80	6 (14%)	45,82,82	1.94	8 (17%)
14	HEM	D	401	4	41,50,50	1.99	6 (14%)	45,82,82	2.06	14 (31%)
15	AOQ	C	4003	-	29,29,29	1.76	7 (24%)	40,42,42	1.61	9 (22%)
16	3PE	C	4004	-	26,26,50	1.37	2 (7%)	29,31,55	1.42	5 (17%)
17	UQ6	C	4005	-	43,43,43	1.19	3 (6%)	51,55,55	2.25	20 (39%)
18	FES	E	301	5	0,4,4	-	-	-		
13	3PH	E	302	-	37,37,47	1.10	2 (5%)	41,42,52	1.27	2 (4%)
14	HEM	C	4001	3	41,50,50	2.03	8 (19%)	45,82,82	1.97	13 (28%)
12	UMQ	A	501	-	35,35,35	0.47	0	46,46,46	1.19	4 (8%)
13	3PH	C	4006	-	34,34,47	1.17	2 (5%)	38,39,52	1.66	8 (21%)

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
13	3PH	A	502	-	-	14/32/32/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEM	C	4002	3	-	4/12/54/54	-
14	HEM	D	401	4	-	4/12/54/54	-
15	AOQ	C	4003	-	-	4/8/38/38	0/4/4/4
16	3PE	C	4004	-	-	16/30/30/54	-
17	UQ6	C	4005	-	-	14/39/39/39	0/1/1/1
18	FES	E	301	5	-	-	0/1/1/1
13	3PH	E	302	-	-	19/39/39/49	-
14	HEM	C	4001	3	-	2/12/54/54	-
12	UMQ	A	501	-	-	3/20/60/60	0/2/2/2
13	3PH	C	4006	-	-	13/36/36/49	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	C3D-C2D	8.34	1.54	1.36
14	C	4001	HEM	C3D-C2D	8.29	1.54	1.36
14	C	4002	HEM	C3D-C2D	7.35	1.52	1.36
15	C	4003	AOQ	C9-C1	-4.64	1.39	1.48
16	C	4004	3PE	O21-C21	4.50	1.47	1.34

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	4002	HEM	C4D-ND-C1D	7.27	112.58	105.07
14	D	401	HEM	C4D-ND-C1D	6.99	112.30	105.07
14	C	4001	HEM	CBA-CAA-C2A	-5.66	102.97	112.62
14	C	4001	HEM	C4D-ND-C1D	5.63	110.89	105.07
17	C	4005	UQ6	C10-C9-C11	4.74	123.25	115.27

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	502	3PH	C22-C21-O21-C2
13	E	302	3PH	C1-O11-P-O13
13	E	302	3PH	C1-O11-P-O14
13	E	302	3PH	C1-O11-P-O12
15	C	4003	AOQ	C11-C16-C2-C1

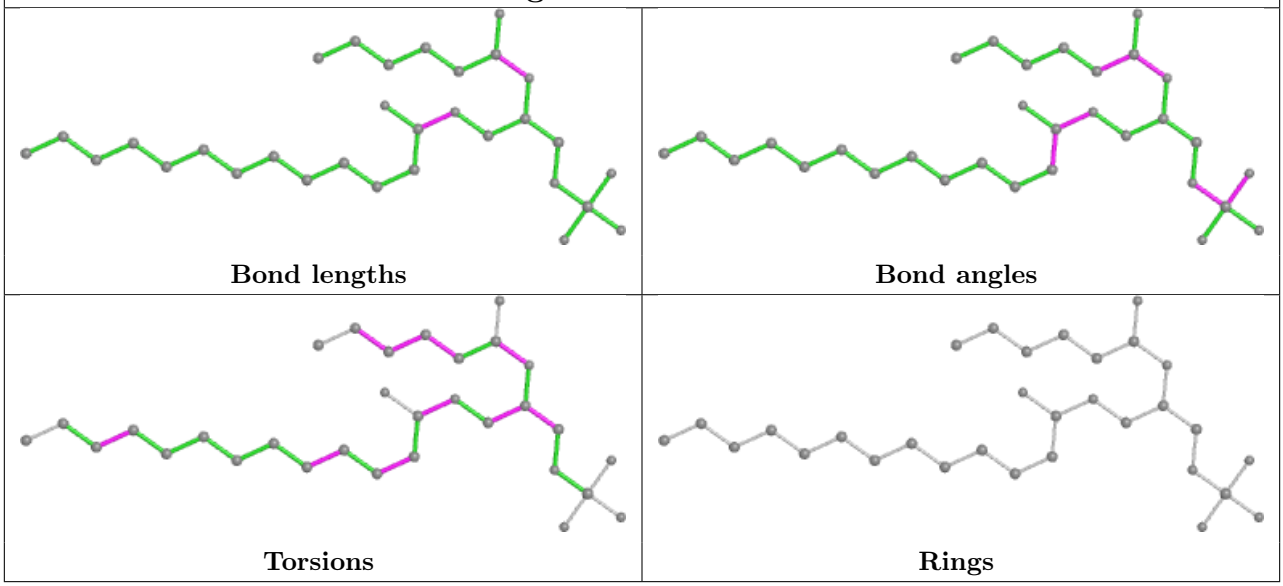
There are no ring outliers.

10 monomers are involved in 47 short contacts:

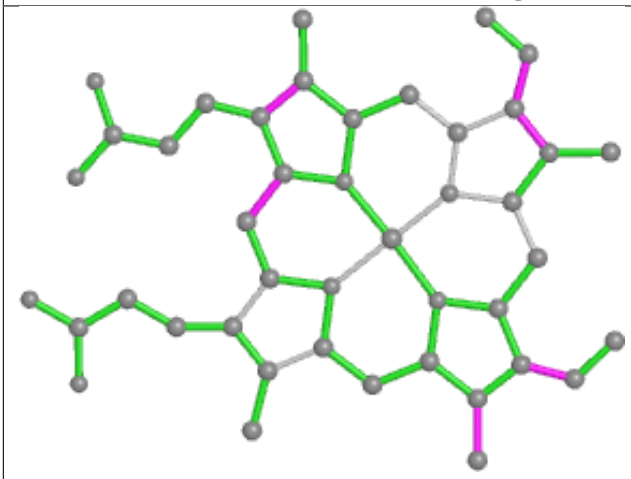
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	502	3PH	2	0
14	C	4002	HEM	8	0
14	D	401	HEM	11	0
15	C	4003	AOQ	3	0
16	C	4004	3PE	1	0
17	C	4005	UQ6	5	0
13	E	302	3PH	6	0
14	C	4001	HEM	7	0
12	A	501	UMQ	3	0
13	C	4006	3PH	1	0

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.

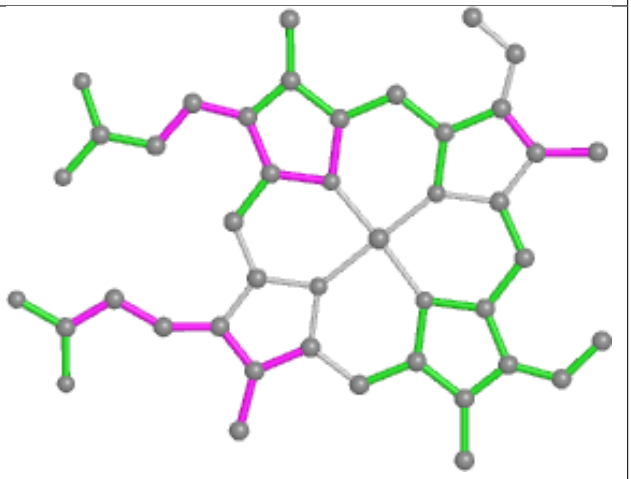
Ligand 3PH A 502



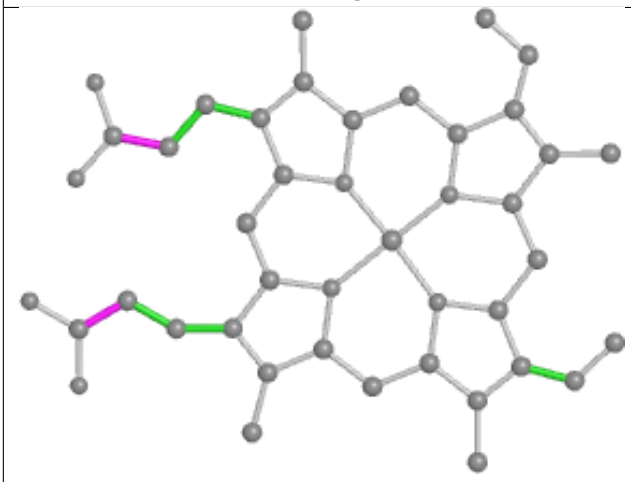
Ligand HEM C 4002



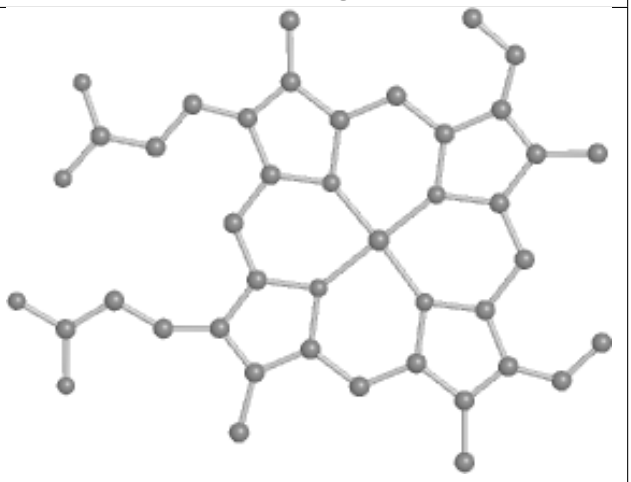
Bond lengths



Bond angles

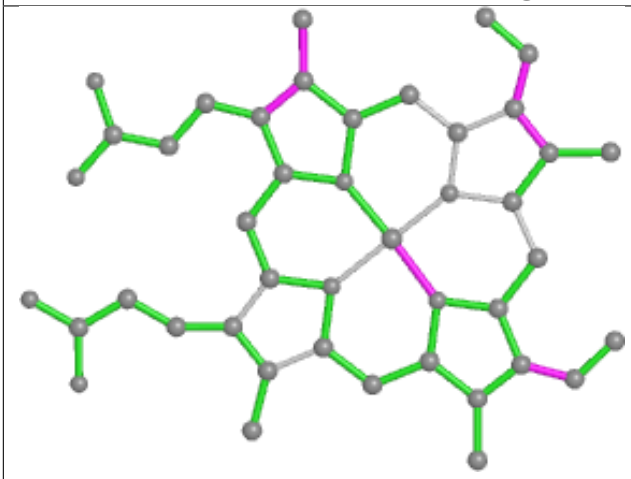


Torsions

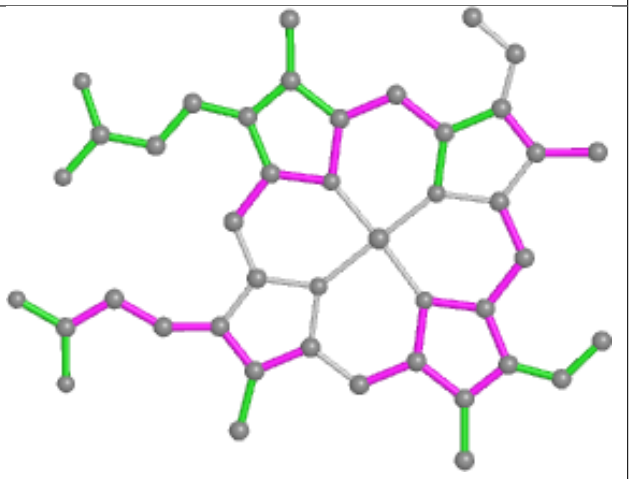


Rings

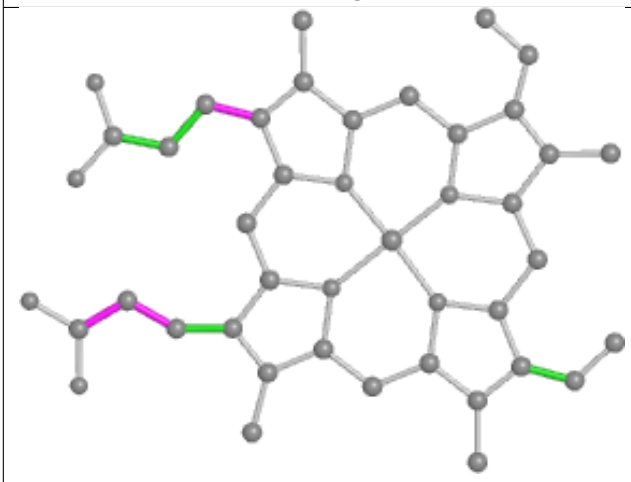
Ligand HEM D 401



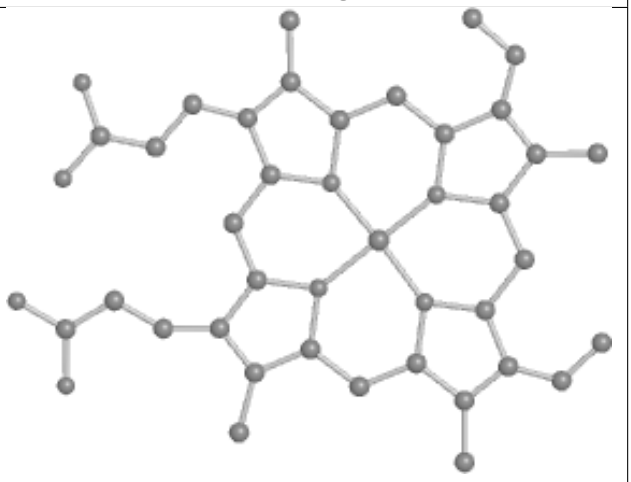
Bond lengths



Bond angles

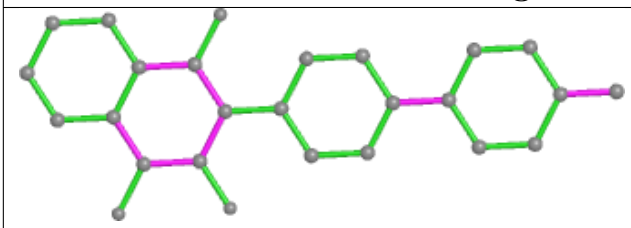


Torsions

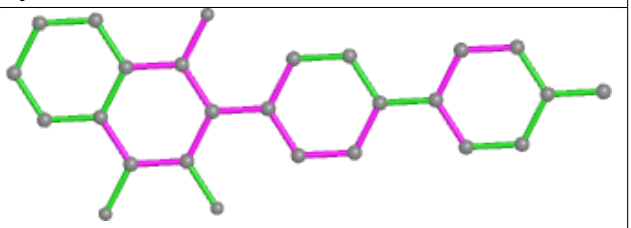


Rings

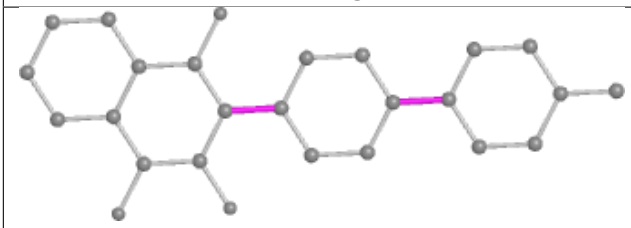
Ligand AOQ C 4003



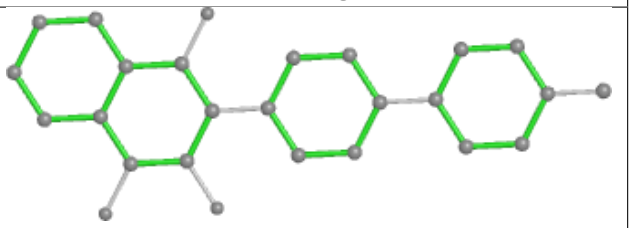
Bond lengths



Bond angles

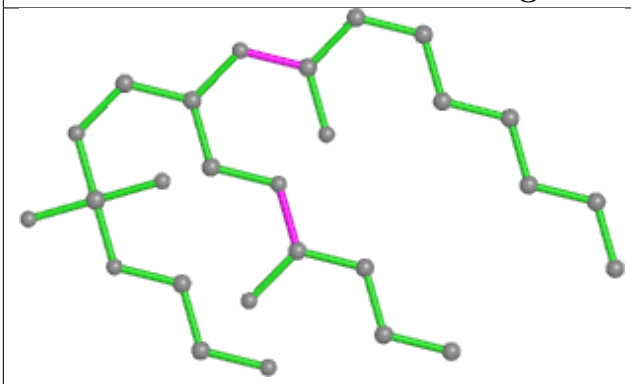


Torsions

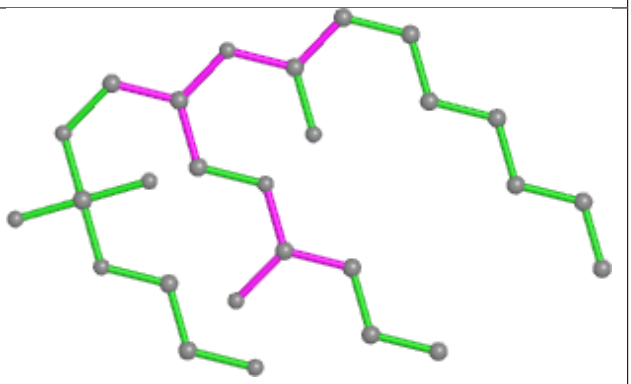


Rings

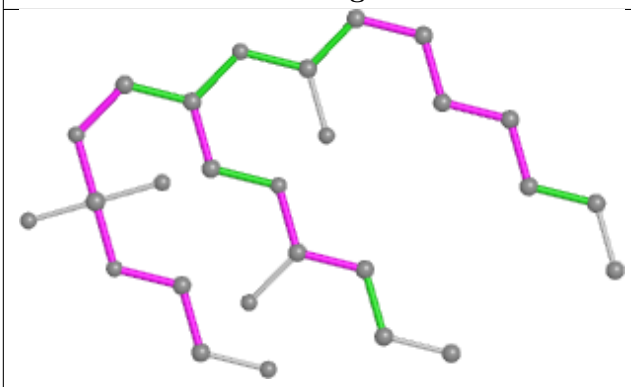
Ligand 3PE C 4004



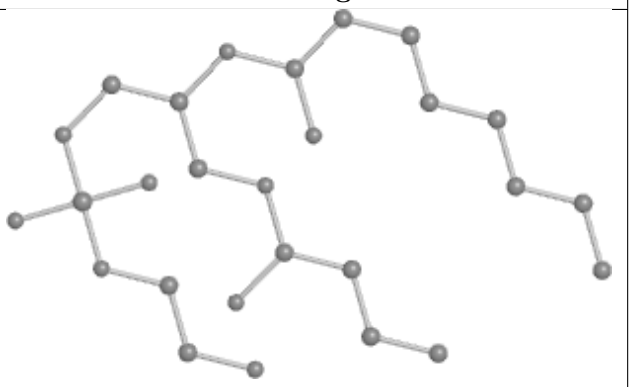
Bond lengths



Bond angles

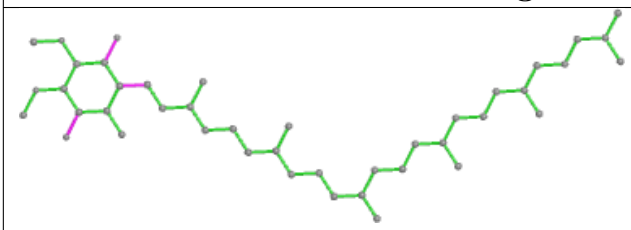


Torsions

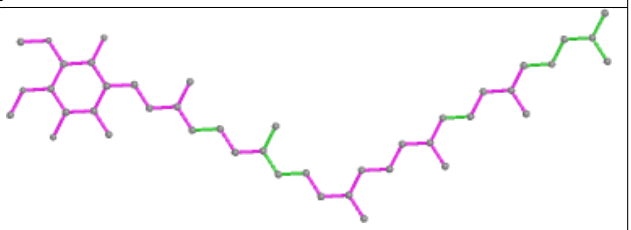


Rings

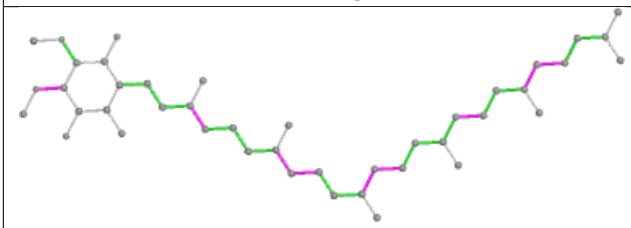
Ligand UQ6 C 4005



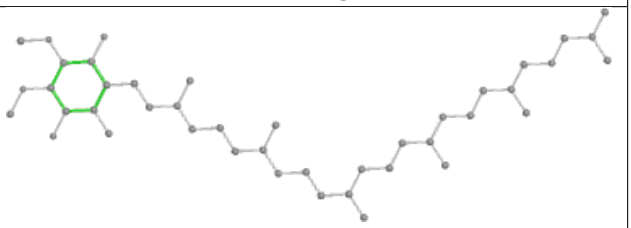
Bond lengths



Bond angles

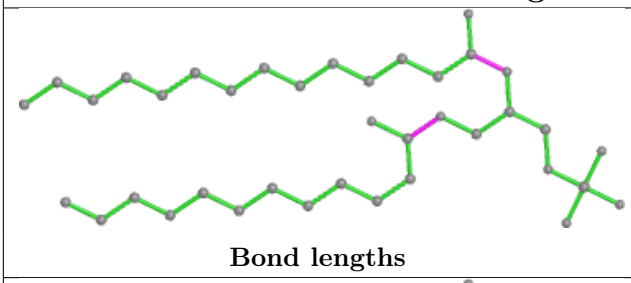


Torsions

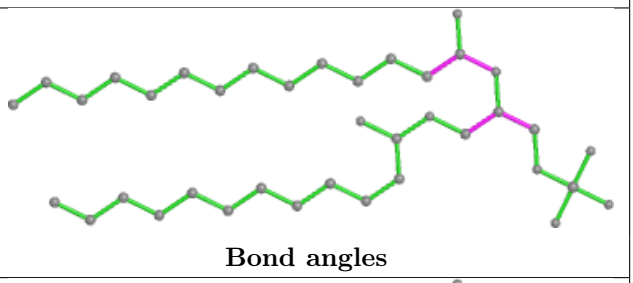


Rings

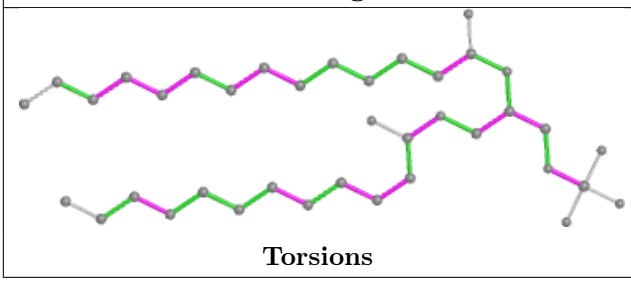
Ligand 3PH E 302



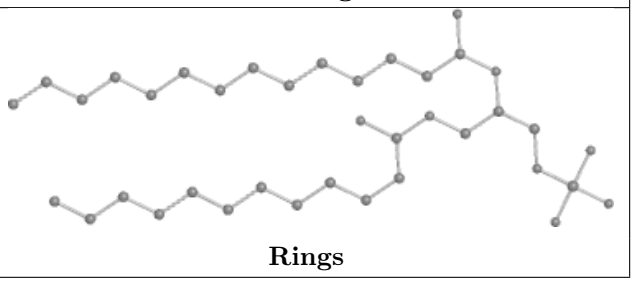
Bond lengths



Bond angles

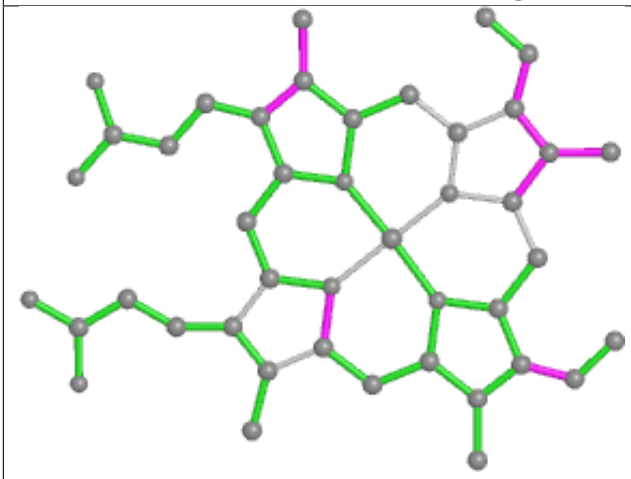


Torsions

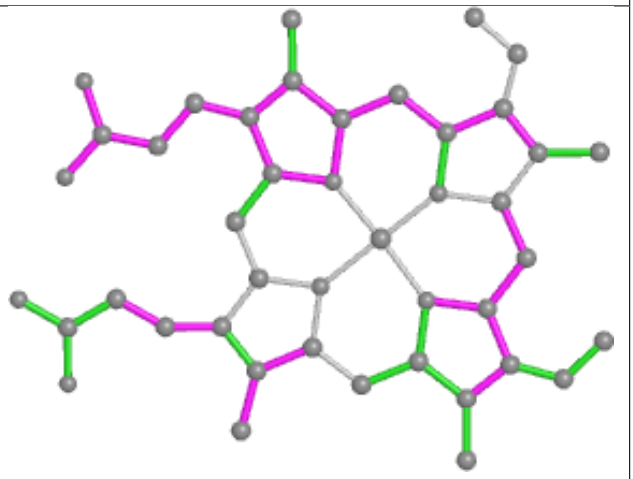


Rings

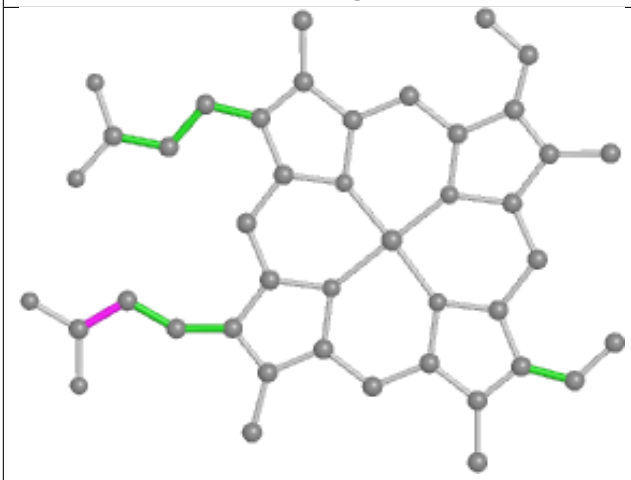
Ligand HEM C 4001



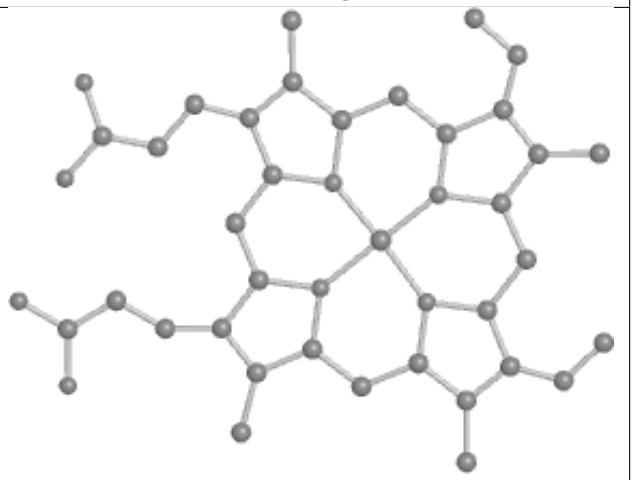
Bond lengths



Bond angles

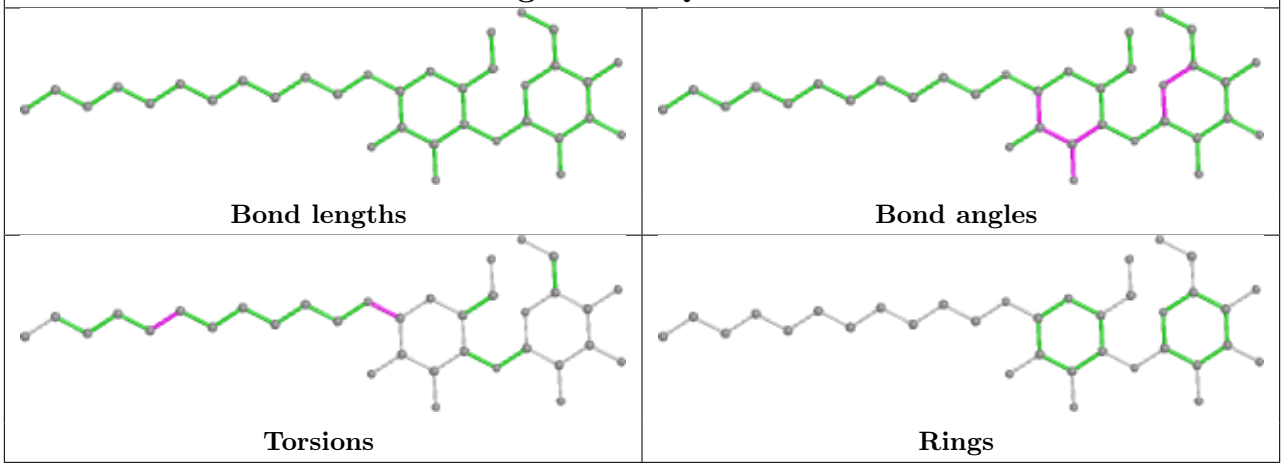


Torsions

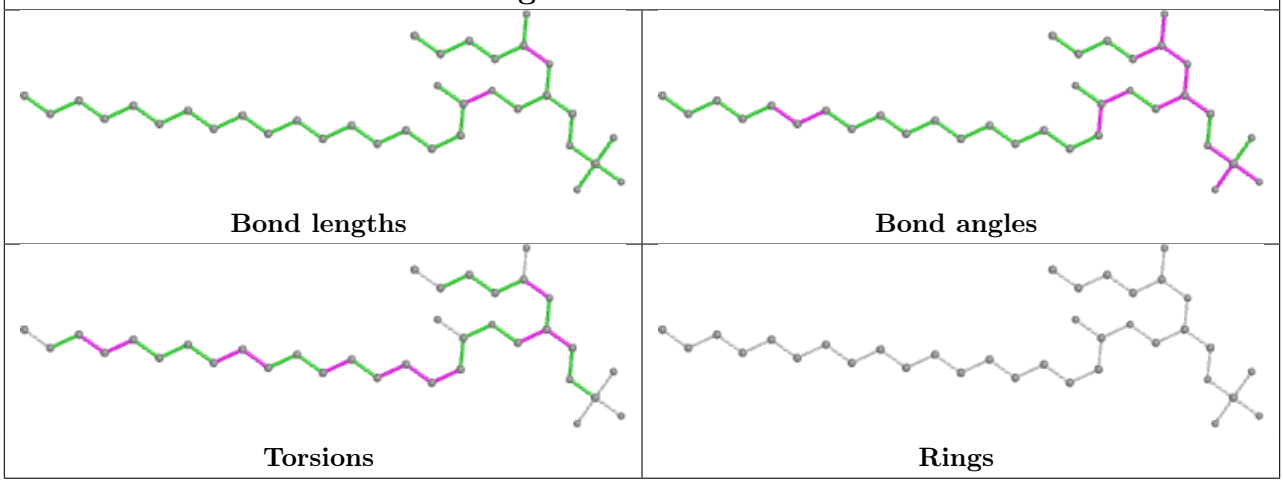


Rings

Ligand UMQ A 501



Ligand 3PH C 4006



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^{th} 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	417/431 (96%)	0.42	37 (8%) 9 3	17, 69, 116, 122	0
2	B	344/352 (97%)	0.55	30 (8%) 10 3	29, 71, 104, 127	0
3	C	384/385 (99%)	-0.25	1 (0%) 94 83	0, 7, 18, 69	0
4	D	248/248 (100%)	0.14	5 (2%) 65 36	16, 40, 63, 83	1 (0%)
5	E	182/185 (98%)	0.03	8 (4%) 34 13	4, 26, 70, 112	0
6	F	74/74 (100%)	0.35	6 (8%) 12 3	38, 61, 92, 94	0
7	G	126/126 (100%)	-0.19	2 (1%) 72 44	6, 27, 48, 67	0
8	H	82/93 (88%)	0.21	4 (4%) 29 11	7, 29, 67, 88	1 (1%)
9	I	57/57 (100%)	0.02	2 (3%) 44 19	24, 45, 78, 102	0
10	J	127/127 (100%)	0.14	3 (2%) 59 30	27, 44, 63, 68	0
11	K	107/107 (100%)	0.38	8 (7%) 14 4	36, 67, 105, 116	0
All	All	2148/2185 (98%)	0.18	106 (4%) 29 11	0, 42, 102, 127	2 (0%)

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	8.9
3	C	384	ASN	7.9
9	I	58	ALA	7.7
2	B	282	GLY	5.7
6	F	119	HIS	5.5

6.2 Non-standard residues in protein, DNA, RNA chains

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)

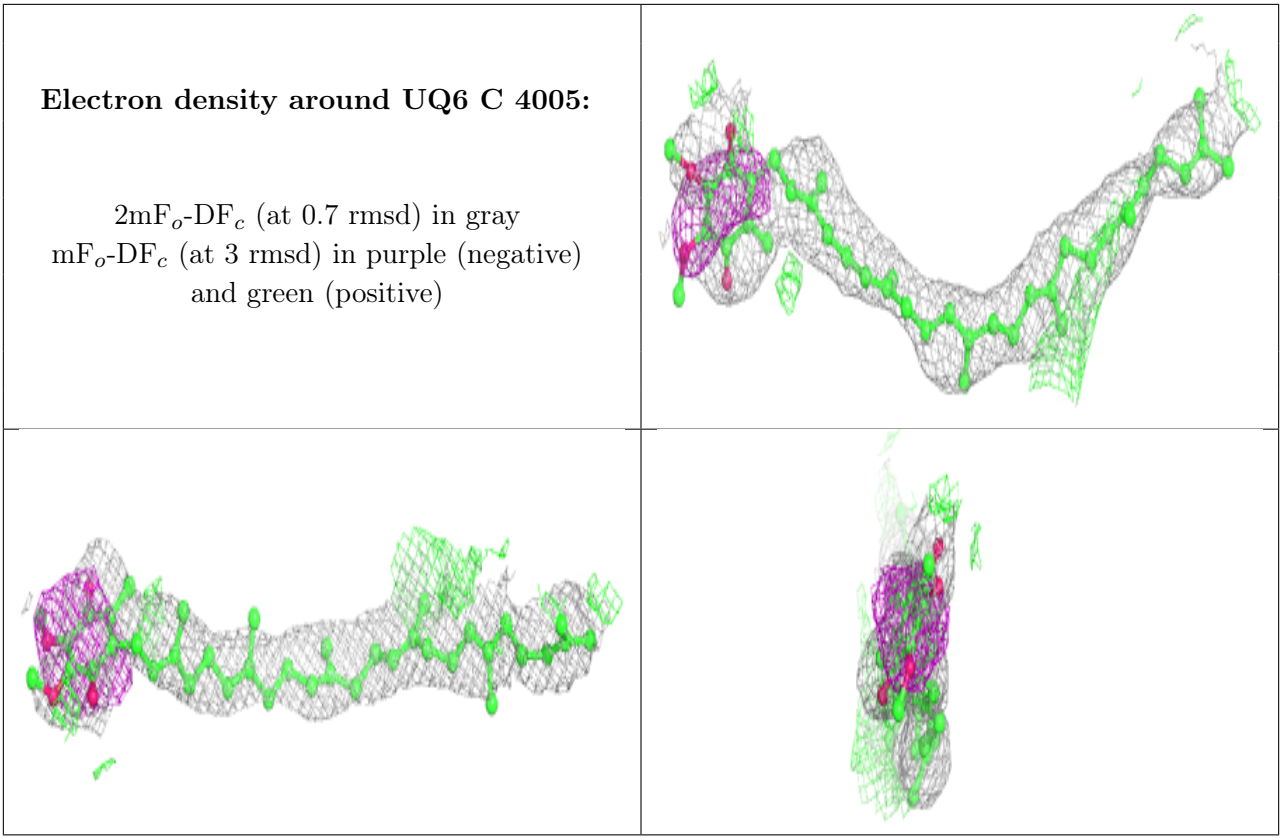
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
17	UQ6	C	4005	43/43	0.83	0.35	6,12,21,24	0
13	3PH	C	4006	35/48	0.88	0.25	3,17,29,39	0
12	UMQ	A	501	34/34	0.89	0.24	13,31,43,48	0
13	3PH	E	302	38/48	0.91	0.26	7,15,21,23	0
13	3PH	A	502	31/48	0.91	0.22	13,20,33,38	0
16	3PE	C	4004	27/51	0.93	0.27	4,8,12,14	0
14	HEM	D	401	43/43	0.94	0.25	22,31,37,43	0
15	AOQ	C	4003	26/26	0.96	0.17	7,12,16,22	0
14	HEM	C	4001	43/43	0.98	0.25	0,2,7,20	0
14	HEM	C	4002	43/43	0.98	0.27	2,5,10,11	0
18	FES	E	301	4/4	0.99	0.18	6,7,7,13	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.

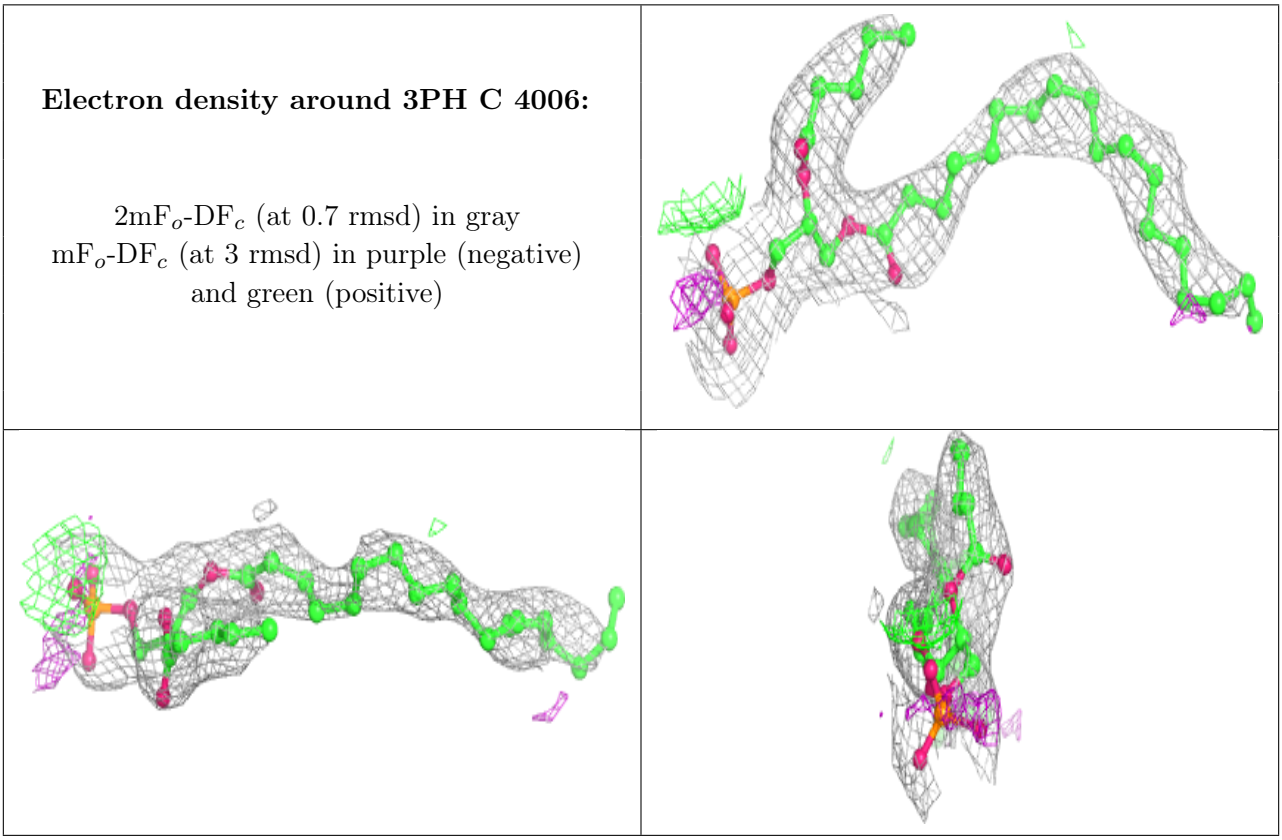
Electron density around UQ6 C 4005:

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



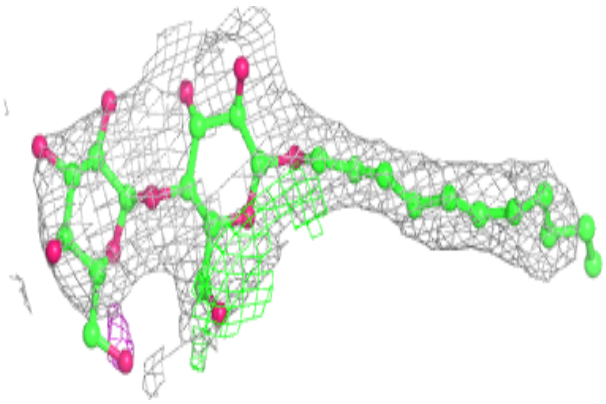
Electron density around 3PH C 4006:

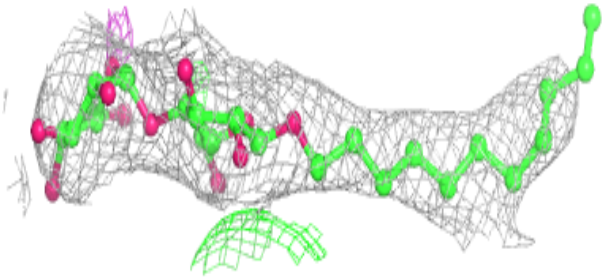
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

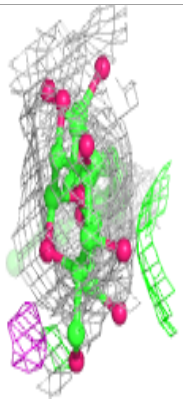


Electron density around UMQ A 501:

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

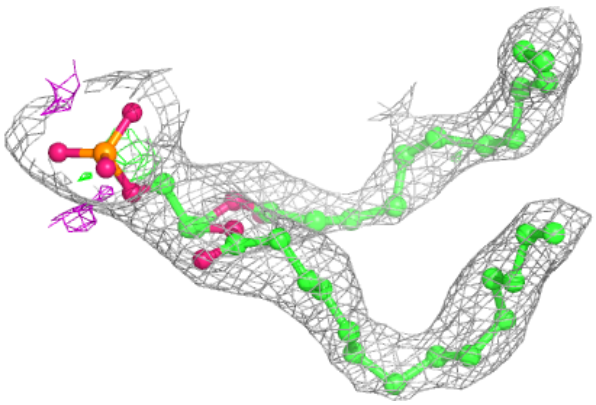


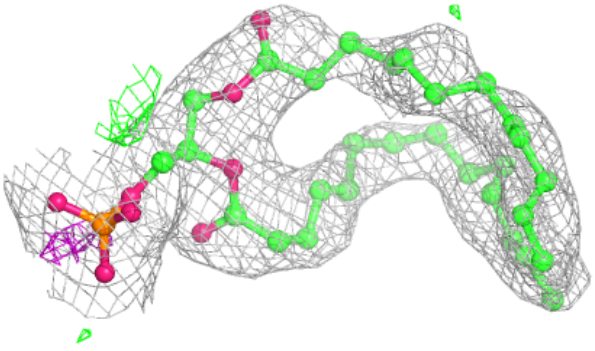


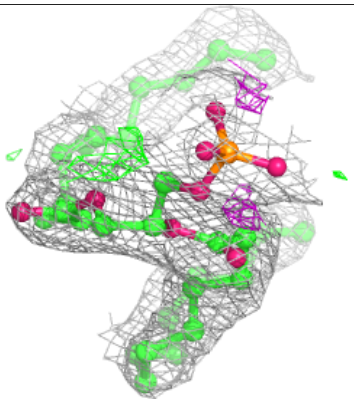


Electron density around 3PH E 302:

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

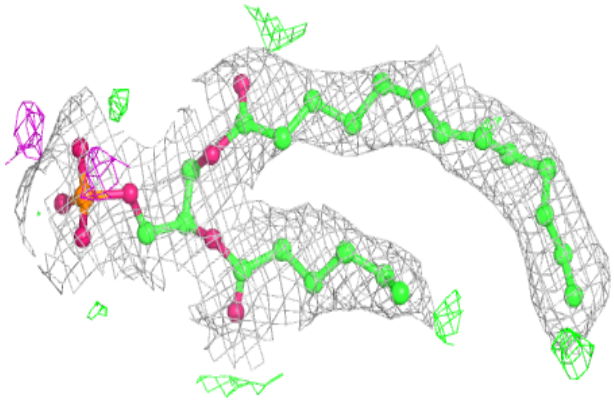


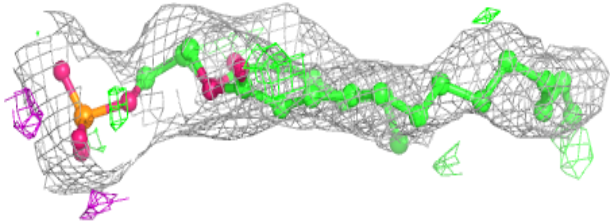


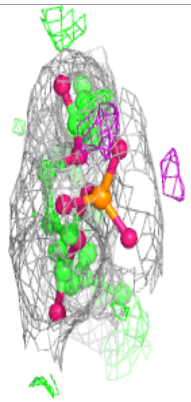


Electron density around 3PH A 502:

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

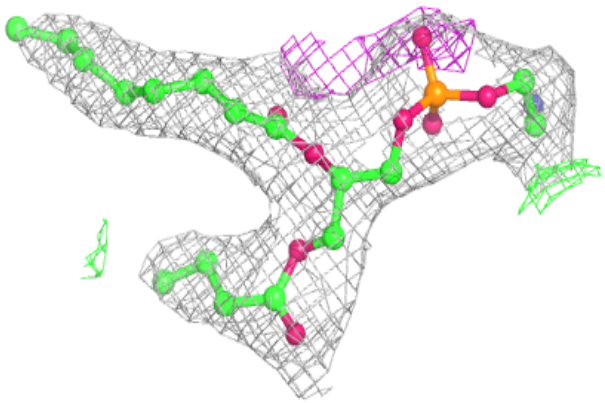


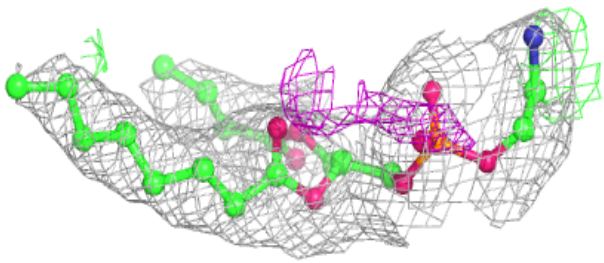


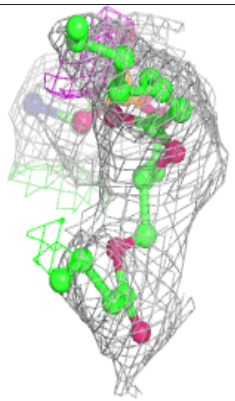


Electron density around 3PE C 4004:

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

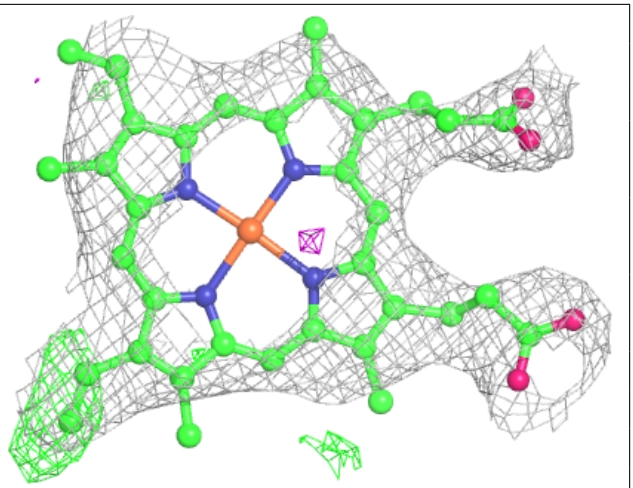


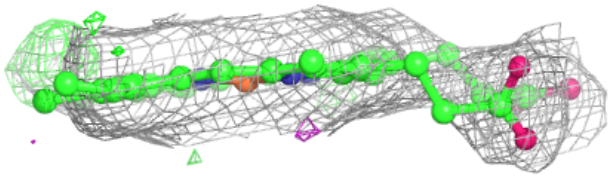


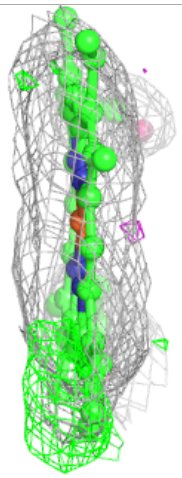


Electron density around HEM D 401:

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

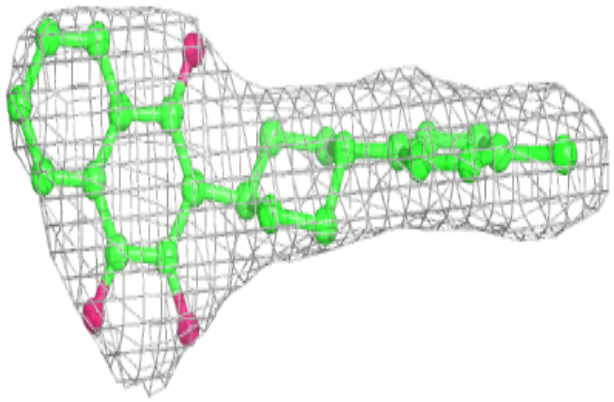


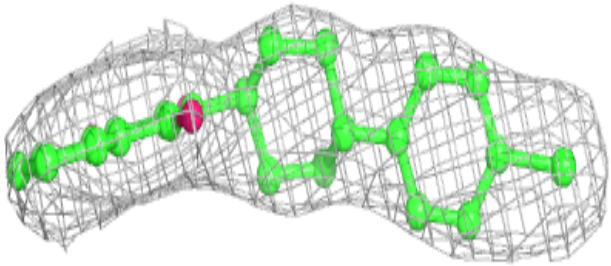


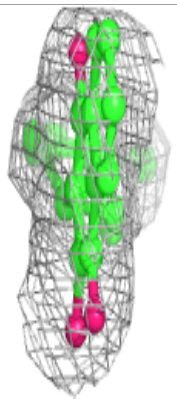


Electron density around AOQ C 4003:

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

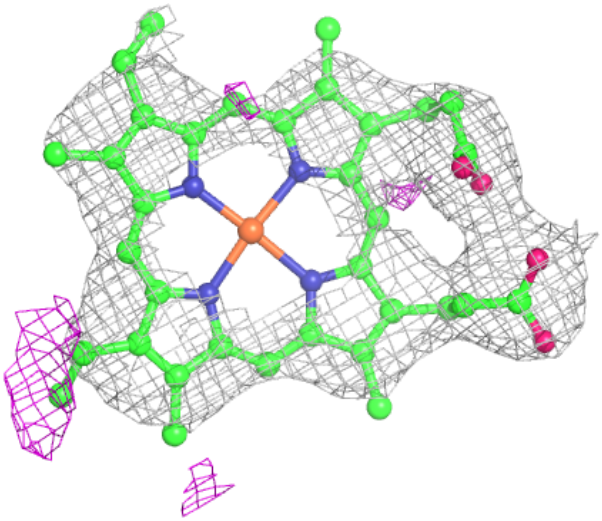


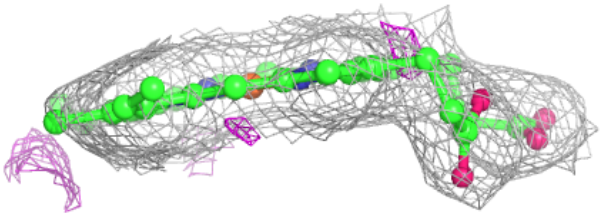


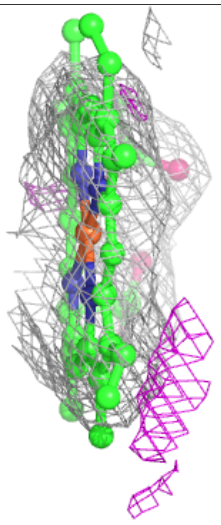


Electron density around HEM C 4001:

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

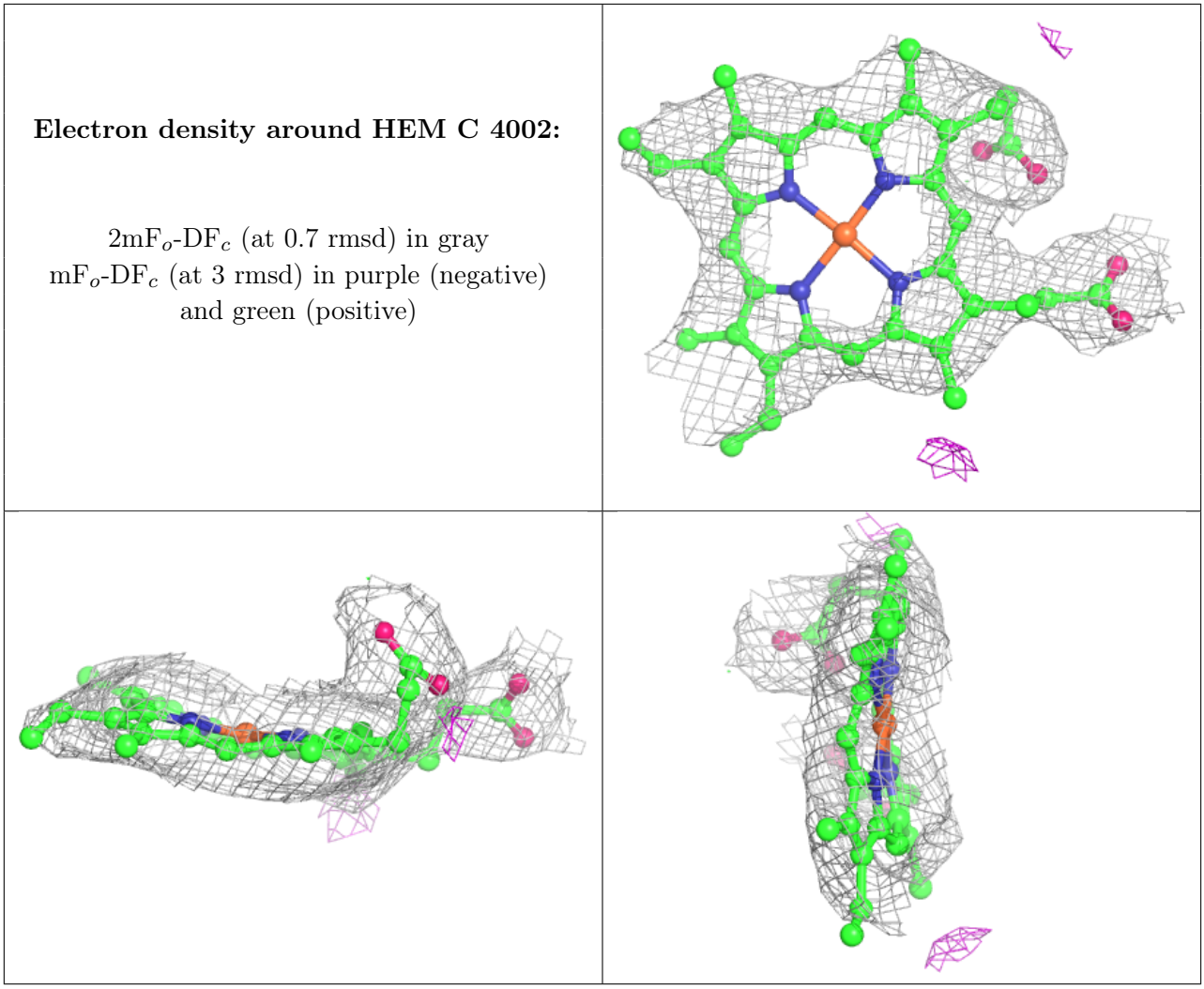






Electron density around HEM C 4002:

$2mF_o$-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.