wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 02:30 AM JST

PDB ID	:	4YTN / pdb_00004ytn
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with N-[3-(pentafluorophenoxy)phenyl]-2-(trifluoromethyl)benzamide
Authors	:	Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on	:	2015-03-18
Resolution	:	3.00 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:

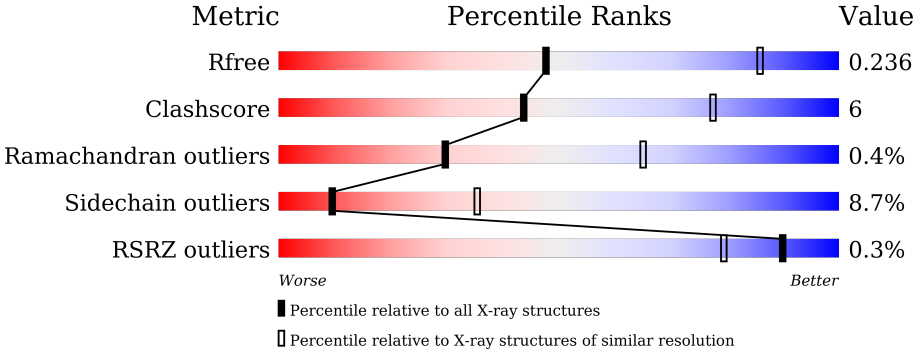
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	645	74% 19% • •
1	E	645	77% 17% • •
2	B	282	73% 15% • 11%
2	F	282	75% 12% • 11%
3	C	188	% 65% 14% • 19%
3	G	188	2% 64% 17% • 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	156	65% 15% • 17%
4	H	156	2% 63% 17% • 17%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18320 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 Succinate dehydrogenase flavoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	616	4787	3004	855	900	28	0	0	0
1	E	616	4787	3004	855	900	28	0	0	0

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	250	1985	1263	338	361	23	0	0	0
2	F	250	1985	1263	338	361	23	0	0	0

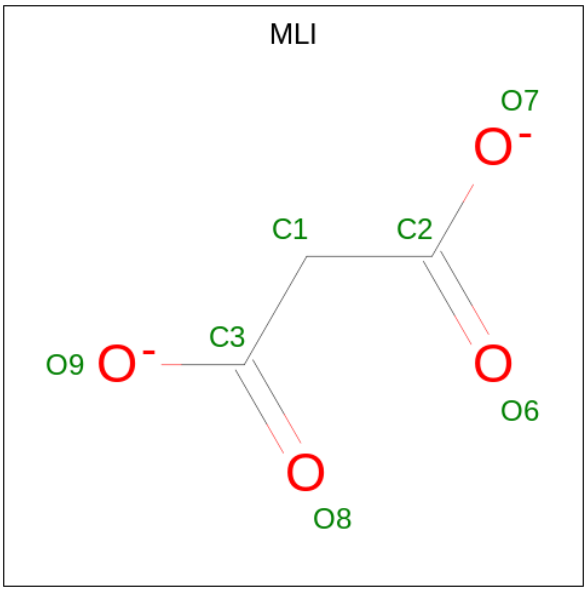
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	153	1217	813	204	194	6	0	0	0
3	G	153	1217	813	204	194	6	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

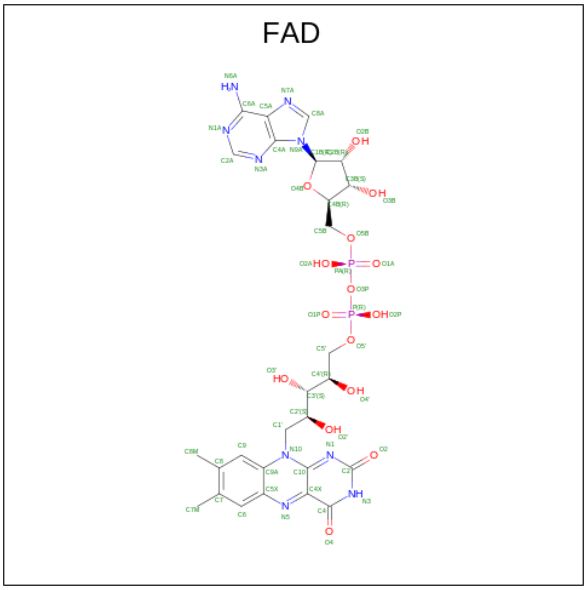
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	129	998	659	165	169	5	0	0	0
4	H	129	998	659	165	169	5	0	0	0

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



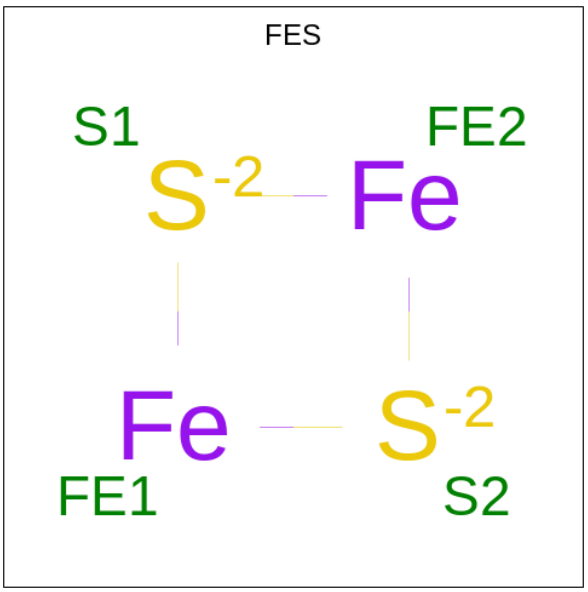
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	3	4		0	0
			Total	C	O			
5	E	1	7	3	4		0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



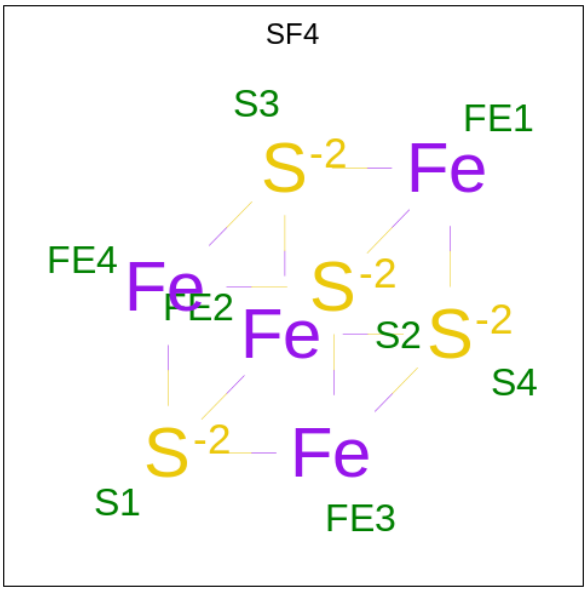
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
6	E	1	53	27	9	15	2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0
7	F	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



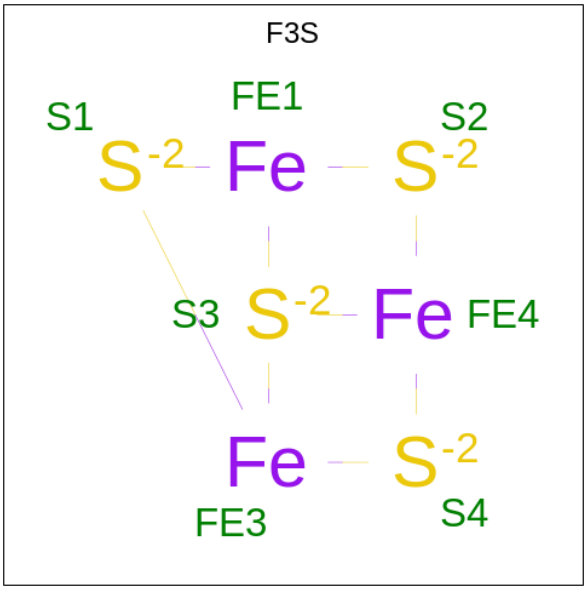
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

Continued on next page...

Continued from previous page...

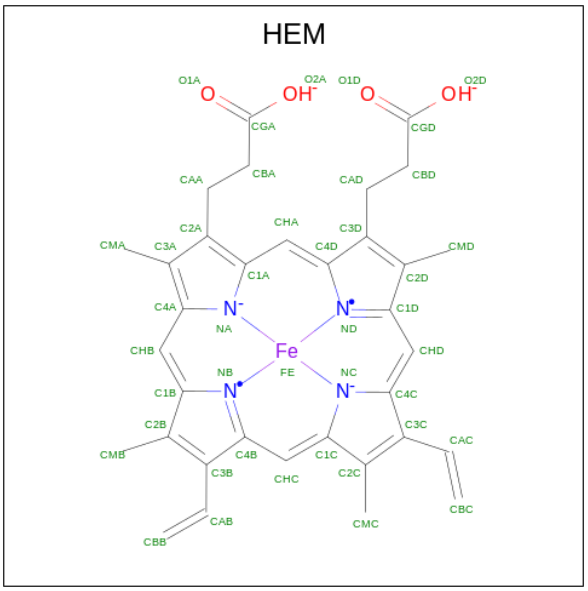
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	F	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



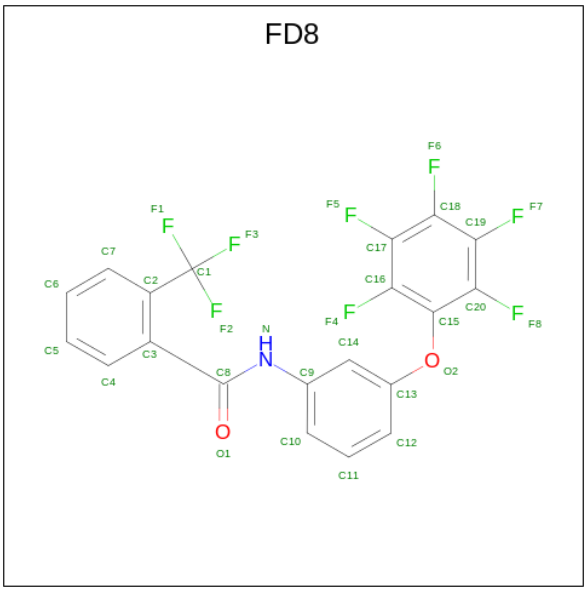
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0
9	F	1	7	3	4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is N-[3-(pentafluorophenoxy)phenyl]-2-(trifluoromethyl)benzamide (CCD ID: FD8) (formula: $C_{20}H_9F_8NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
11	C	1	31	20	8	1	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
11	F	1	31	20	8	1	2	0	0

- Molecule 12 is water.

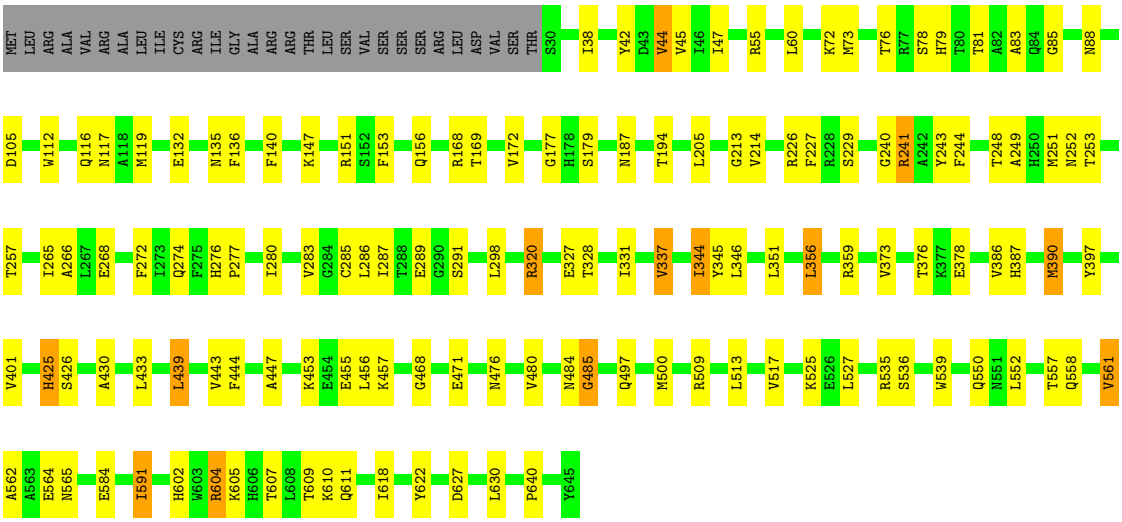
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	17	17	17	0	0
12	B	4	4	4	0	0
12	C	4	4	4	0	0
12	D	2	2	2	0	0
12	E	12	12	12	0	0
12	H	1	1	1	0	0

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.

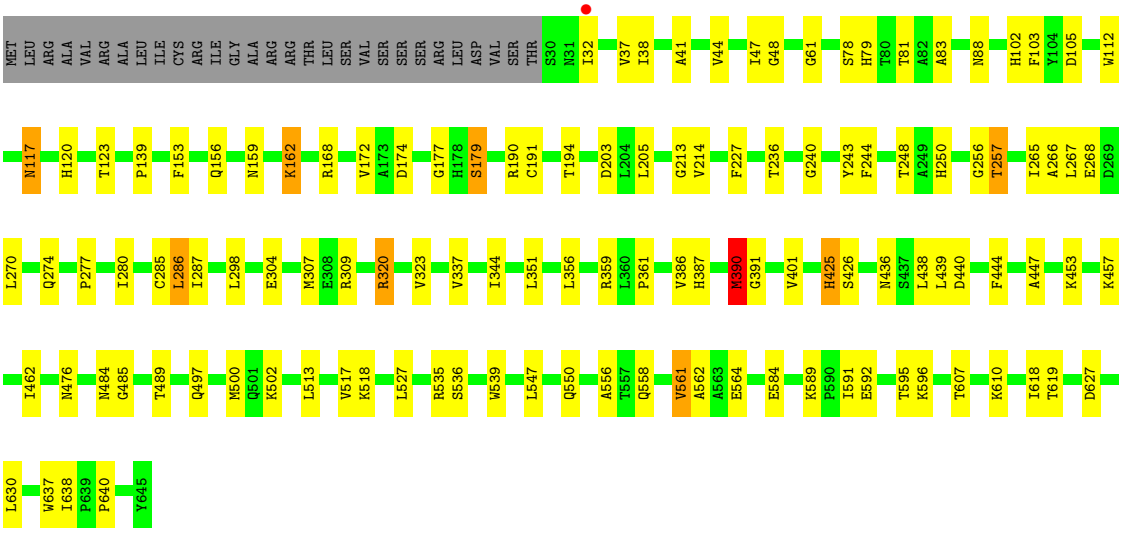
• Molecule 1: Succinate dehydrogenase flavoprotein

Chain A:



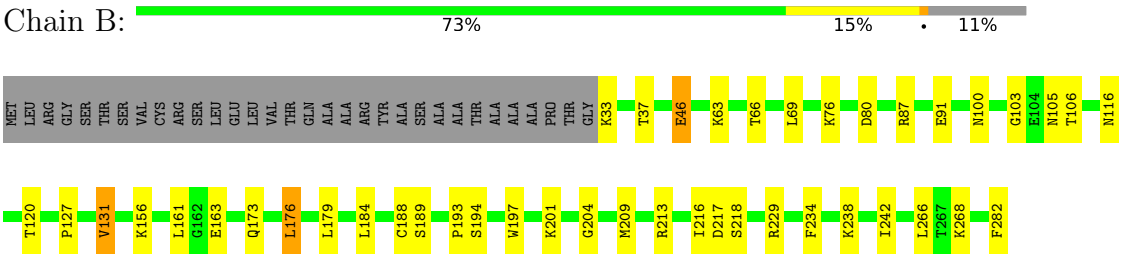
• Molecule 1: Succinate dehydrogenase flavoprotein

Chain E:



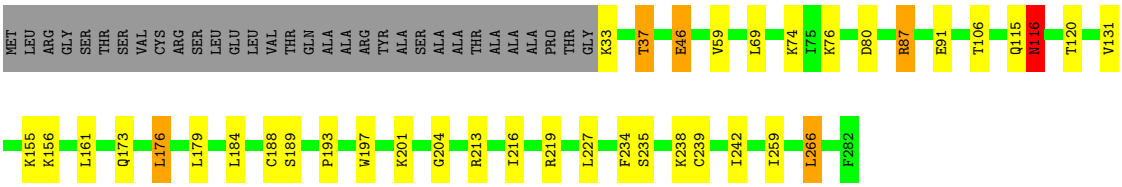
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



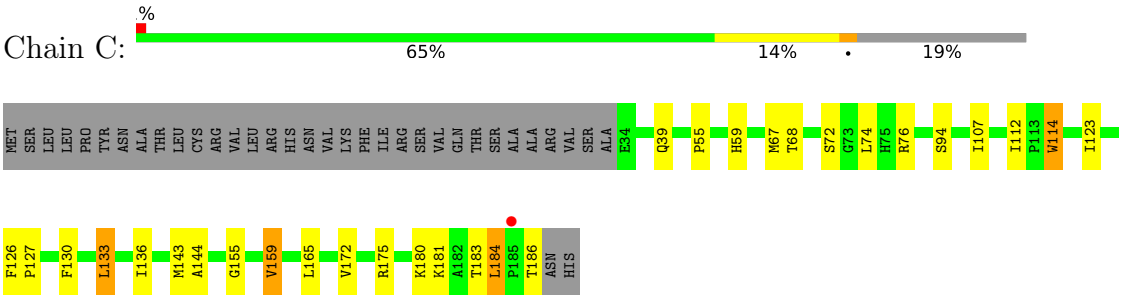
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



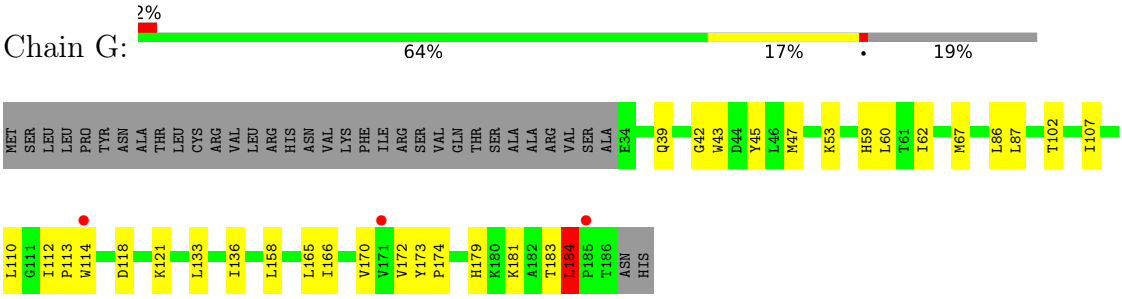
• Molecule 3: Cytochrome b-large subunit

Chain C:



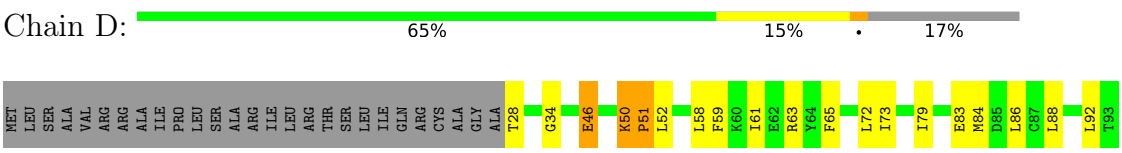
• Molecule 3: Cytochrome b-large subunit

Chain G:



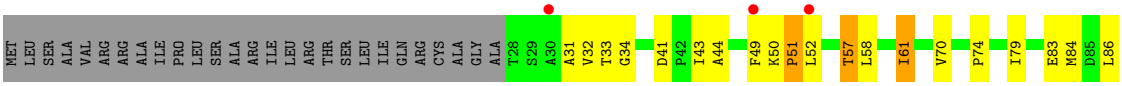
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:



• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.61Å 125.48Å 219.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-3.00) 93.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.190 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	3264 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18320	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FAD, F3S, MLI, FD8, SF4, FES

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	0.52	0/4889	0.83	1/6605 (0.0%)
1	E	0.52	0/4889	0.82	2/6605 (0.0%)
2	B	0.54	0/2029	0.82	3/2739 (0.1%)
2	F	0.52	0/2029	0.78	3/2739 (0.1%)
3	C	0.51	0/1255	0.80	1/1709 (0.1%)
3	G	0.54	0/1255	0.84	1/1709 (0.1%)
4	D	0.55	0/1030	0.80	0/1406
4	H	0.52	0/1030	0.79	0/1406
All	All	0.52	0/18406	0.82	11/24918 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	184	LEU	N-CA-C	7.51	114.98	108.22
2	B	163	GLU	N-CA-C	6.55	118.22	111.14
2	F	161	LEU	N-CA-C	6.20	117.70	111.07
2	B	204	GLY	CA-C-N	5.88	125.58	119.05
2	B	204	GLY	C-N-CA	5.88	125.58	119.05

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	4787	0	4720	78	0
1	E	4787	0	4720	63	0
2	B	1985	0	2001	21	0
2	F	1985	0	2001	18	0
3	C	1217	0	1265	17	0
3	G	1217	0	1265	14	0
4	D	998	0	985	14	0
4	H	998	0	985	17	0
5	A	7	0	2	1	0
5	E	7	0	2	1	0
6	A	53	0	31	9	0
6	E	53	0	31	6	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	2	0
10	G	43	0	30	3	0
11	C	31	0	9	2	0
11	F	31	0	9	1	0
12	A	17	0	0	0	0
12	B	4	0	0	1	0
12	C	4	0	0	0	0
12	D	2	0	0	0	0
12	E	12	0	0	0	0
12	H	1	0	0	0	0
All	All	18320	0	18086	220	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 6.

The worst 5 of 220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:CE1	6:A:702:FAD:HM82	1.84	1.11
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.76	1.00
1:E:79:HIS:NE2	6:E:702:FAD:HM81	1.82	0.92
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.53	0.90
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.40	0.84

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	614/645 (95%)	585 (95%)	27 (4%)	2 (0%)	36	70
1	E	614/645 (95%)	583 (95%)	29 (5%)	2 (0%)	36	70
2	B	248/282 (88%)	229 (92%)	19 (8%)	0	100	100
2	F	248/282 (88%)	235 (95%)	12 (5%)	1 (0%)	30	65
3	C	151/188 (80%)	146 (97%)	5 (3%)	0	100	100
3	G	151/188 (80%)	148 (98%)	2 (1%)	1 (1%)	18	53
4	D	127/156 (81%)	122 (96%)	4 (3%)	1 (1%)	16	50
4	H	127/156 (81%)	118 (93%)	7 (6%)	2 (2%)	7	34
All	All	2280/2542 (90%)	2166 (95%)	105 (5%)	9 (0%)	30	65

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY
3	G	113	PRO
4	D	51	PRO
1	E	485	GLY
1	A	604	ARG

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	502/527 (95%)	466 (93%)	36 (7%)	13	43
1	E	502/527 (95%)	462 (92%)	40 (8%)	11	38
2	B	220/242 (91%)	203 (92%)	17 (8%)	12	40
2	F	220/242 (91%)	204 (93%)	16 (7%)	13	42
3	C	127/158 (80%)	115 (91%)	12 (9%)	8	32
3	G	127/158 (80%)	109 (86%)	18 (14%)	3	16
4	D	98/119 (82%)	85 (87%)	13 (13%)	4	18
4	H	98/119 (82%)	85 (87%)	13 (13%)	4	18
All	All	1894/2092 (90%)	1729 (91%)	165 (9%)	9	35

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	596	LYS
3	G	133	LEU
2	F	37	THR
2	F	176	LEU
3	G	183	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	436	ASN
2	F	44	ASN
1	E	484	ASN
1	E	551	ASN
2	F	100	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
8	SF4	B	302	2	0,12,12	-	-	-		
11	FD8	C	202	-	33,33,33	1.88	6 (18%)	49,49,49	1.40	6 (12%)
11	FD8	F	304	-	33,33,33	1.88	7 (21%)	49,49,49	1.34	2 (4%)
5	MLI	A	701	-	6,6,6	1.05	0	7,7,7	1.34	1 (14%)
5	MLI	E	701	-	6,6,6	1.04	0	7,7,7	1.03	0
10	HEM	G	201	3,4	50,50,50	1.59	7 (14%)	66,82,82	1.88	18 (27%)
7	FES	F	301	2	0,4,4	-	-	-		
9	F3S	B	303	2	0,9,9	-	-	-		
6	FAD	A	702	-	56,58,58	1.42	8 (14%)	81,89,89	1.97	26 (32%)
6	FAD	E	702	-	56,58,58	1.43	7 (12%)	81,89,89	1.93	25 (30%)
9	F3S	F	303	2	0,9,9	-	-	-		
10	HEM	C	201	3,4	50,50,50	1.59	5 (10%)	66,82,82	1.69	15 (22%)
8	SF4	F	302	2	0,12,12	-	-	-		
7	FES	B	301	2	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SF4	B	302	2	-	-	0/6/5/5
8	SF4	F	302	2	-	-	0/6/5/5
11	FD8	C	202	-	-	12/18/18/18	0/3/3/3
5	MLI	A	701	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	E	701	-	-	0/4/4/4	-
10	HEM	G	201	3,4	-	6/14/54/54	-
10	HEM	C	201	3,4	-	6/14/54/54	-
7	FES	F	301	2	-	-	0/1/1/1
6	FAD	A	702	-	-	6/34/50/50	0/6/6/6
6	FAD	E	702	-	-	9/34/50/50	0/6/6/6
9	F3S	B	303	2	-	-	0/3/3/3
9	F3S	F	303	2	-	-	0/3/3/3
11	FD8	F	304	-	-	2/18/18/18	0/3/3/3
7	FES	B	301	2	-	-	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	201	HEM	FE-NB	5.57	2.12	1.94
10	G	201	HEM	FE-NB	5.46	2.11	1.94
6	E	702	FAD	C9A-C5X	5.00	1.49	1.41
6	A	702	FAD	C9A-C5X	4.94	1.49	1.41
11	C	202	FD8	F7-C19	4.83	1.42	1.35

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	304	FD8	C13-O2-C15	6.25	128.53	118.48
6	E	702	FAD	C5A-C4A-N3A	-5.94	119.00	126.75
10	G	201	HEM	CAD-C3D-C4D	5.73	134.68	124.66
6	A	702	FAD	C5A-C4A-N3A	-5.59	119.46	126.75
6	E	702	FAD	N3A-C4A-N9A	4.58	134.63	127.08

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'

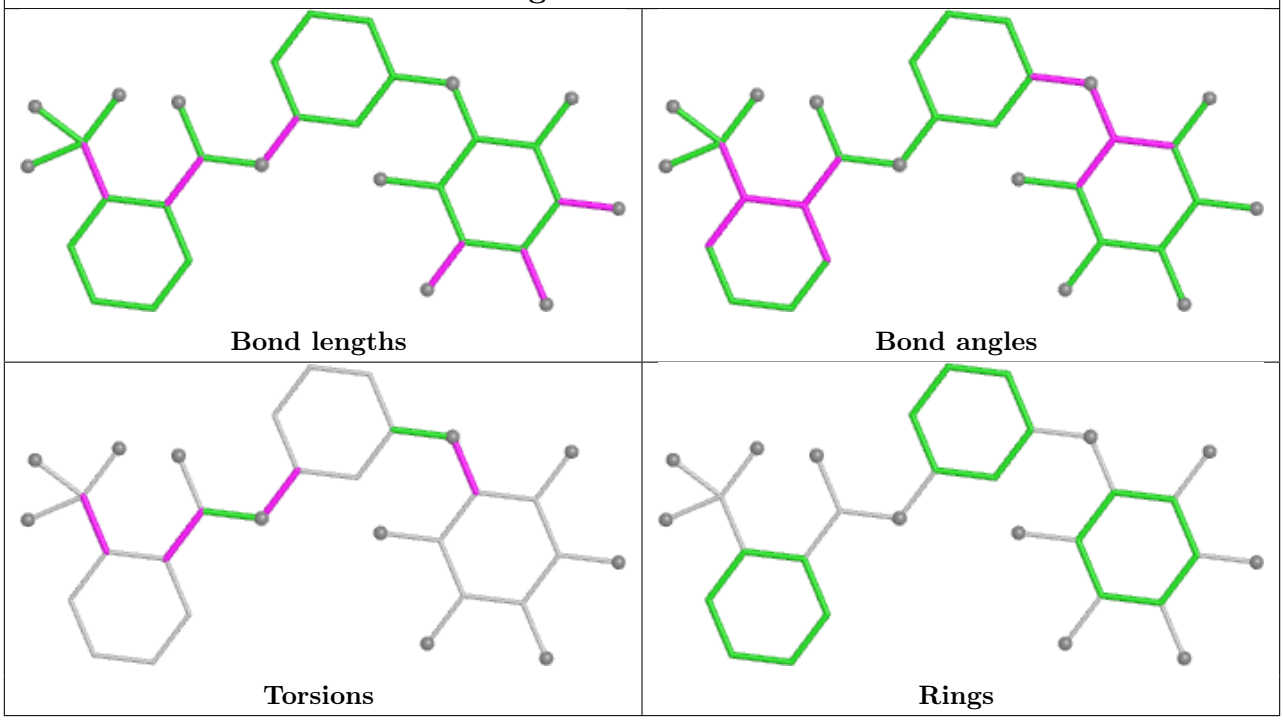
There are no ring outliers.

8 monomers are involved in 25 short contacts:

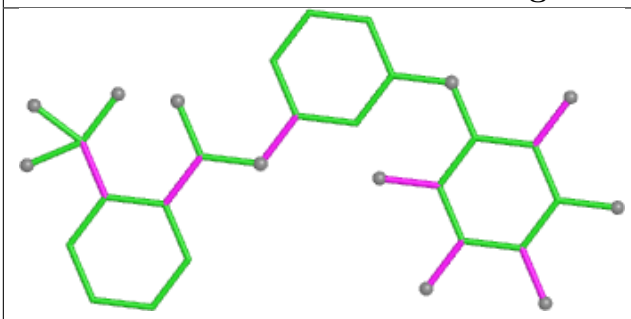
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	202	FD8	2	0
11	F	304	FD8	1	0
5	A	701	MLI	1	0
5	E	701	MLI	1	0
10	G	201	HEM	3	0
6	A	702	FAD	9	0
6	E	702	FAD	6	0
10	C	201	HEM	2	0

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.

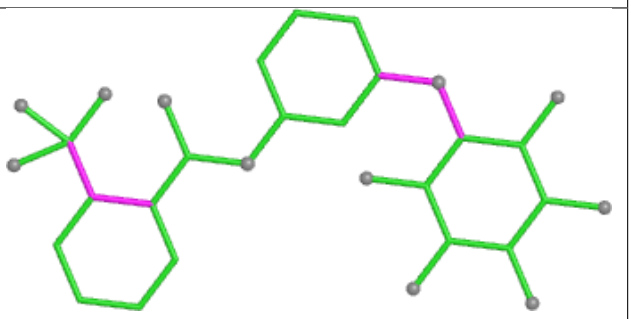
Ligand FD8 C 202



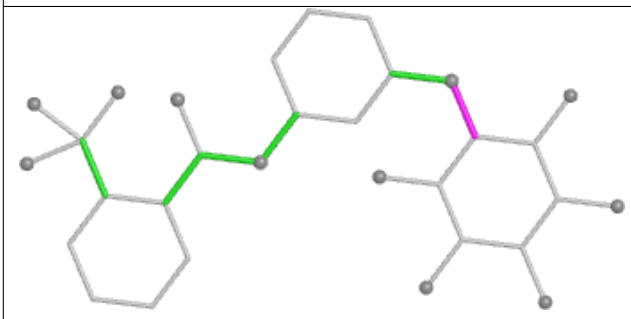
Ligand FD8 F 304



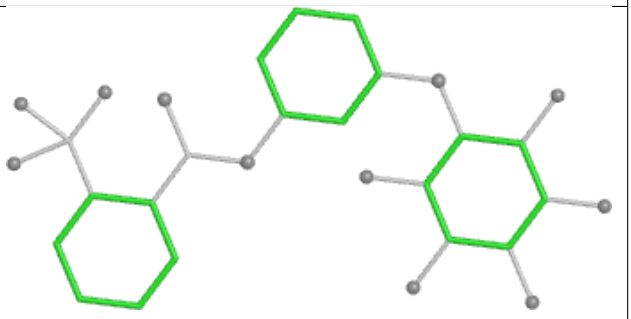
Bond lengths



Bond angles

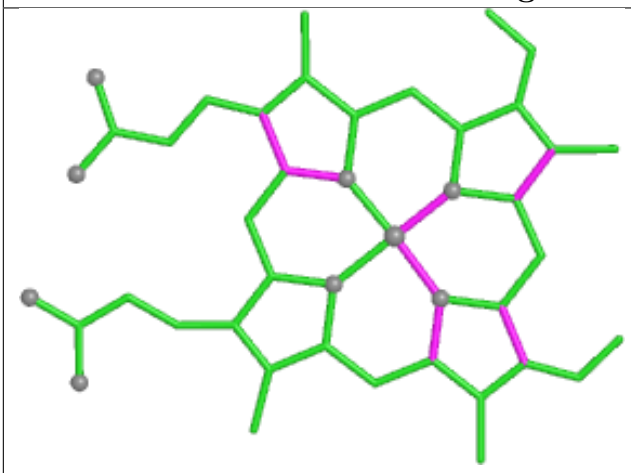


Torsions

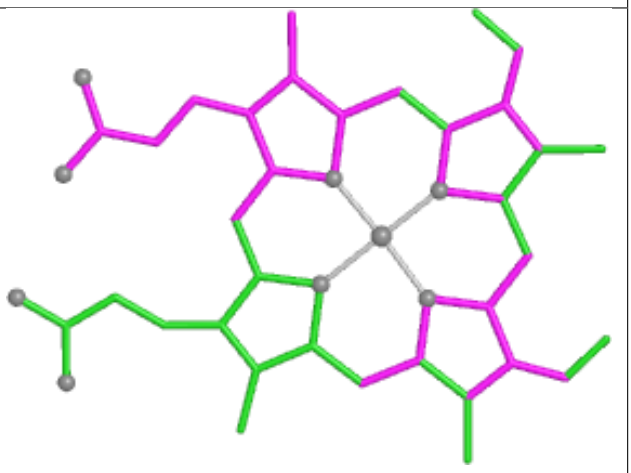


Rings

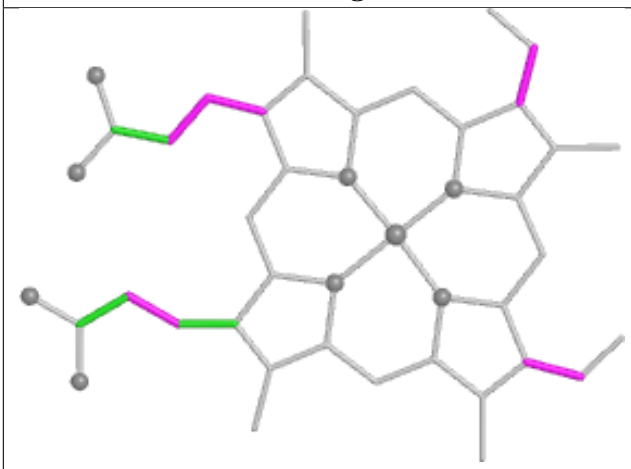
Ligand HEM G 201



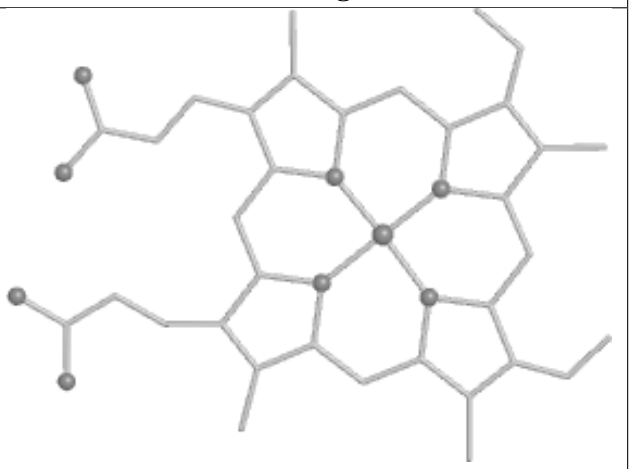
Bond lengths



Bond angles

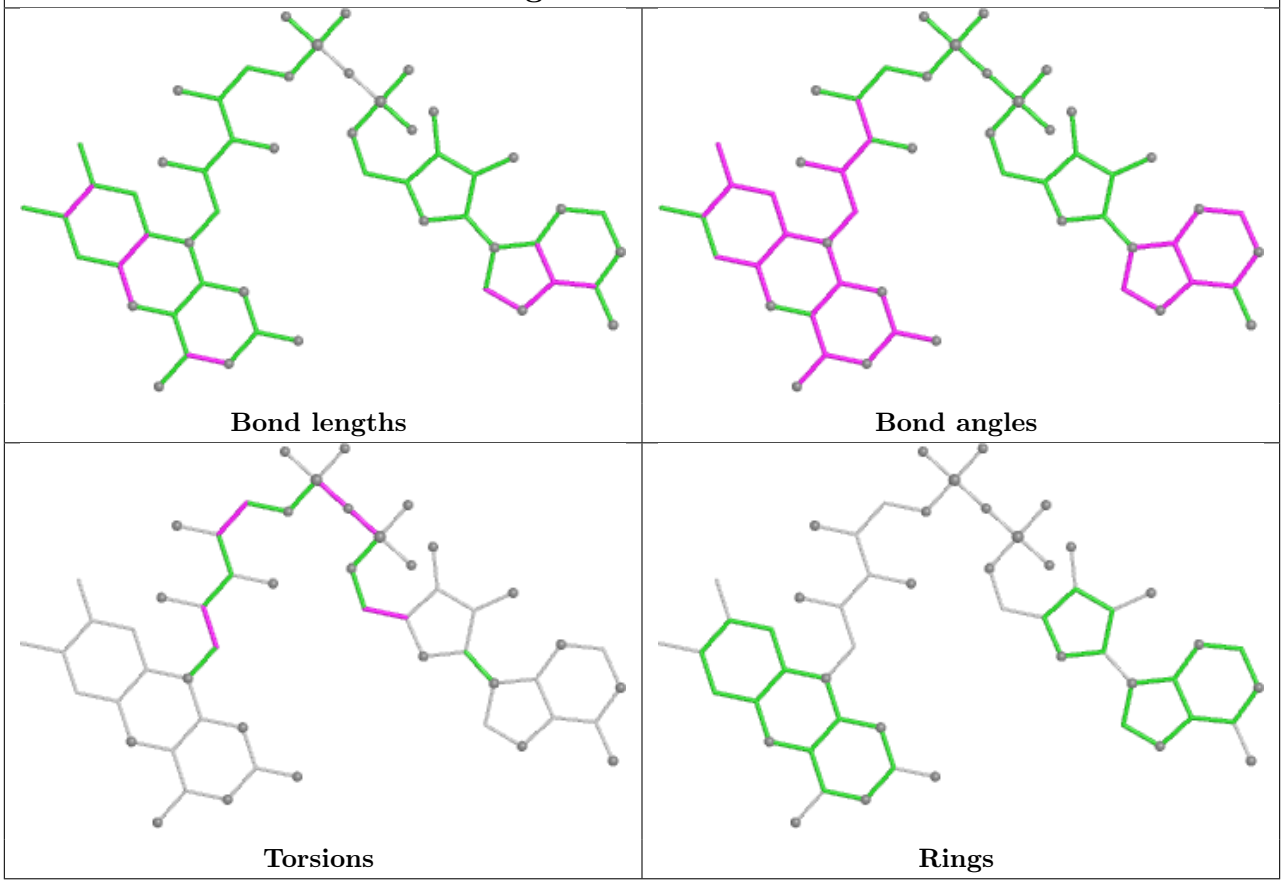


Torsions

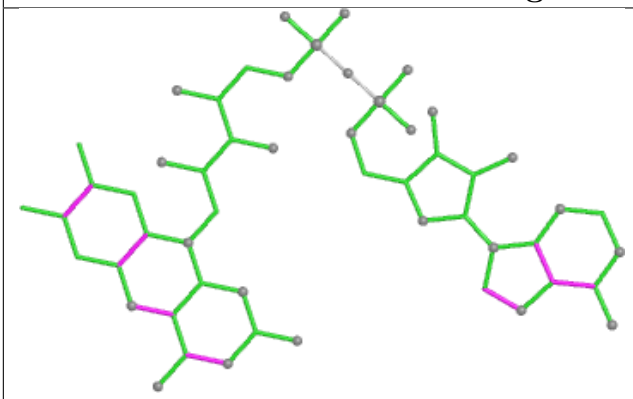


Rings

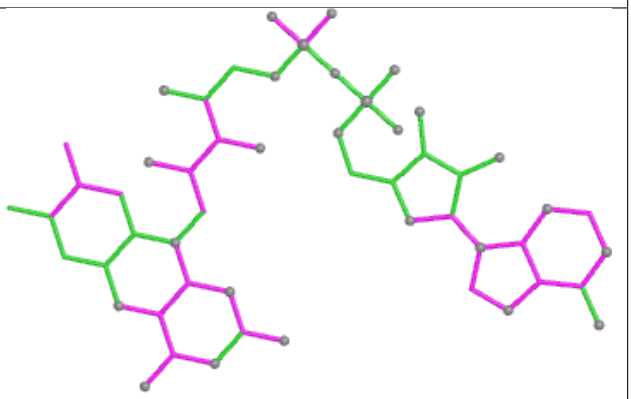
Ligand FAD A 702



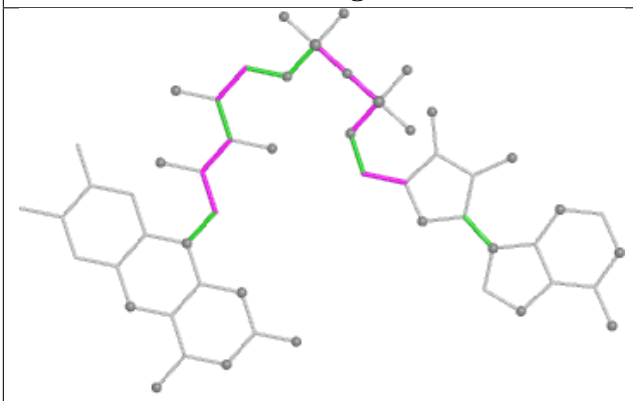
Ligand FAD E 702



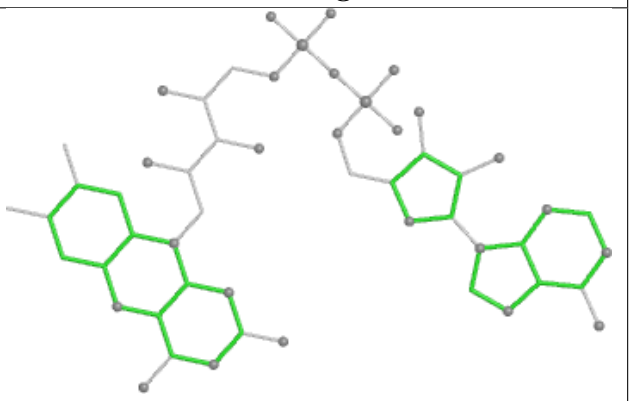
Bond lengths



Bond angles

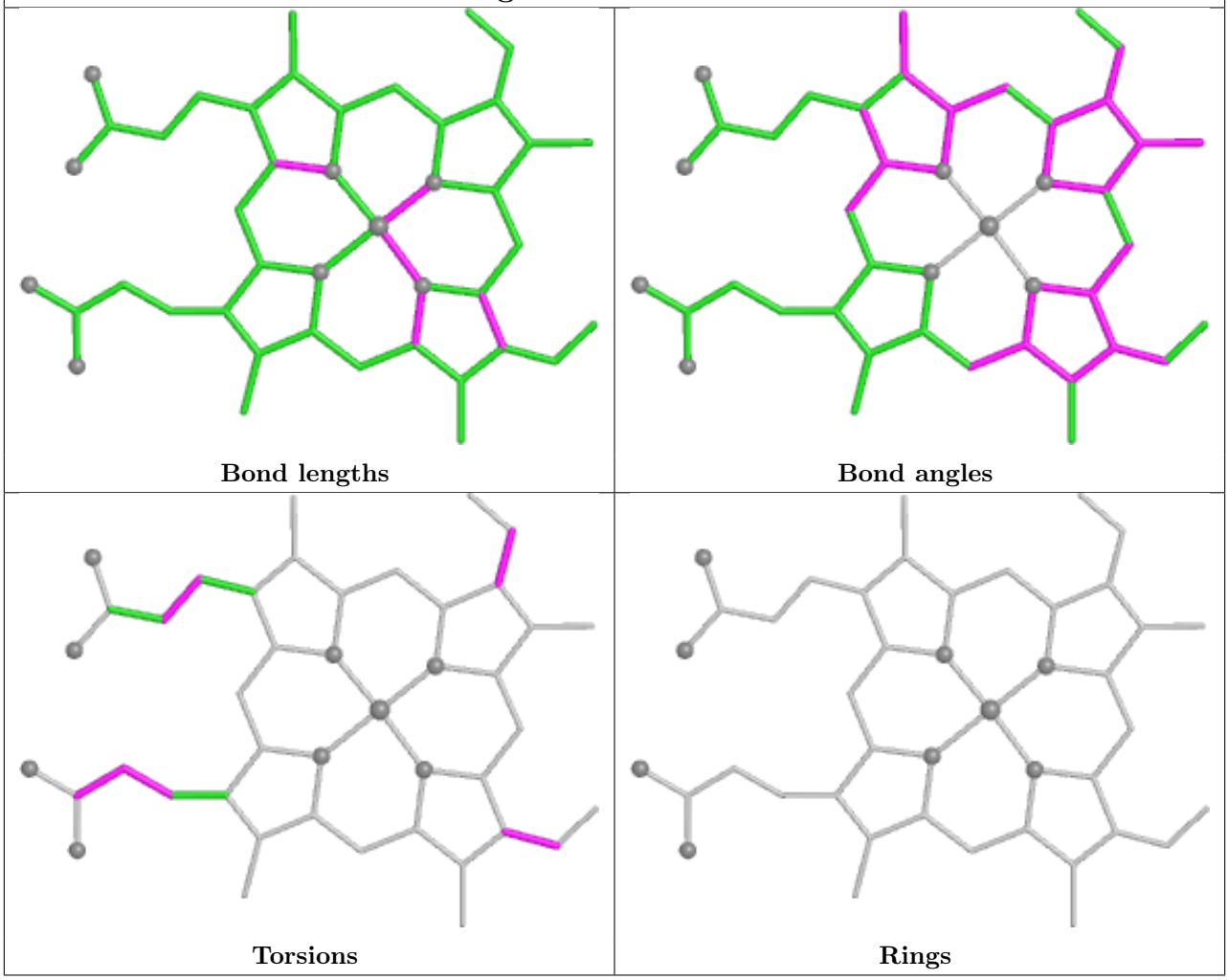


Torsions



Rings

Ligand HEM C 201



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	616/645 (95%)	-0.57	0	100	100	34, 55, 81, 115	0
1	E	616/645 (95%)	-0.54	1 (0%)	91	83	38, 59, 85, 120	0
2	B	250/282 (88%)	-0.51	0	100	100	39, 55, 81, 100	0
2	F	250/282 (88%)	-0.56	0	100	100	39, 56, 82, 106	0
3	C	153/188 (81%)	-0.30	1 (0%)	84	66	40, 64, 106, 173	0
3	G	153/188 (81%)	-0.06	3 (1%)	65	41	51, 75, 142, 177	0
4	D	129/156 (82%)	-0.31	0	100	100	54, 67, 106, 144	0
4	H	129/156 (82%)	-0.20	3 (2%)	61	38	56, 73, 123, 157	0
All	All	2296/2542 (90%)	-0.47	8 (0%)	90	79	34, 60, 98, 177	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	4.2
3	G	185	PRO	3.2
3	G	114	TRP	2.8
4	H	49	PHE	2.6
4	H	52	LEU	2.5

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 oligosaccharides in this entry.

6.4 Ligands (i)

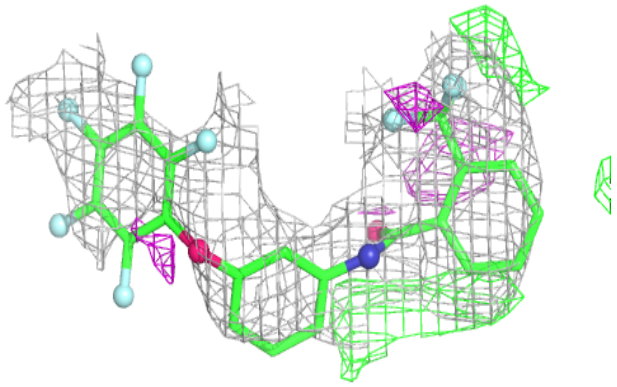
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

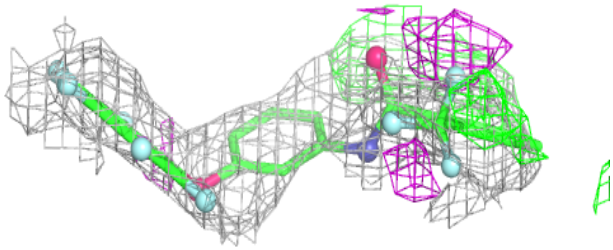
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	FD8	C	202	31/31	0.67	0.23	115,139,146,147	0
11	FD8	F	304	31/31	0.73	0.18	99,126,143,144	0
5	MLI	E	701	7/7	0.96	0.07	49,51,52,56	0
10	HEM	G	201	43/43	0.96	0.12	62,80,87,89	0
10	HEM	C	201	43/43	0.97	0.10	56,67,72,81	0
5	MLI	A	701	7/7	0.97	0.08	50,51,52,52	0
6	FAD	A	702	53/53	0.97	0.07	35,38,44,45	0
6	FAD	E	702	53/53	0.97	0.06	38,48,55,60	0
9	F3S	F	303	7/7	0.98	0.05	45,51,56,57	0
8	SF4	B	302	8/8	0.99	0.03	36,38,42,42	0
8	SF4	F	302	8/8	0.99	0.04	38,43,47,49	0
9	F3S	B	303	7/7	0.99	0.04	45,51,53,54	0
7	FES	B	301	4/4	0.99	0.03	33,36,36,41	0
7	FES	F	301	4/4	1.00	0.03	42,45,45,47	0

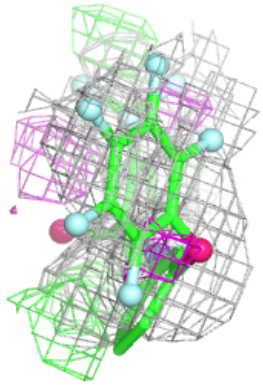
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FD8 C 202:

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

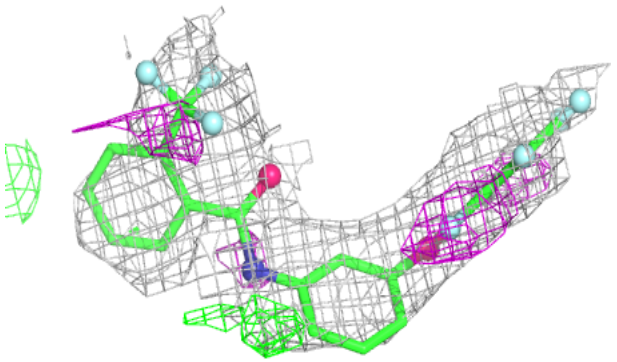


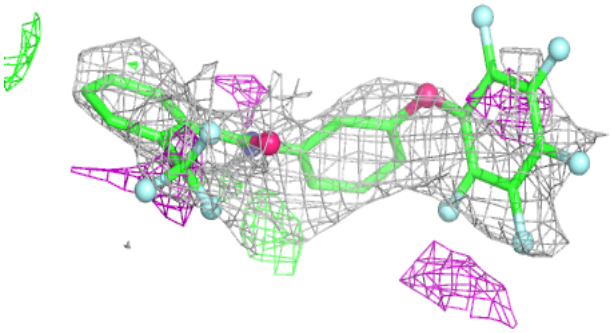


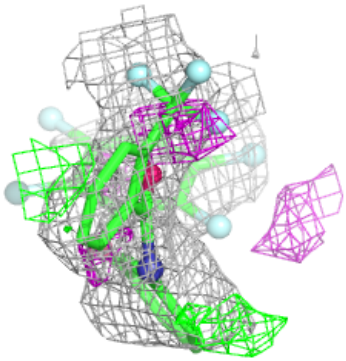


Electron density around FD8 F 304:

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

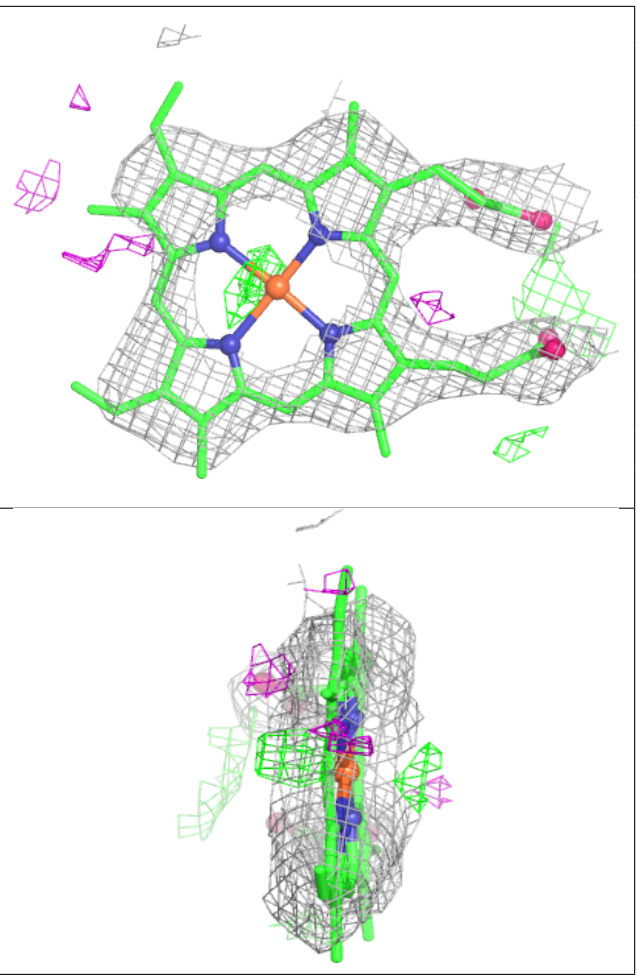






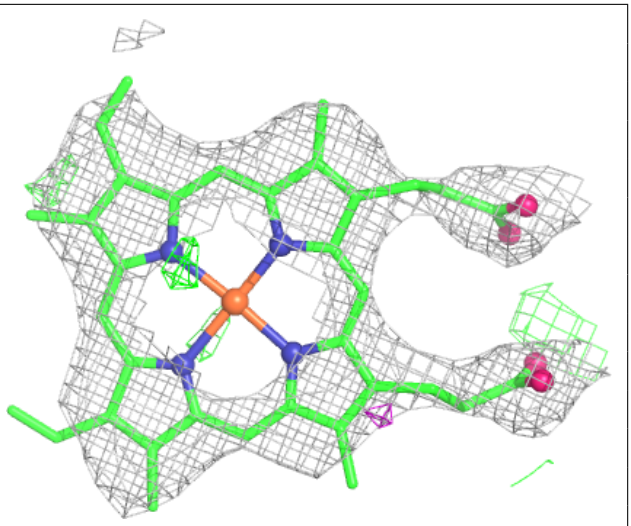
Electron density around HEM G 201:

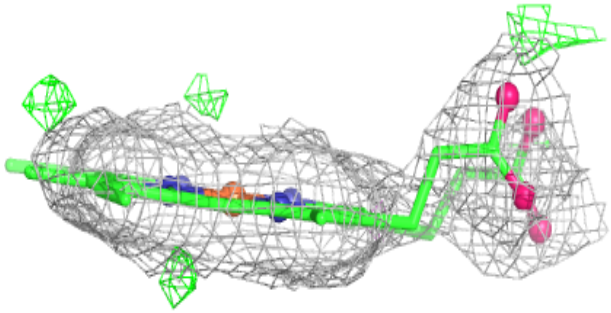
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

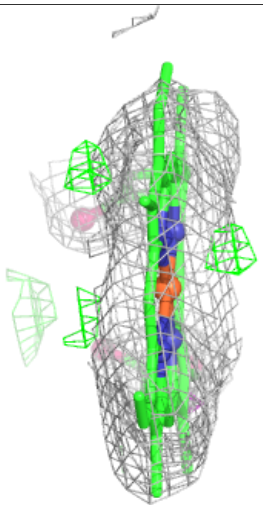


Electron density around HEM C 201:

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

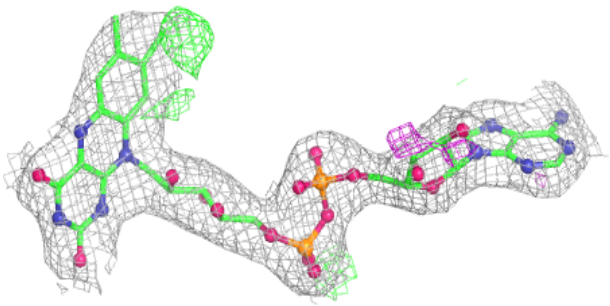


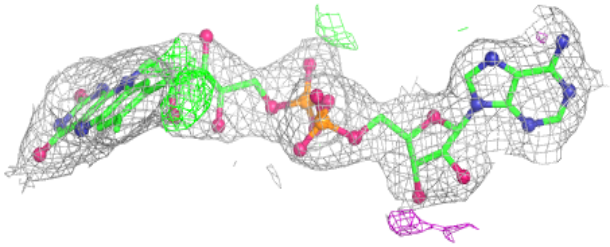


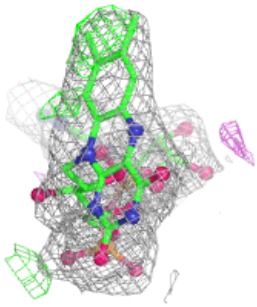


Electron density around FAD A 702:

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

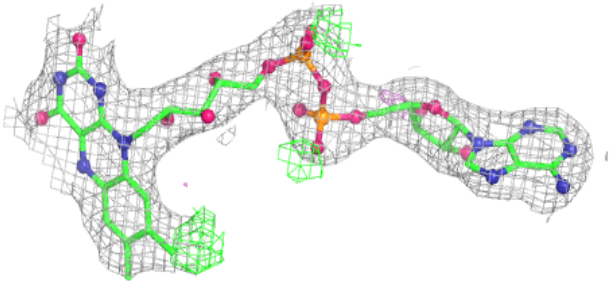


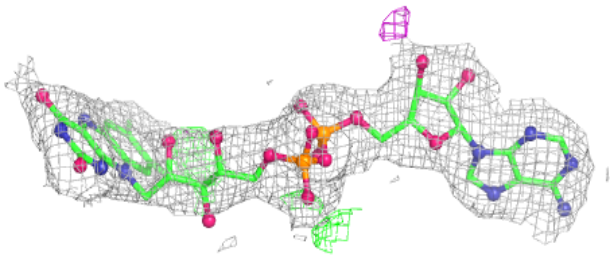


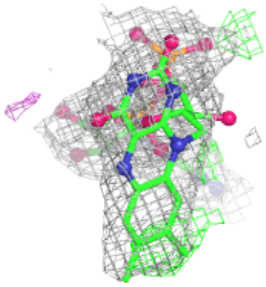


Electron density around FAD E 702:

$2mF_o$-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.