wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 04:10 AM JST

PDB ID	:	5C3J / pdb_00005c3j
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with Ubiquinone-1
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	:	2015-06-17
Resolution	:	2.80 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 (1)) were used in the production of this report:

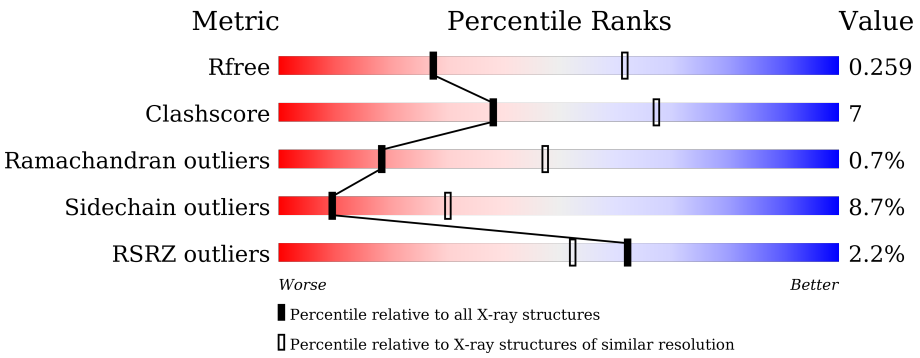
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	73% 21% • •
1	E	645	75% 19% • •
2	B	282	% 72% 15% • 11%
2	F	282	72% 15% • 11%
3	C	188	% 65% 15% • 19%

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Mol	Chain	Length	Quality of chain
3	G	188	16% 62% 14% 5% • 19%
4	D	156	2% 61% 21% • 17%
4	H	156	4% 63% 17% • 17%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18342 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 [ubiquinone] flavoprotein subunit, mitochondrial.

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

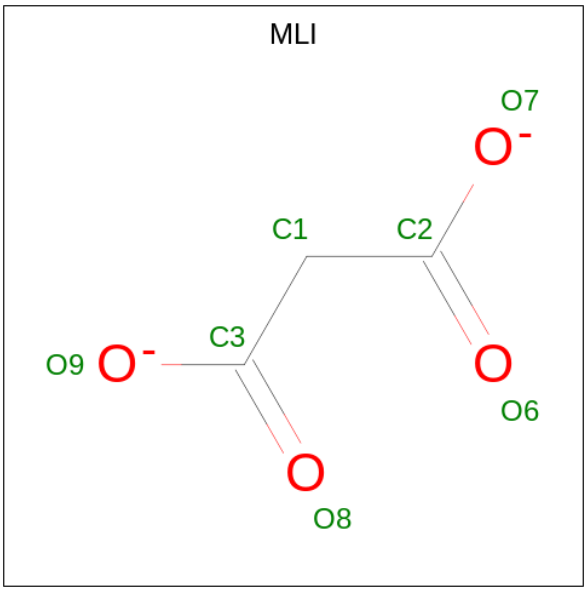
- Molecule 3 is a protein called Cytochrome b-large subunit.

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.

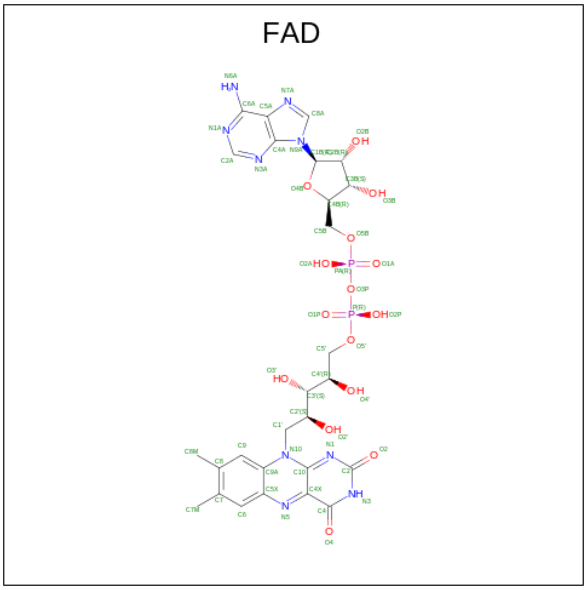
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	129	998	659	165	169	5	0	0	0
4	H	129	998	659	165	169	5	0	0	0

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



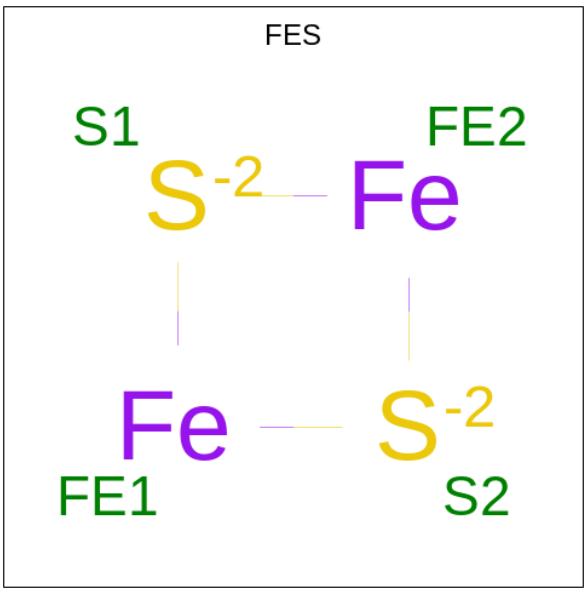
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	3	4		0	0
5	E	1	7	3	4		0	0

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



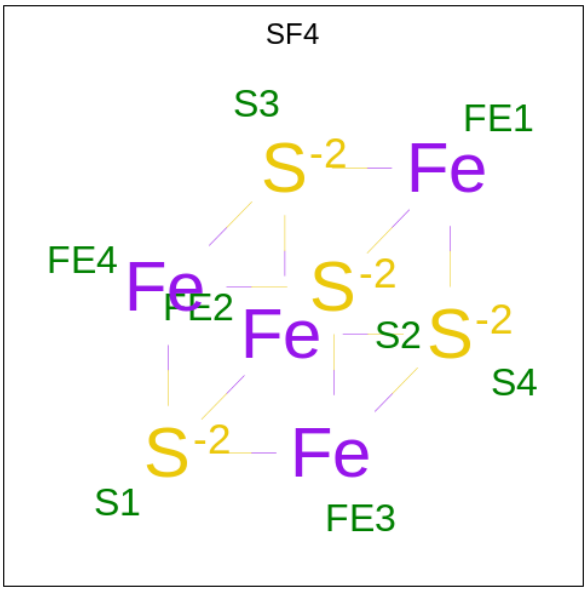
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	53	27	9	15	2	0	0
6	E	1	53	27	9	15	2	0	0

- 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

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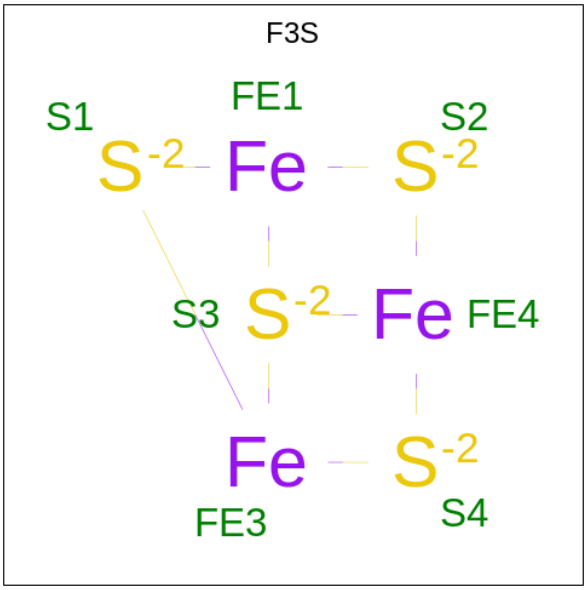
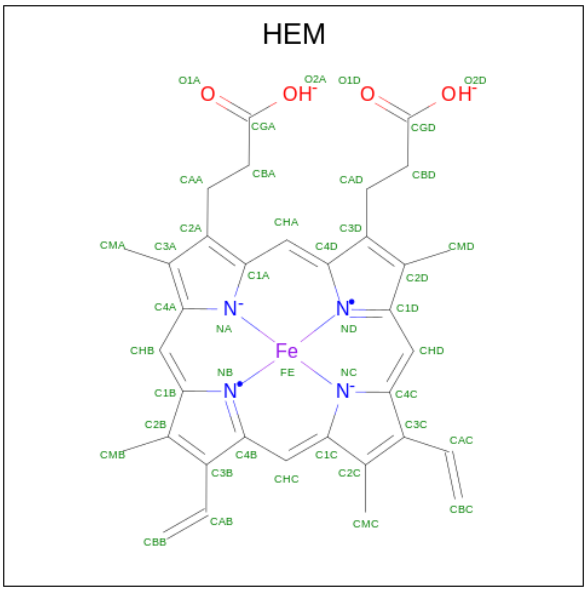
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	F	1	8	4	4	0	0

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



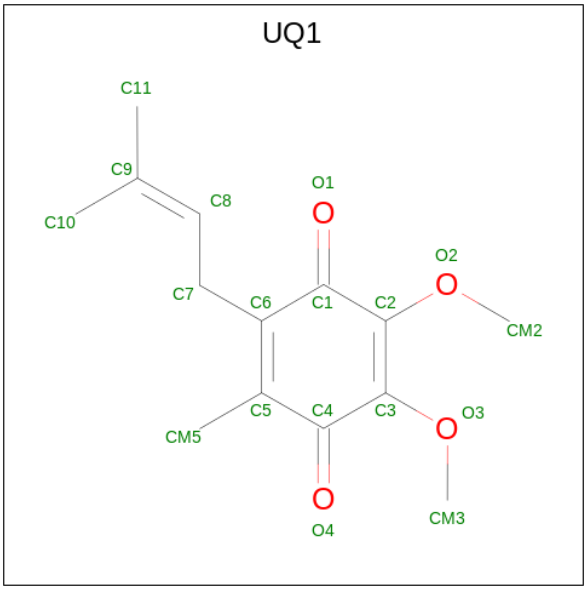
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0
9	F	1	7	3	4	0	0

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



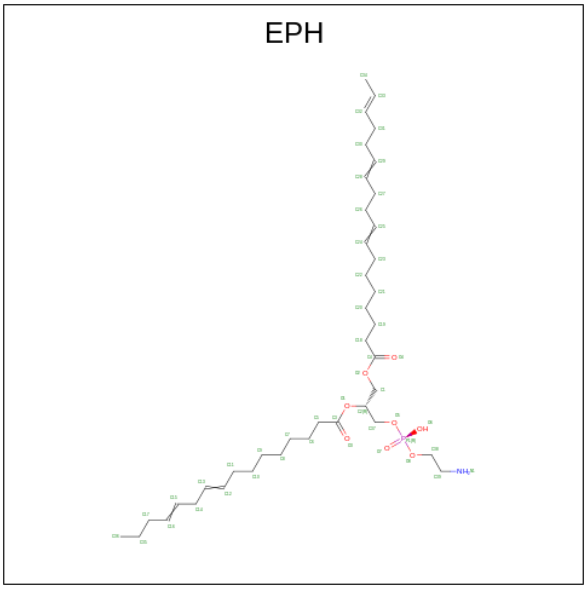
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
10	G	1	43	34	1	4	4	0	0

- Molecule 11 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	C	1	18	14	4	0	0
			Total	C	O		
11	G	1	18	14	4	0	0

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: $C_{39}H_{68}NO_8P$).



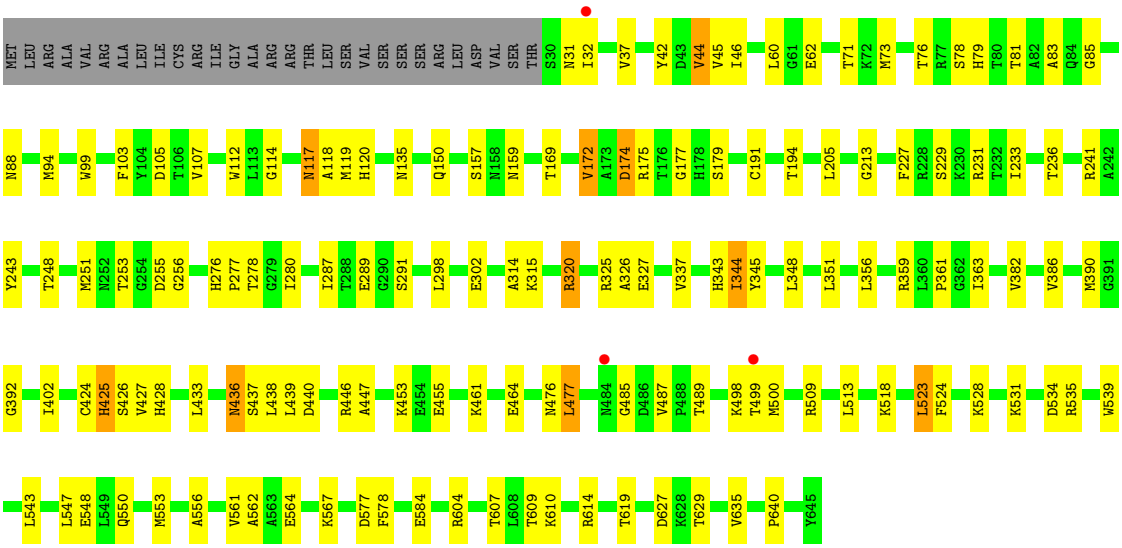
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	D	1	44	34	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	44	34	1	8	1	0	0

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.

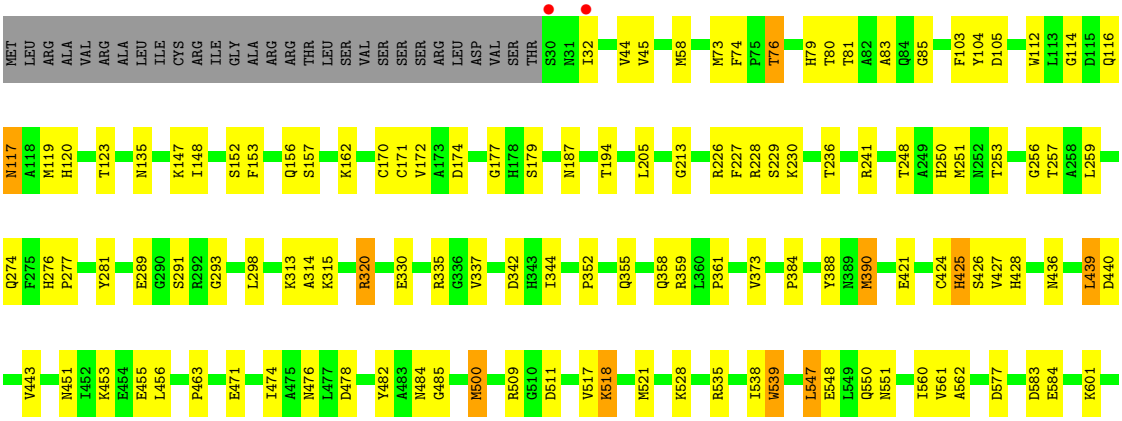
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A:



• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain E:

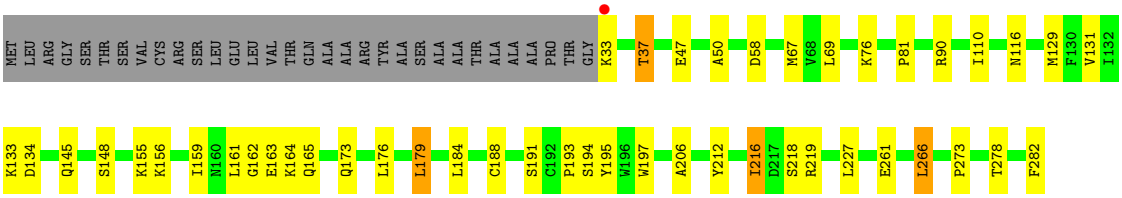


• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:

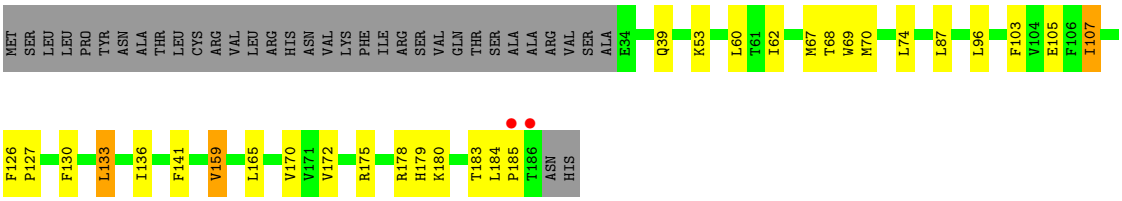
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



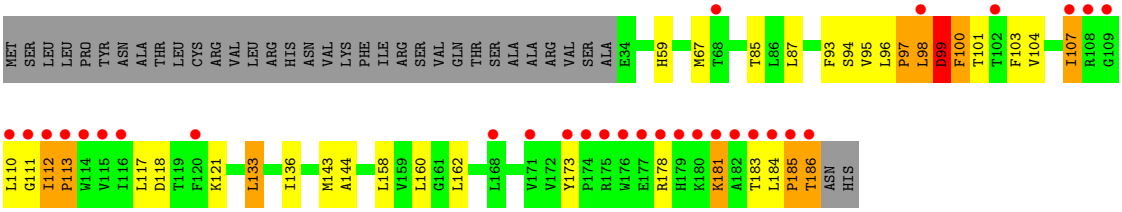
• Molecule 3: Cytochrome b-large subunit

Chain C:



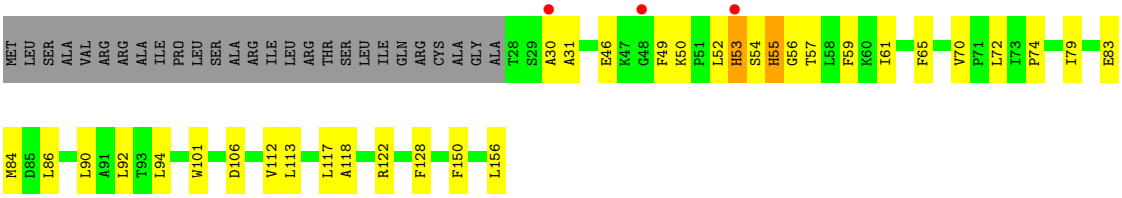
• Molecule 3: Cytochrome b-large subunit

Chain G:



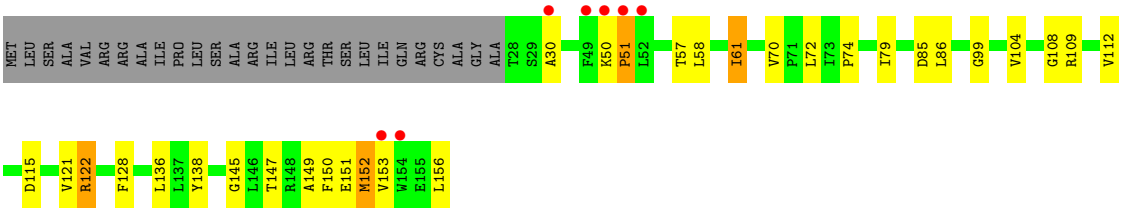
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

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	123.75Å 126.83Å 220.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (20.00-2.80) 88.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.260 0.204 , 0.259	Depositor DCC
R_{free} test set	3841 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18342	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, HEM, UQ1, FAD, SF4, F3S, FES, EPH

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	0.67	3/4889 (0.1%)	0.93	7/6605 (0.1%)
1	E	0.67	2/4889 (0.0%)	0.90	5/6605 (0.1%)
2	B	0.64	0/2029	0.86	1/2739 (0.0%)
2	F	0.69	0/2029	0.86	2/2739 (0.1%)
3	C	0.60	0/1255	0.84	0/1709
3	G	0.68	0/1255	0.87	1/1709 (0.1%)
4	D	0.71	1/1030 (0.1%)	0.88	2/1406 (0.1%)
4	H	0.60	0/1030	0.87	1/1406 (0.1%)
All	All	0.66	6/18406 (0.0%)	0.89	19/24918 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
4	D	0	1
4	H	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	172	VAL	C-O	-6.75	1.16	1.24
4	D	55	HIS	CG-ND1	-5.57	1.32	1.38
1	E	539	TRP	NE1-CE2	-5.50	1.31	1.37
1	A	539	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	539	TRP	CA-C	-5.29	1.46	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	55	HIS	N-CA-C	-7.85	97.41	109.65
4	D	53	HIS	N-CA-C	-7.39	100.30	110.35
1	A	31	ASN	N-CA-C	6.54	118.49	111.36
4	H	115	ASP	N-CA-C	6.46	118.86	111.11
1	A	425	HIS	N-CA-C	6.22	119.34	111.69

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	ALA	Peptide
2	F	162	GLY	Peptide
4	H	30	ALA	Peptide

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	4722	74	0
1	E	4787	0	4722	65	0
2	B	1985	0	2001	23	0
2	F	1985	0	2001	21	0
3	C	1217	0	1265	19	0
3	G	1217	0	1265	32	0
4	D	998	0	985	17	0
4	H	998	0	985	16	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	8	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	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	18	0	18	4	0
11	G	18	0	18	1	0
12	D	44	0	53	1	0
12	H	44	0	53	1	0
All	All	18342	0	18214	252	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 252 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:NE2	6:A:702:FAD:HM82	1.30	1.41
3:G:96:LEU:O	3:G:98:LEU:HD12	1.41	1.17
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.14	1.11
3:G:98:LEU:HD13	3:G:98:LEU:H	1.12	1.09
1:E:79:HIS:NE2	6:E:702:FAD:HM83	1.68	1.07

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%)	577 (94%)	35 (6%)	2 (0%)	36 66
1	E	614/645 (95%)	577 (94%)	36 (6%)	1 (0%)	43 72
2	B	248/282 (88%)	231 (93%)	15 (6%)	2 (1%)	16 44
2	F	248/282 (88%)	233 (94%)	14 (6%)	1 (0%)	30 60
3	C	151/188 (80%)	141 (93%)	9 (6%)	1 (1%)	18 47
3	G	151/188 (80%)	134 (89%)	10 (7%)	7 (5%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	127/156 (81%)	121 (95%)	6 (5%)	0	100	100
4	H	127/156 (81%)	119 (94%)	7 (6%)	1 (1%)	16	44
All	All	2280/2542 (90%)	2133 (94%)	132 (6%)	15 (1%)	18	47

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	185	PRO
1	A	485	GLY
2	B	116	ASN
1	E	485	GLY
3	G	97	PRO

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%)	459 (91%)	43 (9%)	10	31
1	E	502/527 (95%)	463 (92%)	39 (8%)	11	35
2	B	220/242 (91%)	204 (93%)	16 (7%)	13	38
2	F	220/242 (91%)	202 (92%)	18 (8%)	10	33
3	C	127/158 (80%)	114 (90%)	13 (10%)	7	23
3	G	127/158 (80%)	113 (89%)	14 (11%)	6	20
4	D	98/119 (82%)	85 (87%)	13 (13%)	4	14
4	H	98/119 (82%)	90 (92%)	8 (8%)	10	33
All	All	1894/2092 (90%)	1730 (91%)	164 (9%)	9	30

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	484	ASN
3	G	67	MET

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Mol	Chain	Res	Type
1	E	535	ARG
2	F	148	SER
3	G	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	252	ASN
1	E	503	HIS
4	H	142	HIS
1	E	347	GLN
1	E	358	GLN

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)

16 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	$\#\|Z\| > 2$
12	EPH	H	201	-	43,43,48	1.11	2 (4%)	45,48,53	1.16	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	F3S	B	303	2	0,9,9	-	-	-		
10	HEM	G	201	4,3	50,50,50	1.56	6 (12%)	66,82,82	1.87	16 (24%)
11	UQ1	C	202	-	18,18,18	2.13	5 (27%)	22,25,25	1.28	3 (13%)
9	F3S	F	303	2	0,9,9	-	-	-		
6	FAD	A	702	-	56,58,58	1.38	10 (17%)	81,89,89	1.93	23 (28%)
10	HEM	C	201	4,3	50,50,50	1.61	7 (14%)	66,82,82	1.70	14 (21%)
5	MLI	E	701	-	6,6,6	1.00	0	7,7,7	1.44	1 (14%)
6	FAD	E	702	-	56,58,58	1.50	9 (16%)	81,89,89	1.93	21 (25%)
12	EPH	D	201	-	43,43,48	1.08	2 (4%)	45,48,53	1.16	5 (11%)
7	FES	F	301	2	0,4,4	-	-	-		
8	SF4	B	302	2	0,12,12	-	-	-		
11	UQ1	G	202	-	18,18,18	2.16	6 (33%)	22,25,25	1.09	2 (9%)
7	FES	B	301	2	0,4,4	-	-	-		
8	SF4	F	302	2	0,12,12	-	-	-		
5	MLI	A	701	-	6,6,6	1.08	0	7,7,7	1.34	1 (14%)

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
12	EPH	H	201	-	-	29/47/47/52	-
9	F3S	B	303	2	-	-	0/3/3/3
10	HEM	G	201	4,3	-	6/14/54/54	-
11	UQ1	C	202	-	-	4/9/33/33	0/1/1/1
9	F3S	F	303	2	-	-	0/3/3/3
6	FAD	A	702	-	-	7/34/50/50	0/6/6/6
10	HEM	C	201	4,3	-	3/14/54/54	-
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	E	702	-	-	4/34/50/50	0/6/6/6
12	EPH	D	201	-	-	24/47/47/52	-
7	FES	F	301	2	-	-	0/1/1/1
8	SF4	B	302	2	-	-	0/6/5/5
11	UQ1	G	202	-	-	0/9/33/33	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/4/4/4	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	FE-NB	5.55	2.12	1.94
10	C	201	HEM	FE-NB	5.35	2.11	1.94
11	C	202	UQ1	CM5-C5	-5.35	1.39	1.50
6	E	702	FAD	C9A-C5X	5.26	1.50	1.41
12	H	201	EPH	O1-C3	4.67	1.47	1.34

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	702	FAD	C5A-C4A-N3A	-6.36	118.45	126.75
6	A	702	FAD	C5A-C4A-N3A	-5.33	119.80	126.75
10	G	201	HEM	CAD-C3D-C4D	5.26	133.86	124.66
6	E	702	FAD	N3A-C4A-N9A	5.21	135.67	127.08
6	E	702	FAD	N3A-C2A-N1A	-4.60	121.41	128.60

There are no chirality outliers.

5 of 77 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	PA-O3P-P-O5'
6	E	702	FAD	N10-C1'-C2'-O2'
10	G	201	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

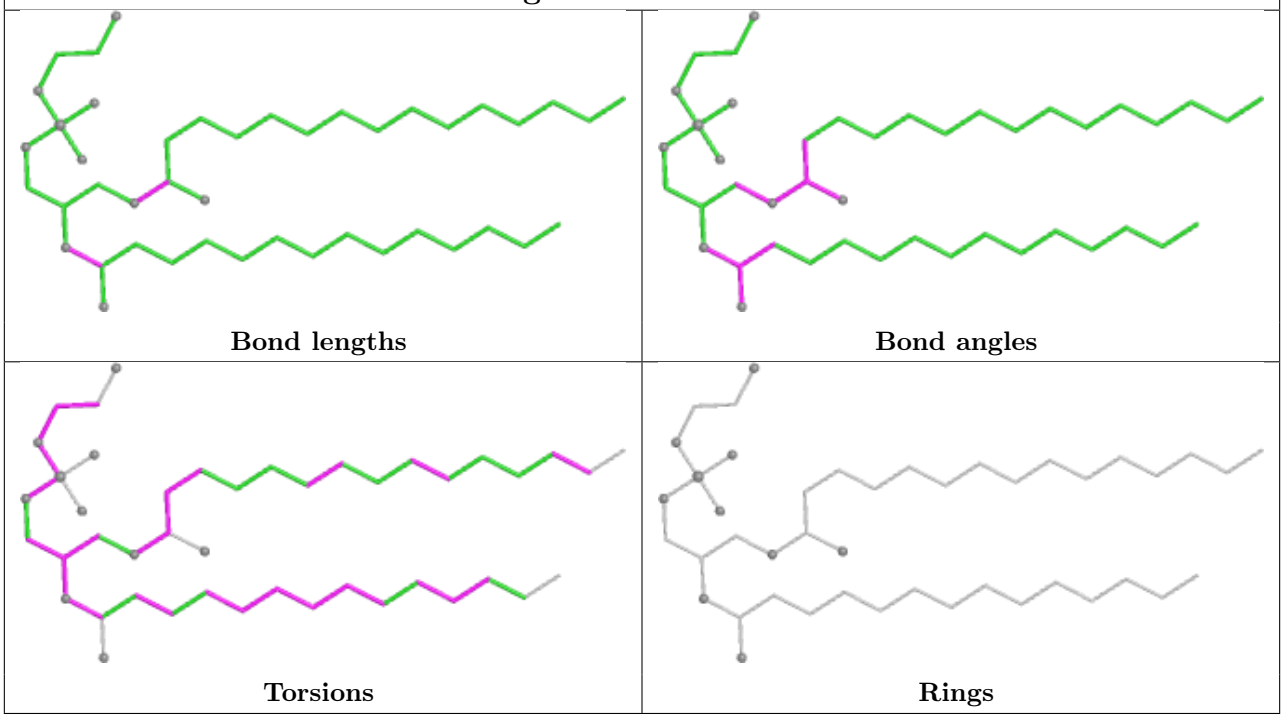
10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	201	EPH	1	0
10	G	201	HEM	4	0
11	C	202	UQ1	4	0
6	A	702	FAD	9	0
10	C	201	HEM	2	0
5	E	701	MLI	1	0
6	E	702	FAD	8	0
12	D	201	EPH	1	0
11	G	202	UQ1	1	0
5	A	701	MLI	1	0

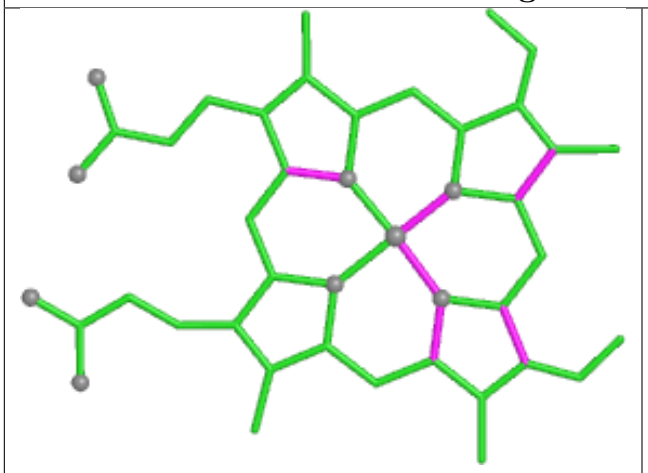
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

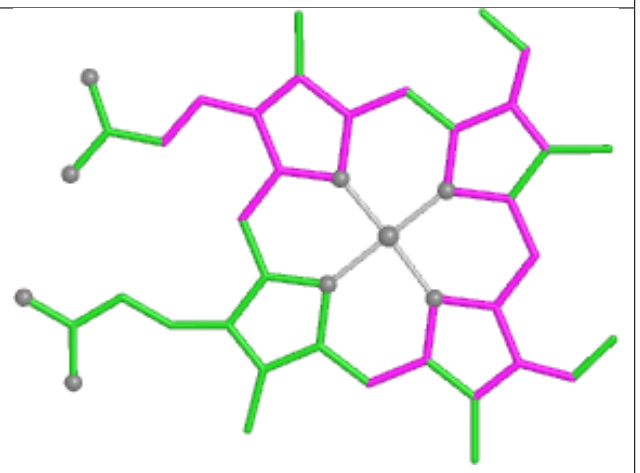
Ligand EPH H 201



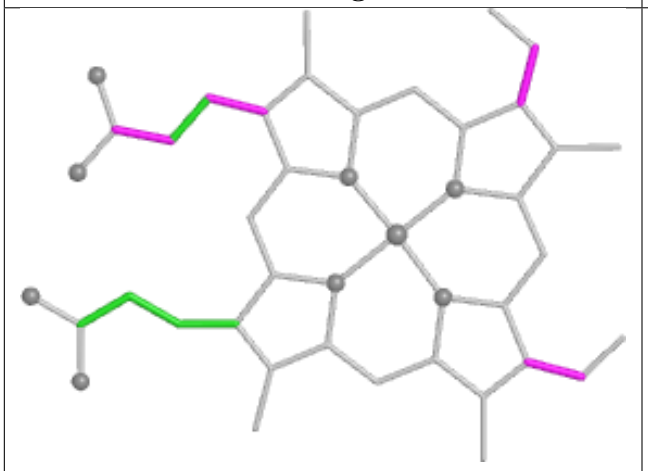
Ligand HEM G 201



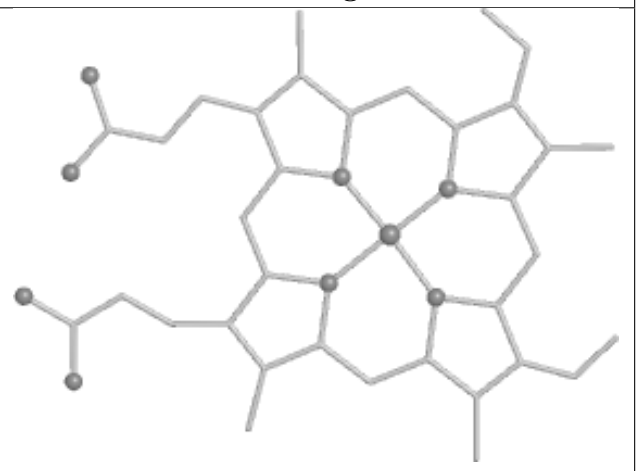
Bond lengths



Bond angles

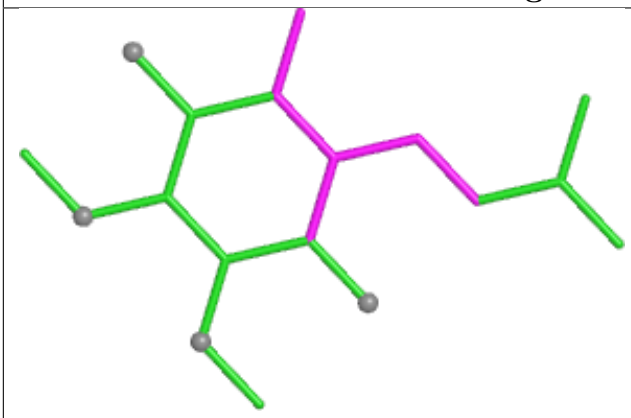


Torsions



Rings

Ligand UQ1 C 202



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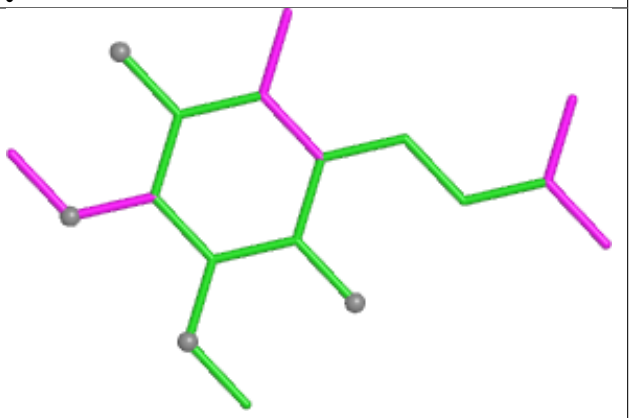

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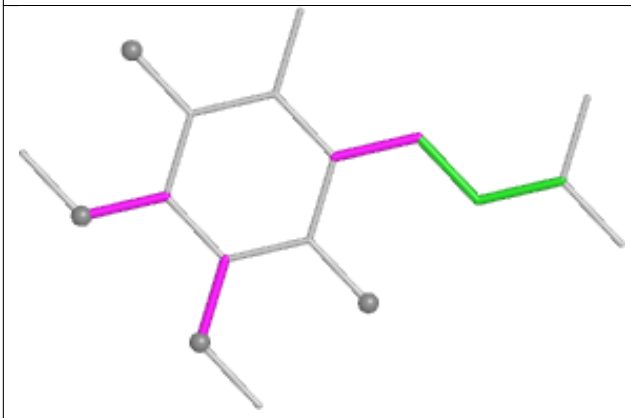
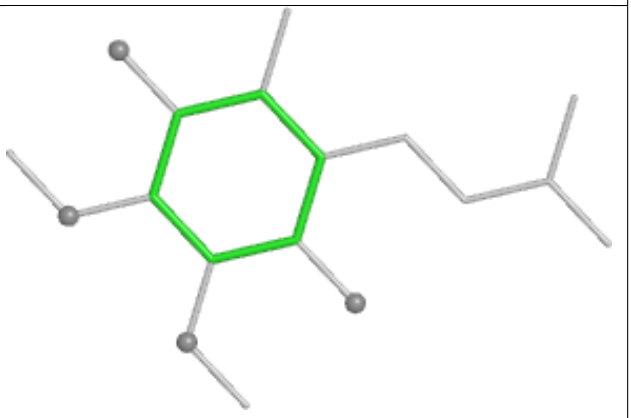
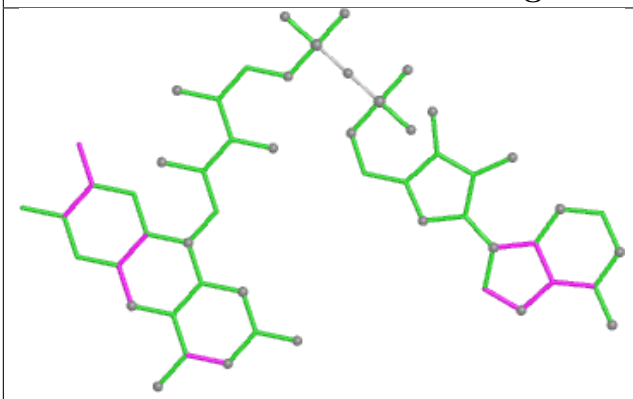


Torsions

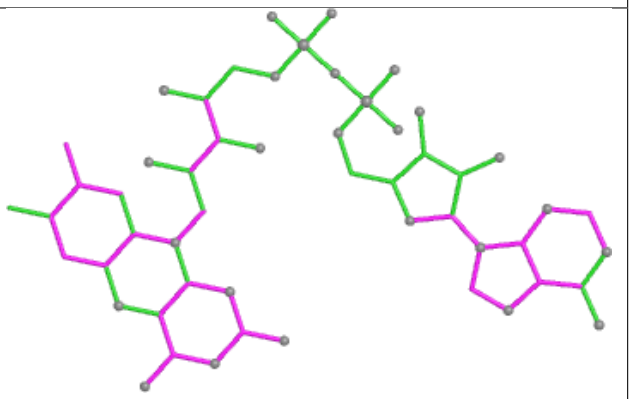


Rings

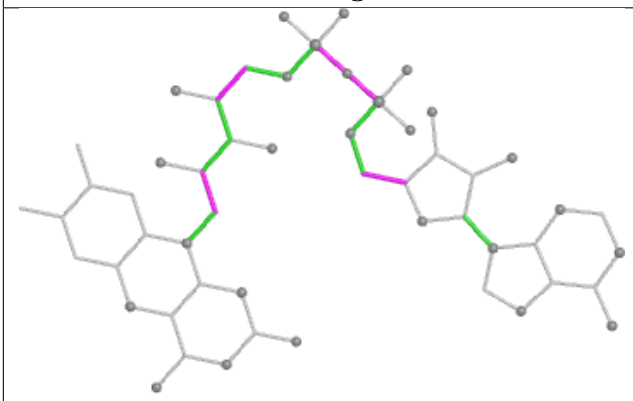
Ligand FAD A 702



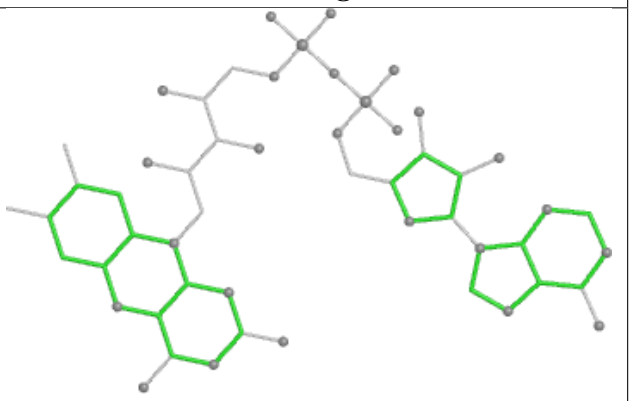
Bond lengths



Bond angles

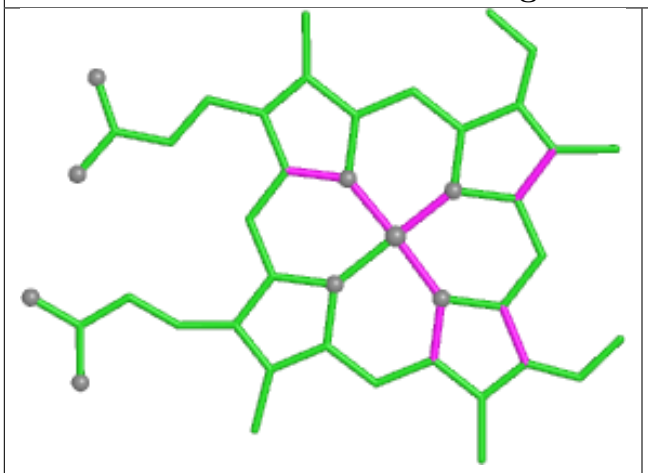


Torsions

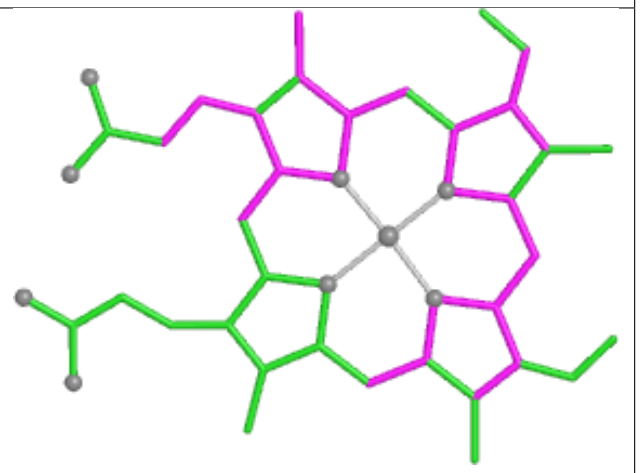


Rings

Ligand HEM C 201



Bond lengths



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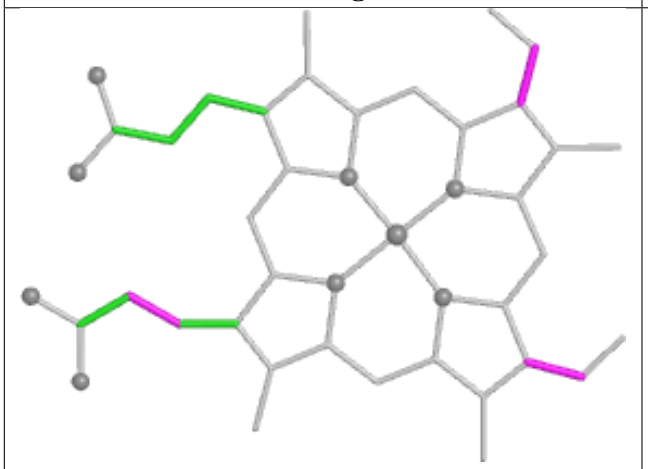
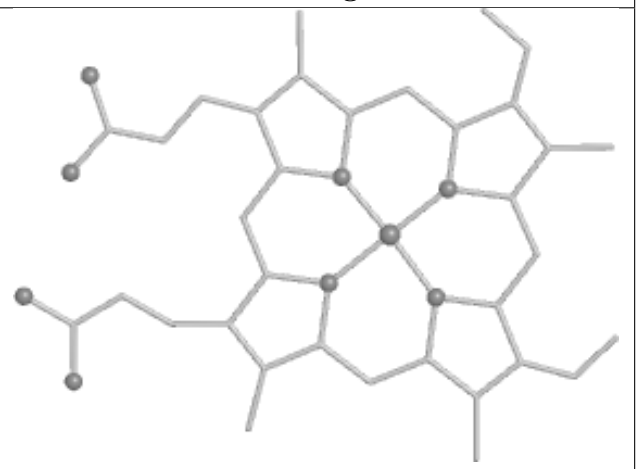
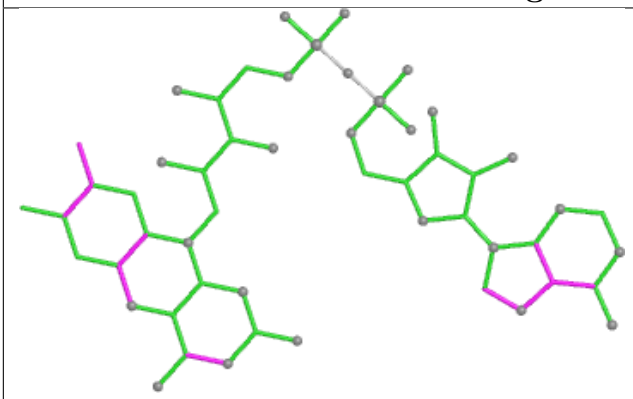


Torsions



Rings

Ligand FAD E 702



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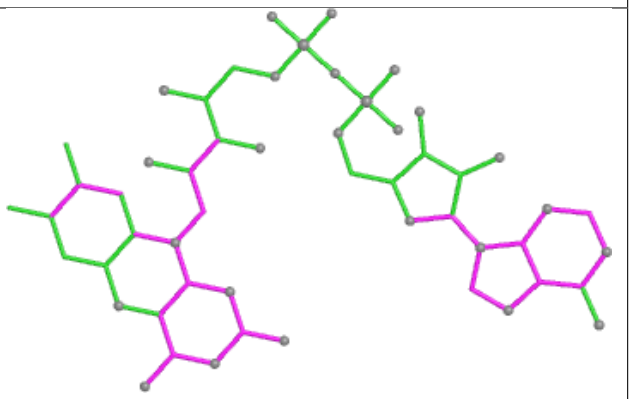
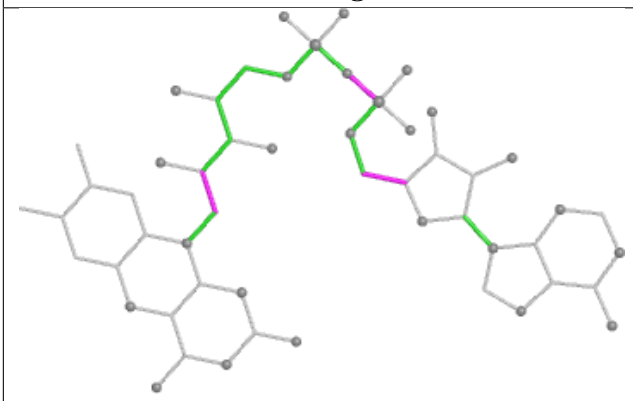
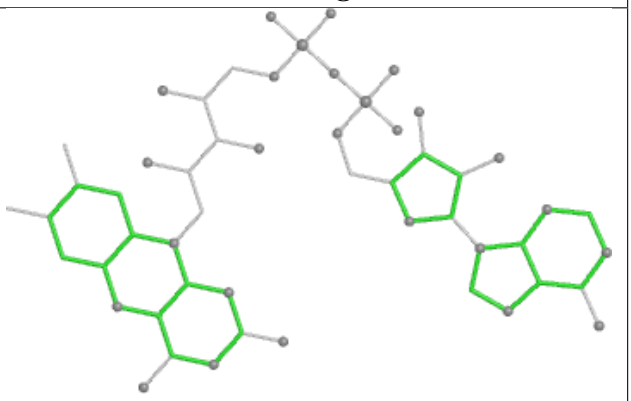


Bond angles

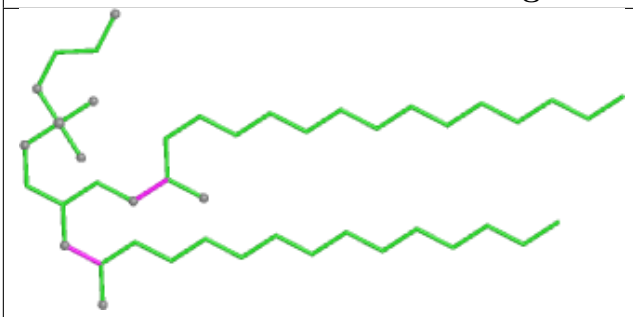


Torsions



Rings

Ligand EPH D 201



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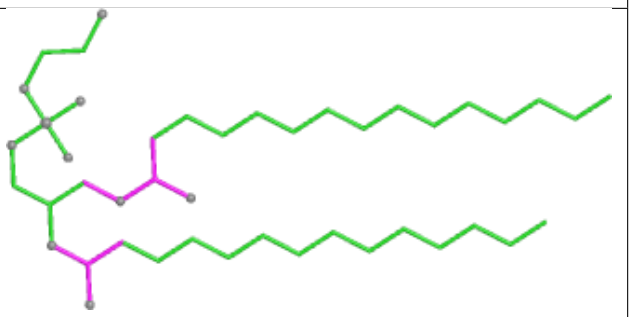
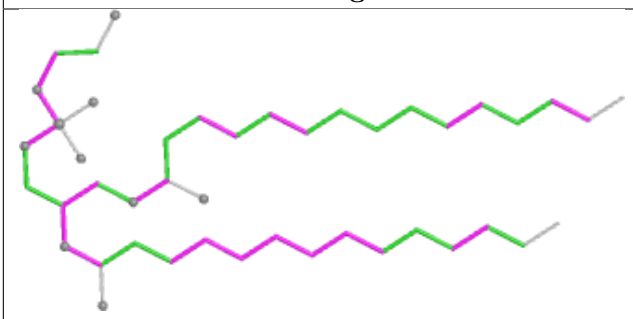
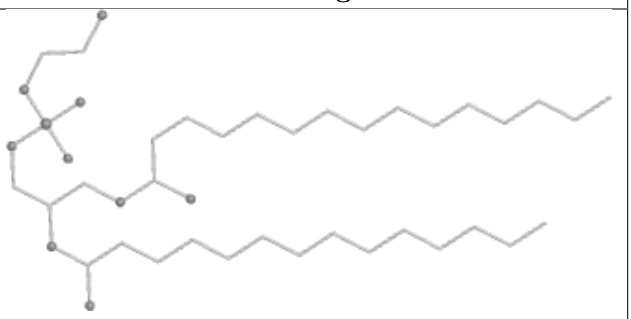


Bond angles

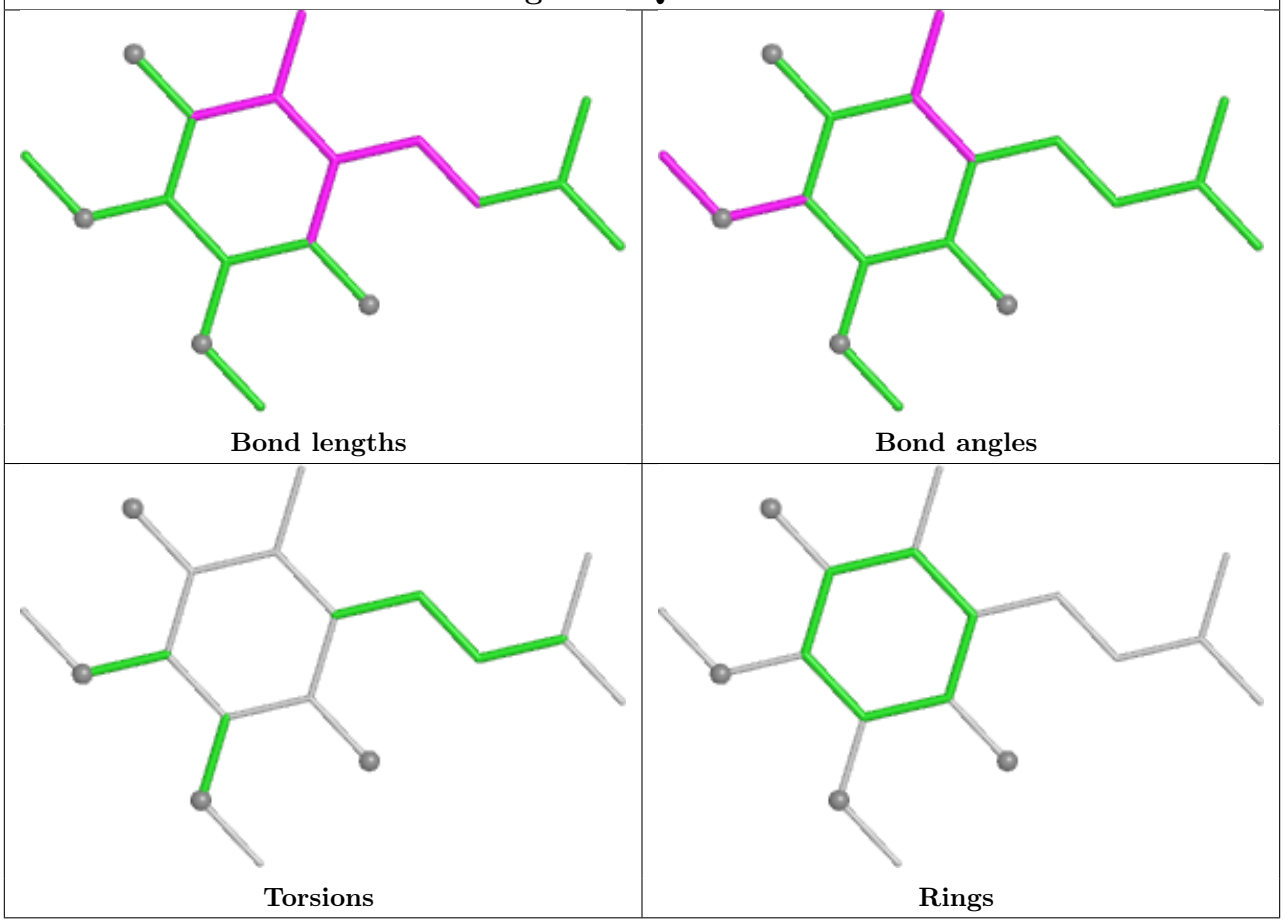


Torsions



Rings

Ligand UQ1 G 202



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%)	-0.25	3 (0%)	87	82	18, 46, 71, 98	1 (0%)
1	E	616/645 (95%)	-0.29	2 (0%)	90	86	24, 45, 71, 98	1 (0%)
2	B	250/282 (88%)	-0.17	2 (0%)	82	75	28, 44, 74, 93	0
2	F	250/282 (88%)	-0.30	1 (0%)	88	84	24, 42, 66, 83	0
3	C	153/188 (81%)	0.16	2 (1%)	75	66	36, 59, 89, 121	0
3	G	153/188 (81%)	0.73	30 (19%)	3	2	34, 64, 153, 181	0
4	D	129/156 (82%)	0.29	3 (2%)	61	51	45, 60, 96, 118	0
4	H	129/156 (82%)	0.29	7 (5%)	31	24	38, 59, 104, 131	0
All	All	2296/2542 (90%)	-0.10	50 (2%)	62	52	18, 48, 84, 181	2 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	115	VAL	6.5
1	A	499	THR	5.9
3	G	114	TRP	5.8
3	G	185	PRO	5.4
3	G	184	LEU	5.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

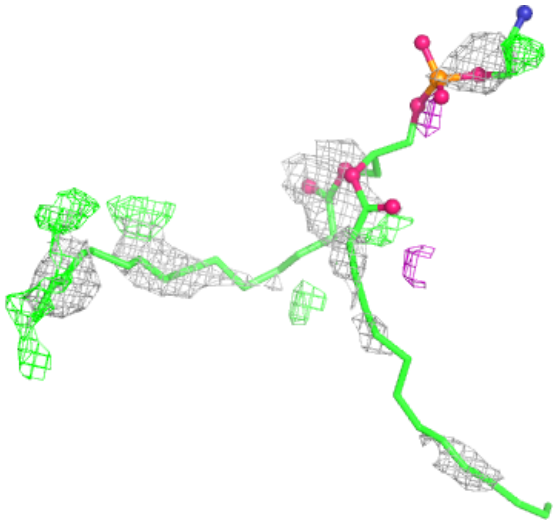
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

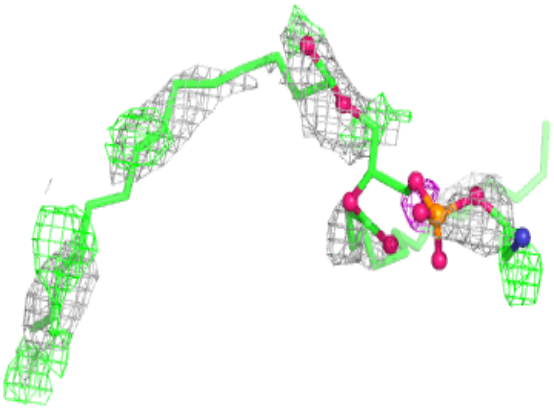
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	EPH	H	201	44/49	0.69	0.39	56,72,103,105	44
11	UQ1	C	202	18/18	0.72	0.28	63,68,71,72	18
12	EPH	D	201	44/49	0.76	0.30	42,56,72,75	44
11	UQ1	G	202	18/18	0.76	0.24	52,63,67,68	18
5	MLI	E	701	7/7	0.93	0.09	31,33,34,35	0
10	HEM	G	201	43/43	0.94	0.12	50,66,75,84	0
10	HEM	C	201	43/43	0.96	0.12	49,65,74,83	0
6	FAD	E	702	53/53	0.96	0.07	25,28,33,35	0
9	F3S	F	303	7/7	0.96	0.06	30,37,43,47	0
5	MLI	A	701	7/7	0.97	0.07	42,43,44,44	0
9	F3S	B	303	7/7	0.97	0.05	36,40,46,46	0
6	FAD	A	702	53/53	0.97	0.06	21,24,31,33	0
8	SF4	F	302	8/8	0.98	0.05	25,27,30,30	0
7	FES	B	301	4/4	0.98	0.04	29,30,33,33	0
8	SF4	B	302	8/8	0.98	0.04	27,29,31,33	0
7	FES	F	301	4/4	0.99	0.04	29,29,32,34	0

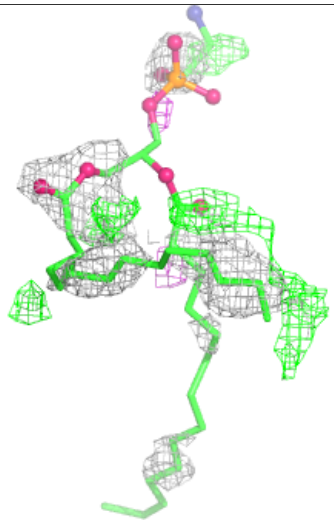
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EPH H 201:

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

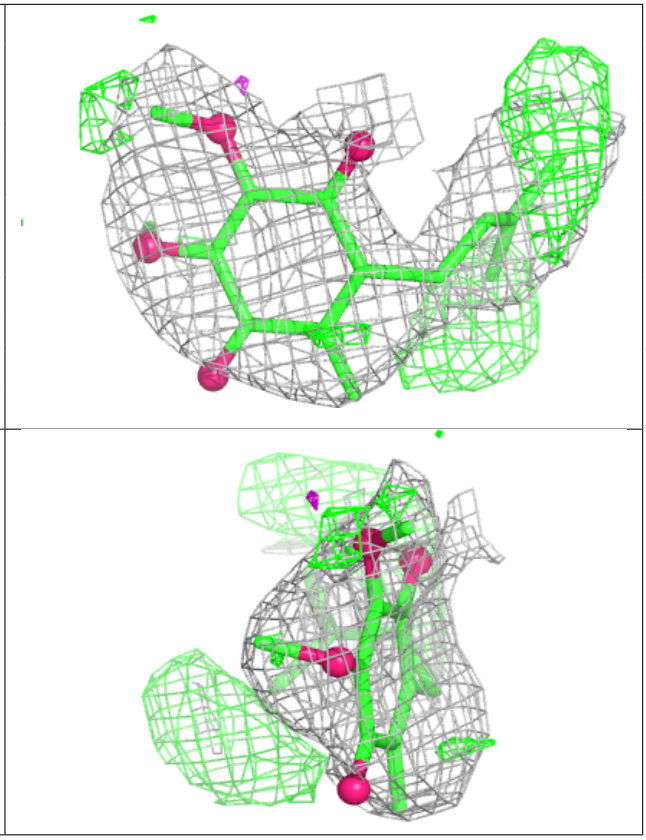






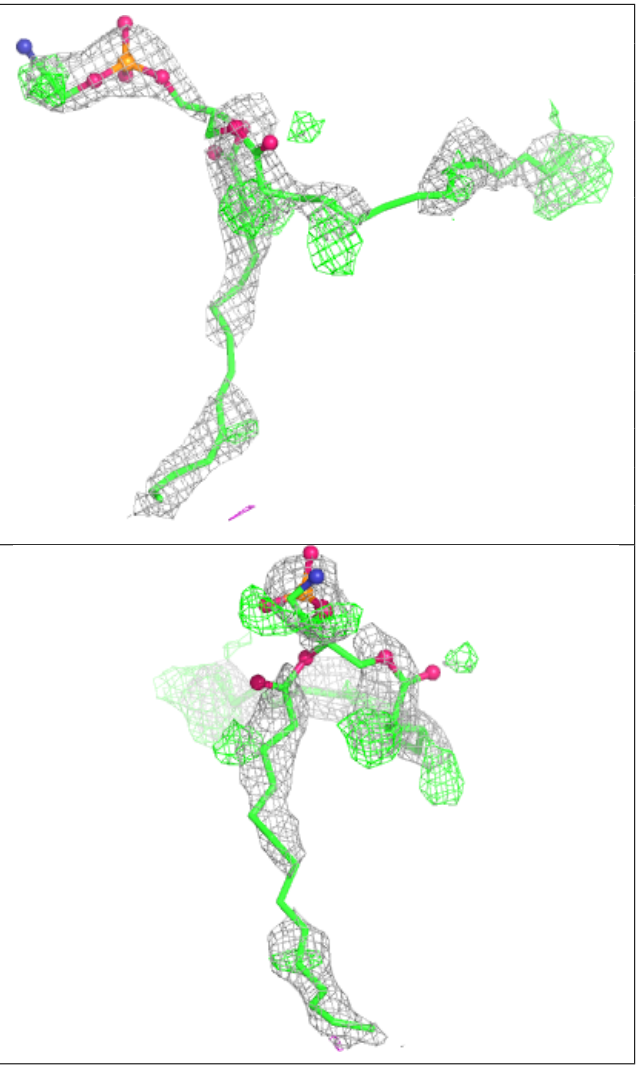
Electron density around UQ1 C 202:

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



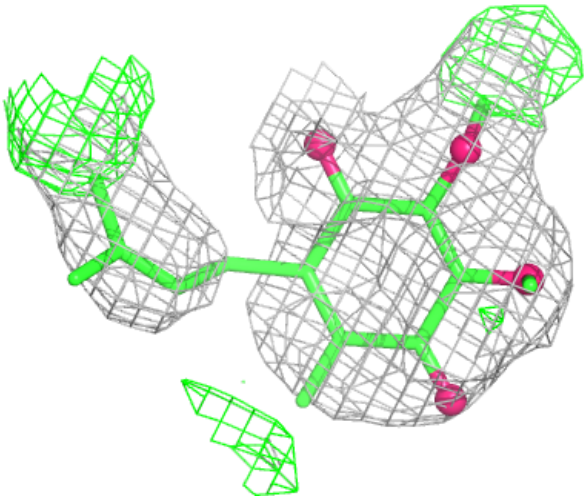
Electron density around EPH D 201:

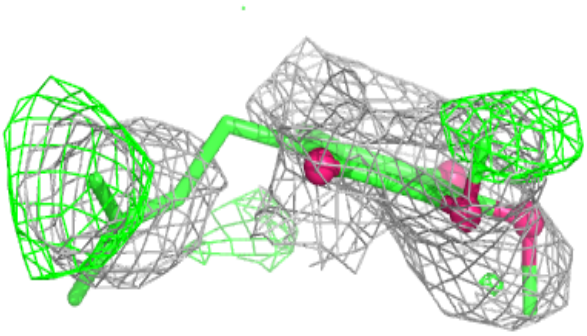
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

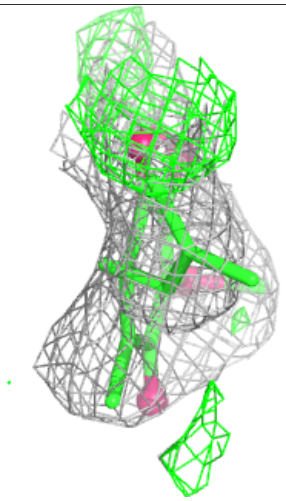


Electron density around UQ1 G 202:

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

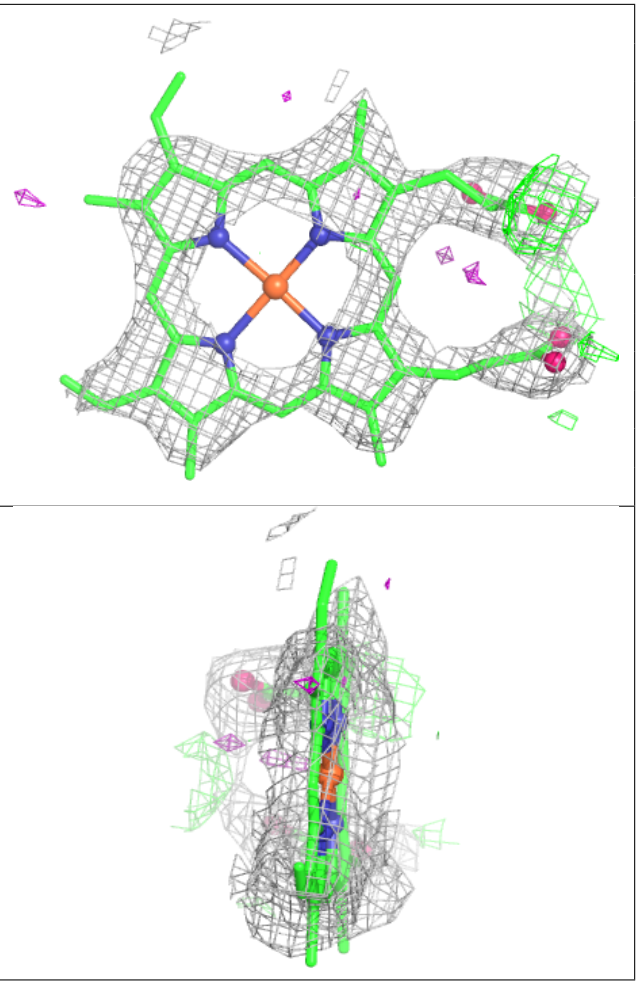






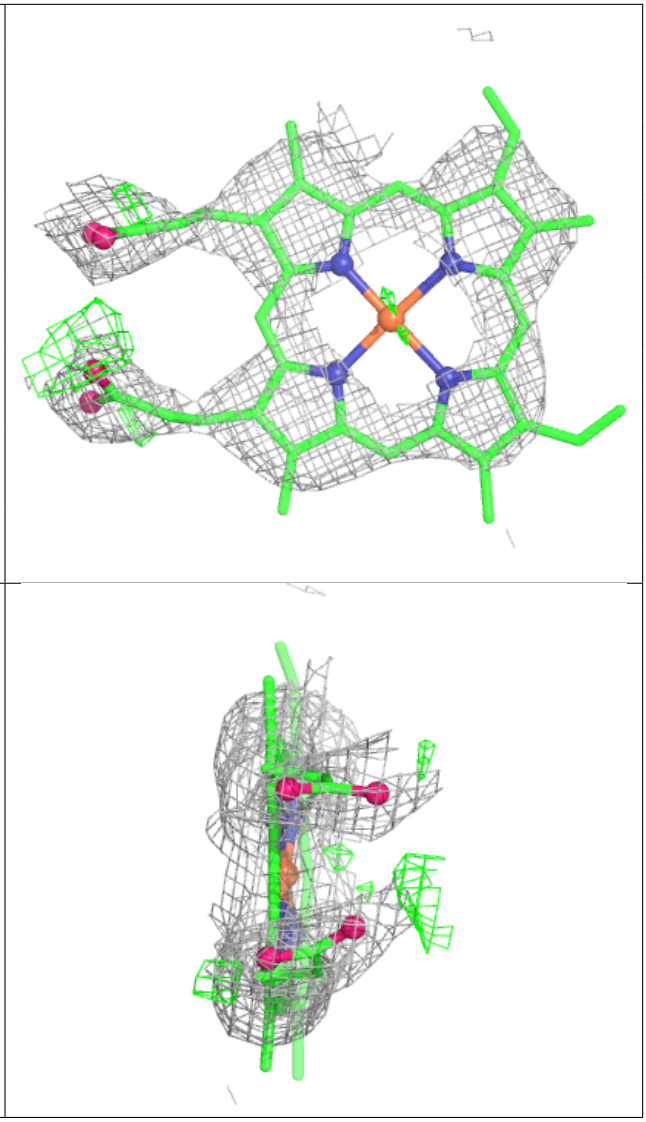
Electron density around HEM G 201:

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



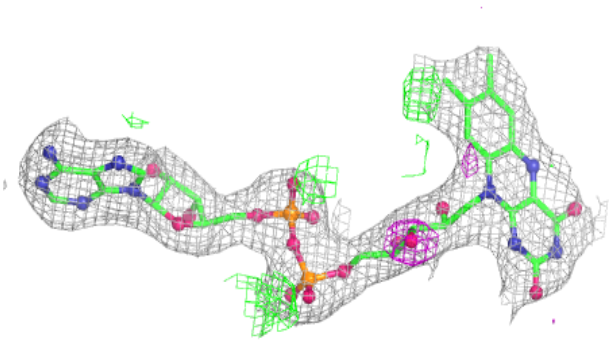
Electron density around HEM C 201:

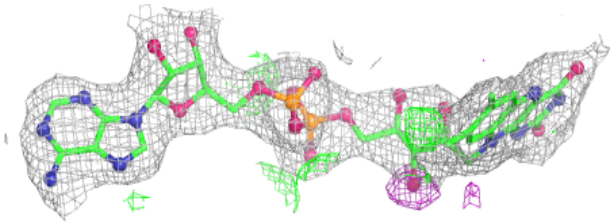
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

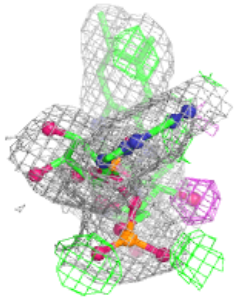


Electron density around FAD E 702:

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

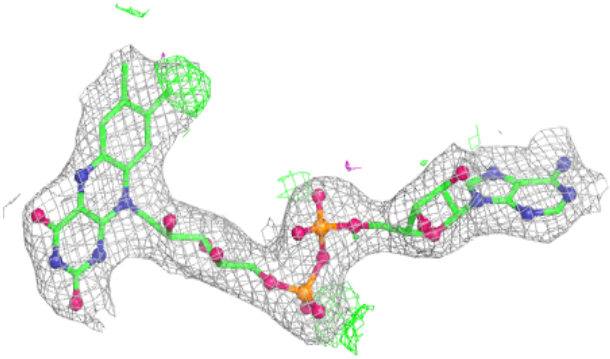


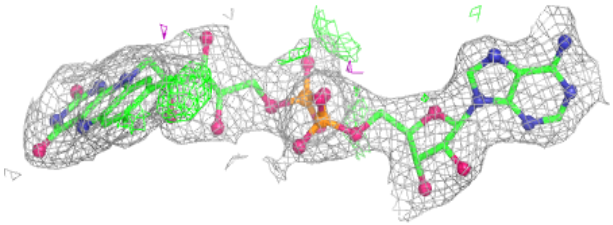


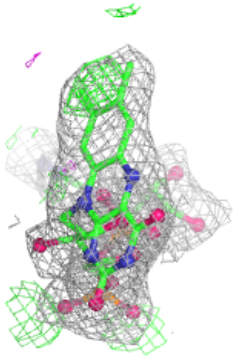


Electron density around FAD A 702:

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







6.5 Other polymers (i)

There are no such residues in this entry.