wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2024 – 07:58 AM JST

PDB ID	:	4YSZ
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with 2-iodo-N-[3-(1-methylethoxy)phenyl]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	:	2015-03-17
Resolution	:	3.30 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:

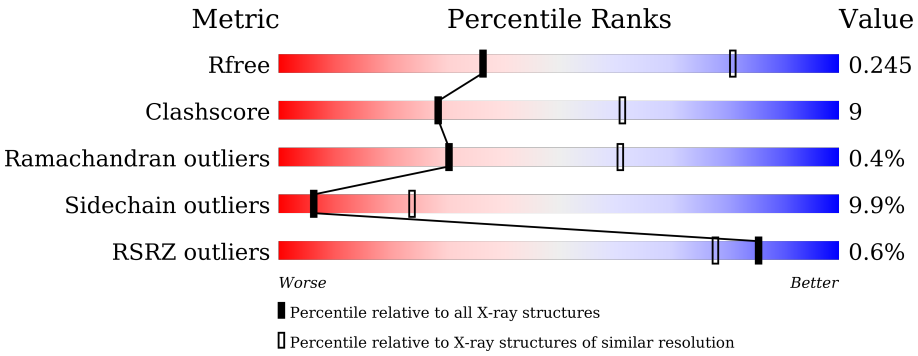
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.30 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	76% 18% • •
2	B	282	71% 16% • 11%
2	F	282	72% 13% • 11%
3	C	188	% 64% 14% • 19%

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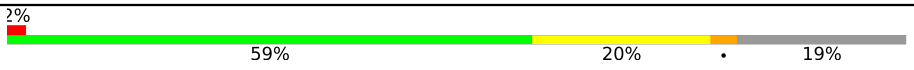
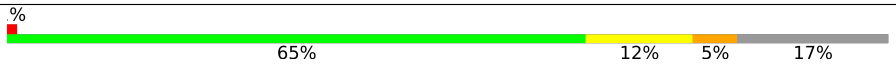
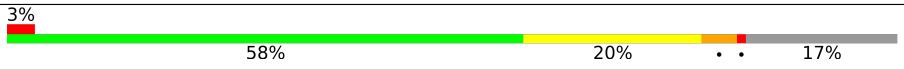
Mol	Chain	Length	Quality of chain
3	G	188	
4	D	156	
4	H	156	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	E	701	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18361 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
1	A	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			
1	E	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			

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

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

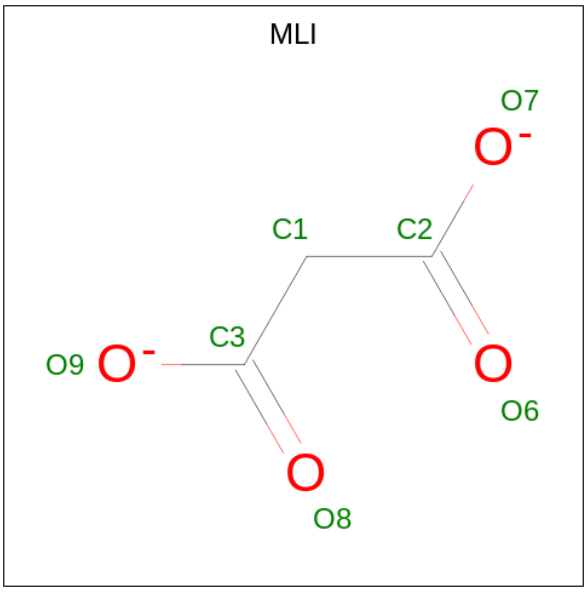
- Molecule 3 is a protein called Cytochrome b-large subunit.

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

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

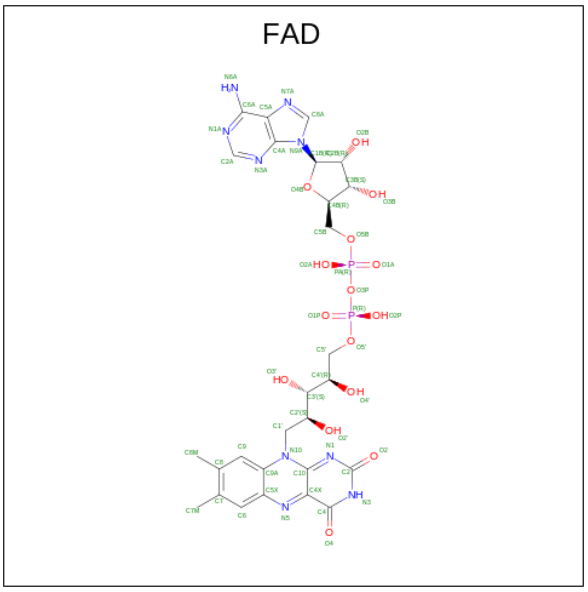
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

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



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

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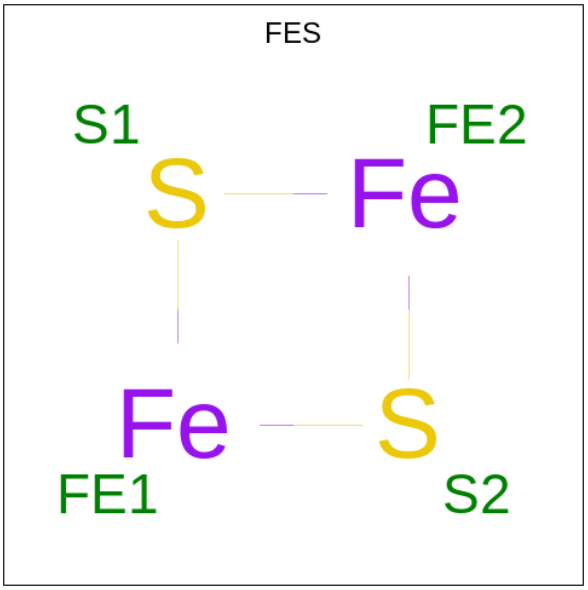
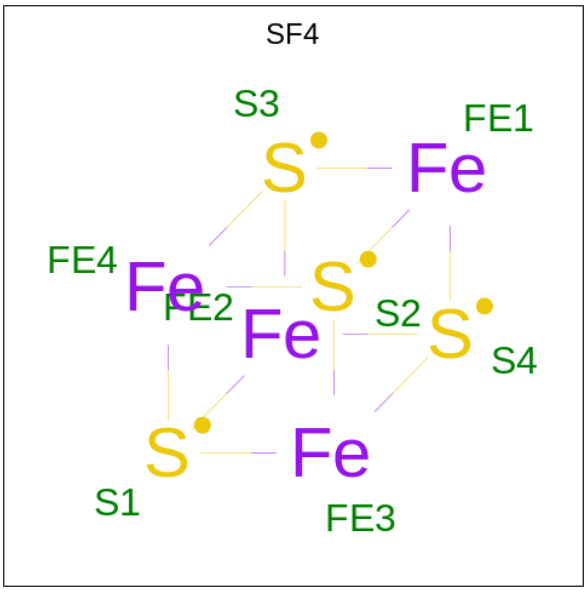
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



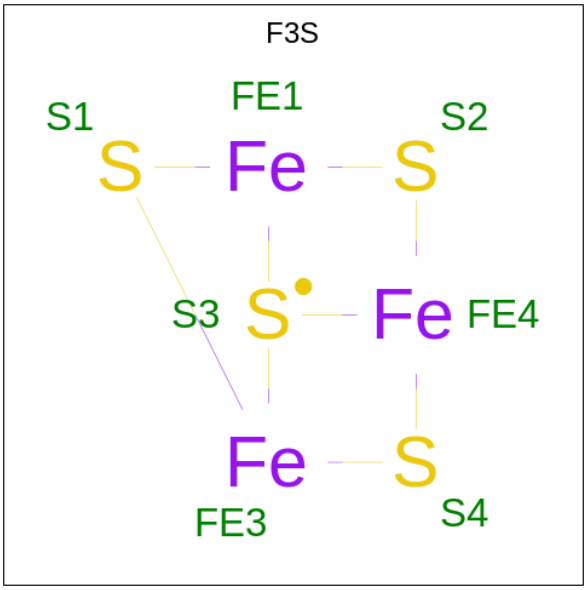
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Fe	S		0	0
			4	2	2			
7	F	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



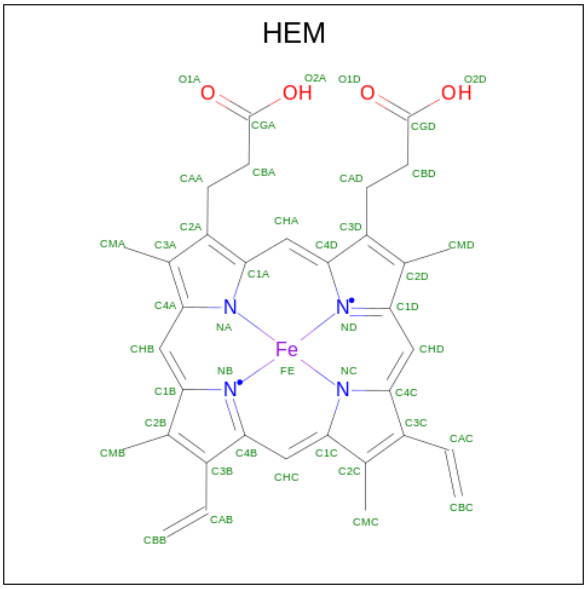
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 8 4 4	0	0
8	F	1	Total Fe S 8 4 4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



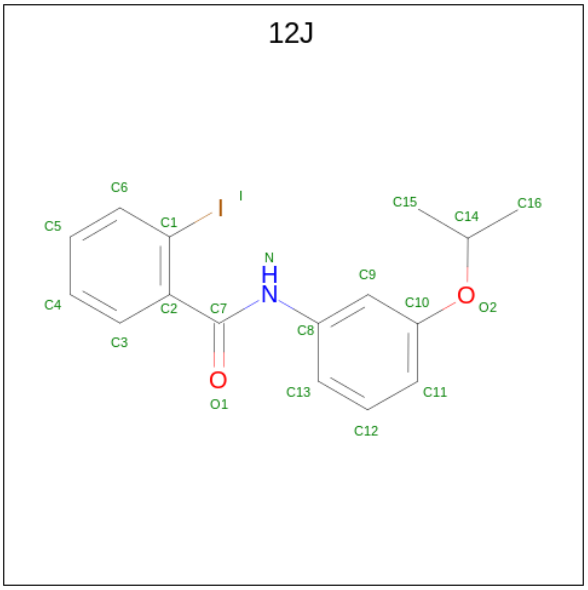
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0
9	F	1	Total Fe S 7 3 4	0	0

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



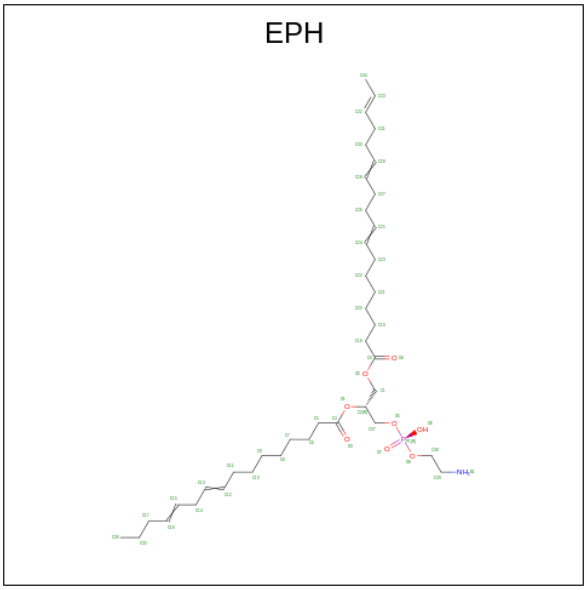
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 2-iodo-N-[3-(1-methylethoxy)phenyl]benzamide (three-letter code: 12J) (formula: $C_{16}H_{16}INO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	I	N	O	0	0
			20	16	1	1	2		
11	G	1	Total	C	I	N	O	0	0
			20	16	1	1	2		

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



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	O	0	0
			4	4		
13	B	2	Total	O	0	0
			2	2		
13	C	1	Total	O	0	0
			1	1		
13	D	1	Total	O	0	0
			1	1		
13	E	6	Total	O	0	0
			6	6		

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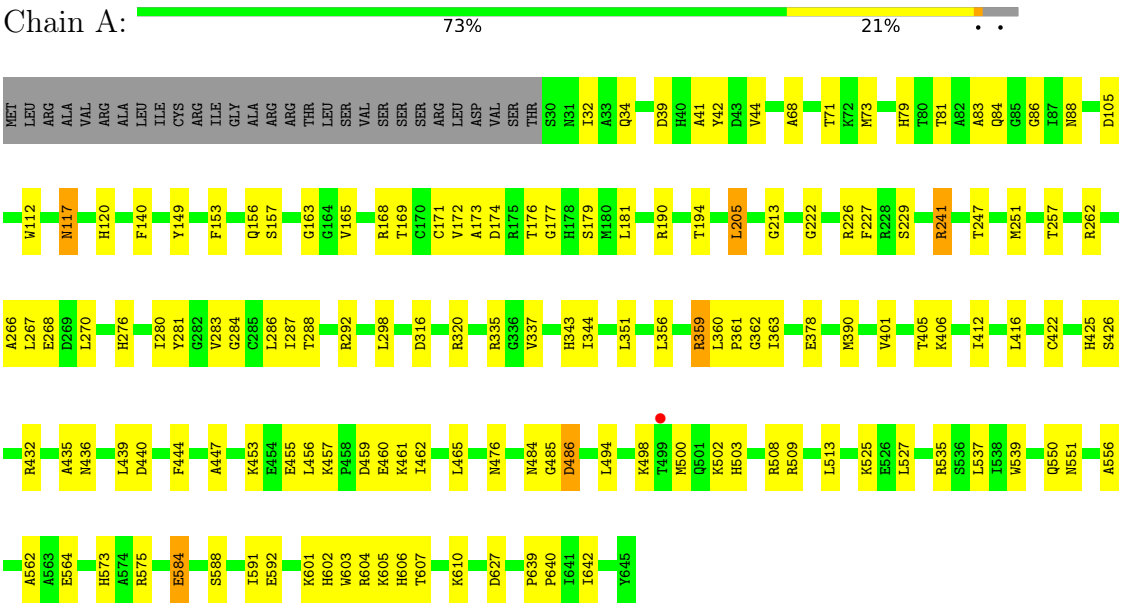
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total O 1 1	0	0

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.

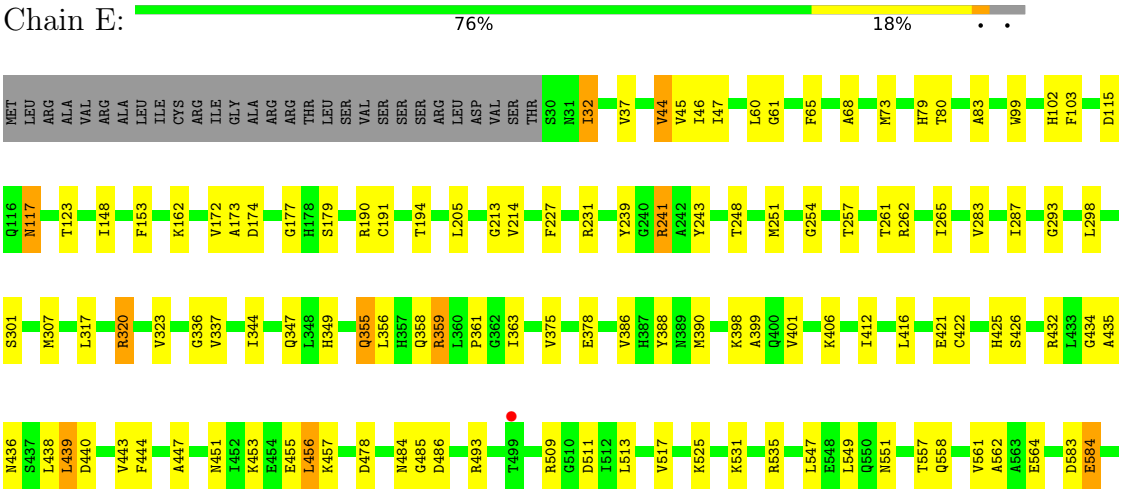
• Molecule 1: Succinate dehydrogenase flavoprotein

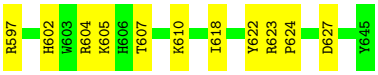
Chain A:



• Molecule 1: Succinate dehydrogenase flavoprotein

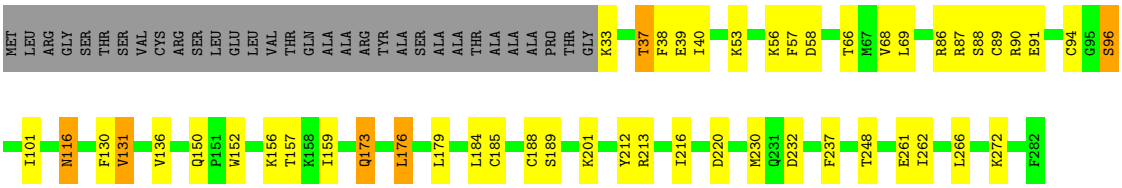
Chain E:





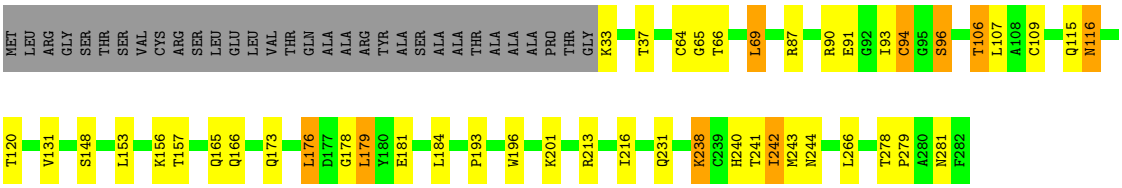
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



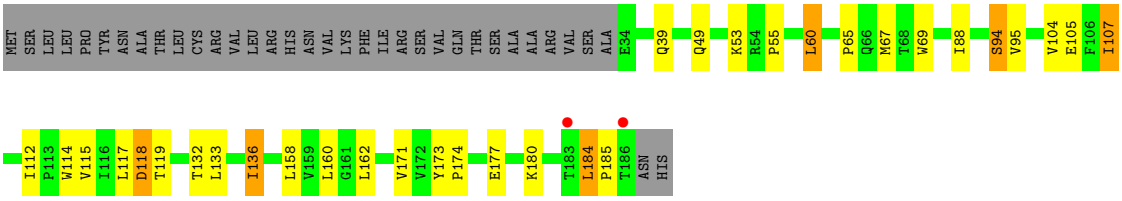
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



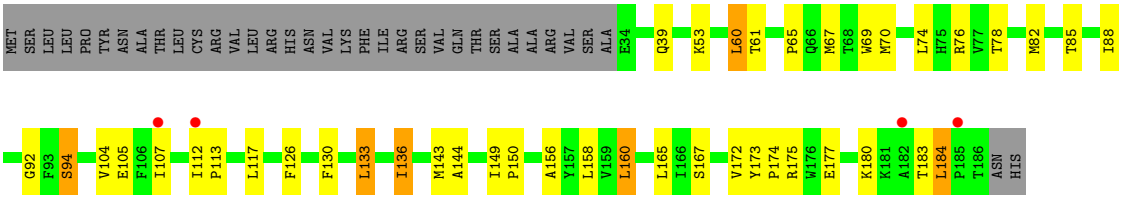
• Molecule 3: Cytochrome b-large subunit

Chain C:



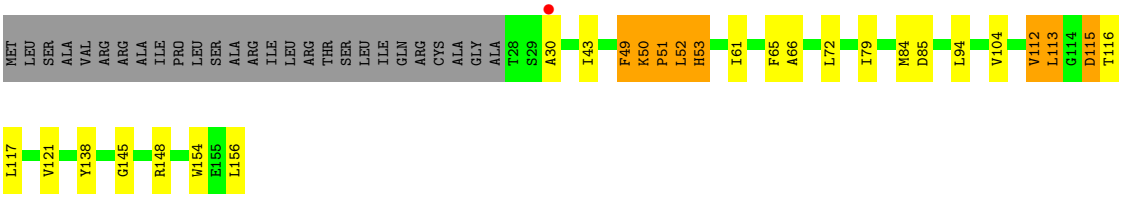
• Molecule 3: Cytochrome b-large subunit

Chain G:



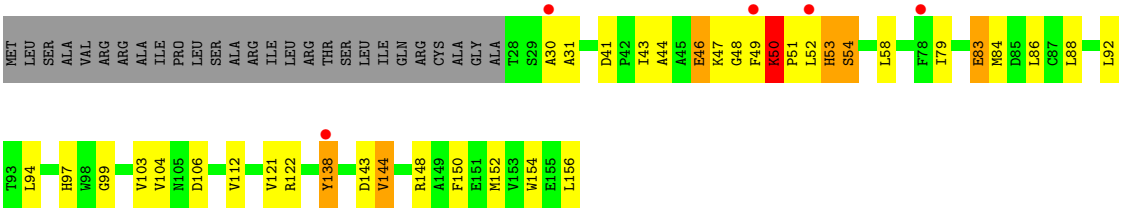
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

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	123.93Å 126.97Å 219.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.30 29.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.82-3.30) 97.3 (29.82-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.250 0.180 , 0.245	Depositor DCC
R_{free} test set	2624 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18361	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MLI, SF4, FES, EPH, FAD, 12J, F3S, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/4889	0.68	0/6605
1	E	0.45	0/4889	0.68	0/6605
2	B	0.43	0/2029	0.66	0/2739
2	F	0.47	1/2029 (0.0%)	0.64	0/2739
3	C	0.43	0/1255	0.62	0/1709
3	G	0.44	0/1255	0.63	0/1709
4	D	0.51	0/1030	0.65	0/1406
4	H	0.51	0/1030	0.64	0/1406
All	All	0.45	1/18406 (0.0%)	0.66	0/24918

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
4	D	0	1
4	H	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	CYS	C-N	5.55	1.43	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	ALA	Peptide
4	H	30	ALA	Peptide
4	H	50	LYS	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	4720	71	0
1	E	4787	0	4720	77	0
2	B	1985	0	2001	19	0
2	F	1985	0	2001	21	0
3	C	1217	0	1265	25	0
3	G	1217	0	1265	23	0
4	D	998	0	985	44	0
4	H	998	0	985	47	0
5	A	7	0	2	1	0
5	E	7	0	2	2	0
6	A	53	0	31	4	0
6	E	53	0	31	5	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	6	0
10	G	43	0	30	5	0
11	C	20	0	16	4	0
11	G	20	0	16	4	0
12	D	44	0	53	0	0
12	H	44	0	53	2	0
13	A	4	0	0	0	0
13	B	2	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
All	All	18361	0	18206	318	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 9.

The worst 5 of 318 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)
4:D:112:VAL:C	4:D:113:LEU:HD23	1.39	1.39
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.48	1.28
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.52	1.23
4:D:112:VAL:HG12	4:D:113:LEU:CD2	1.77	1.13
4:H:50:LYS:N	4:H:50:LYS:HD2	1.59	1.12

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%)	573 (93%)	39 (6%)	2 (0%)	37	66
1	E	614/645 (95%)	583 (95%)	30 (5%)	1 (0%)	44	71
2	B	248/282 (88%)	232 (94%)	14 (6%)	2 (1%)	16	46
2	F	248/282 (88%)	231 (93%)	16 (6%)	1 (0%)	30	61
3	C	151/188 (80%)	142 (94%)	9 (6%)	0	100	100
3	G	151/188 (80%)	140 (93%)	10 (7%)	1 (1%)	19	50
4	D	127/156 (81%)	120 (94%)	6 (5%)	1 (1%)	16	46
4	H	127/156 (81%)	123 (97%)	4 (3%)	0	100	100
All	All	2280/2542 (90%)	2144 (94%)	128 (6%)	8 (0%)	30	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY

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Mol	Chain	Res	Type
1	E	80	THR
2	B	88	SER
2	B	232	ASP
3	G	113	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%)	456 (91%)	46 (9%)	7 26
1	E	502/527 (95%)	465 (93%)	37 (7%)	11 34
2	B	220/242 (91%)	197 (90%)	23 (10%)	5 21
2	F	220/242 (91%)	194 (88%)	26 (12%)	4 17
3	C	127/158 (80%)	114 (90%)	13 (10%)	6 23
3	G	127/158 (80%)	112 (88%)	15 (12%)	4 17
4	D	98/119 (82%)	86 (88%)	12 (12%)	4 16
4	H	98/119 (82%)	82 (84%)	16 (16%)	2 9
All	All	1894/2092 (90%)	1706 (90%)	188 (10%)	6 24

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	406	LYS
2	F	120	THR
1	E	439	LEU
1	E	610	LYS
2	F	184	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	484	ASN

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Mol	Chain	Res	Type
2	F	115	GLN
1	E	503	HIS
2	F	55	GLN
2	F	145	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	D	201	-	43,43,48	1.11	2 (4%)	45,48,53	1.11	4 (8%)
6	FAD	E	702	-	53,58,58	1.33	5 (9%)	68,89,89	1.70	17 (25%)
7	FES	F	301	2	0,4,4	-	-	-		
10	HEM	C	201	3,4	41,50,50	1.40	6 (14%)	45,82,82	2.15	18 (40%)
11	12J	C	202	-	21,21,21	1.50	2 (9%)	28,28,28	1.19	2 (7%)
12	EPH	H	201	-	43,43,48	1.18	2 (4%)	45,48,53	1.21	5 (11%)
9	F3S	B	303	2	0,9,9	-	-	-		
11	12J	G	202	-	21,21,21	1.36	2 (9%)	28,28,28	2.04	2 (7%)

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	-	-	-		
10	HEM	G	201	3,4	41,50,50	1.45	8 (19%)	45,82,82	2.15	16 (35%)
5	MLI	A	701	-	6,6,6	1.15	0	7,7,7	1.08	0
8	SF4	F	302	2	0,12,12	-	-	-		
7	FES	B	301	2	0,4,4	-	-	-		
5	MLI	E	701	-	6,6,6	1.08	0	7,7,7	1.09	0
6	FAD	A	702	-	53,58,58	1.26	4 (7%)	68,89,89	1.49	12 (17%)
9	F3S	F	303	2	0,9,9	-	-	-		

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	D	201	-	-	22/47/47/52	-
6	FAD	E	702	-	-	4/30/50/50	0/6/6/6
11	12J	C	202	-	-	4/12/12/12	0/2/2/2
10	HEM	C	201	3,4	-	4/12/54/54	-
7	FES	F	301	2	-	-	0/1/1/1
12	EPH	H	201	-	-	27/47/47/52	-
9	F3S	B	303	2	-	-	0/3/3/3
11	12J	G	202	-	-	3/12/12/12	0/2/2/2
10	HEM	G	201	3,4	-	5/12/54/54	-
8	SF4	B	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/4/4/4	-
8	SF4	F	302	2	-	-	0/6/5/5
7	FES	B	301	2	-	-	0/1/1/1
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	A	702	-	-	6/30/50/50	0/6/6/6
9	F3S	F	303	2	-	-	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C9A-C5X	5.27	1.50	1.41
12	H	201	EPH	O2-C4	4.91	1.47	1.33
11	C	202	12J	C2-C7	-4.82	1.40	1.50
6	A	702	FAD	C9A-C5X	4.81	1.49	1.41
12	H	201	EPH	O1-C3	4.60	1.47	1.34

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	202	12J	C10-O2-C14	9.20	131.15	119.37
10	G	201	HEM	CAD-C3D-C4D	5.87	134.92	124.66
10	C	201	HEM	C1B-NB-C4B	5.38	110.63	105.07
10	C	201	HEM	CAD-C3D-C4D	5.18	133.71	124.66
6	E	702	FAD	C8M-C8-C9	-4.45	111.26	119.49

There are no chirality outliers.

5 of 75 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'
6	E	702	FAD	N10-C1'-C2'-C3'

There are no ring outliers.

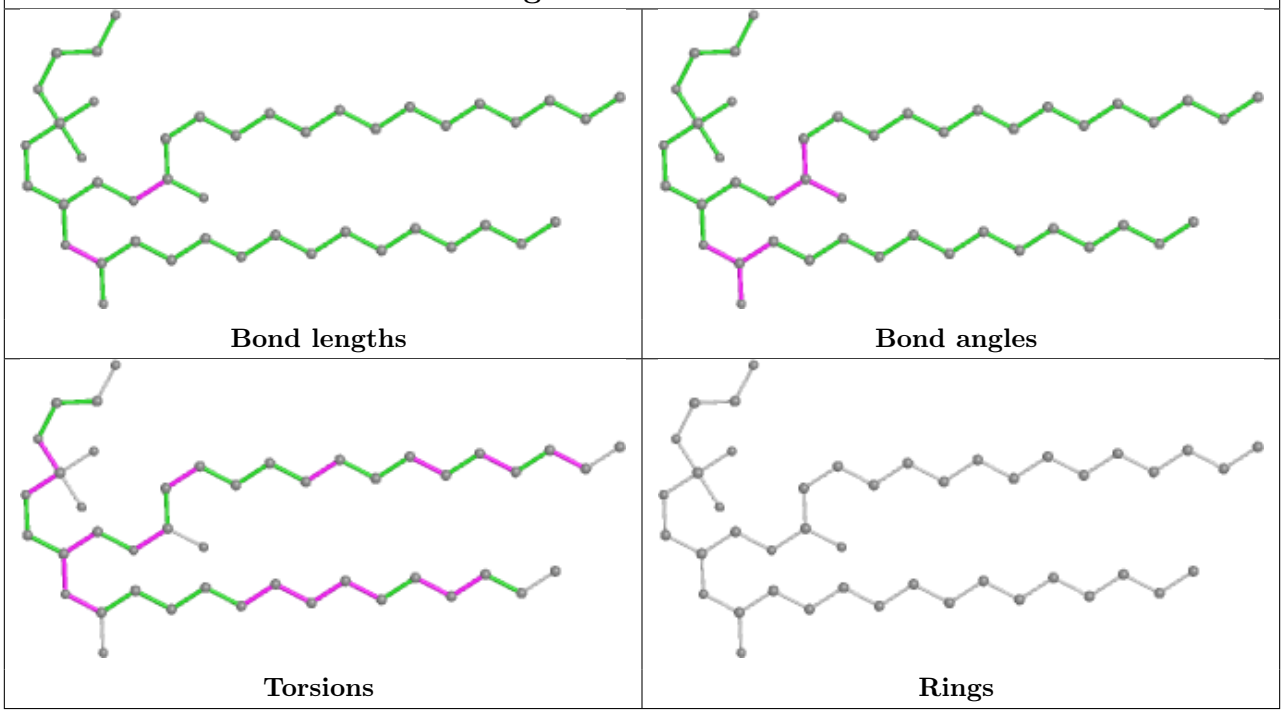
9 monomers are involved in 33 short contacts:

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

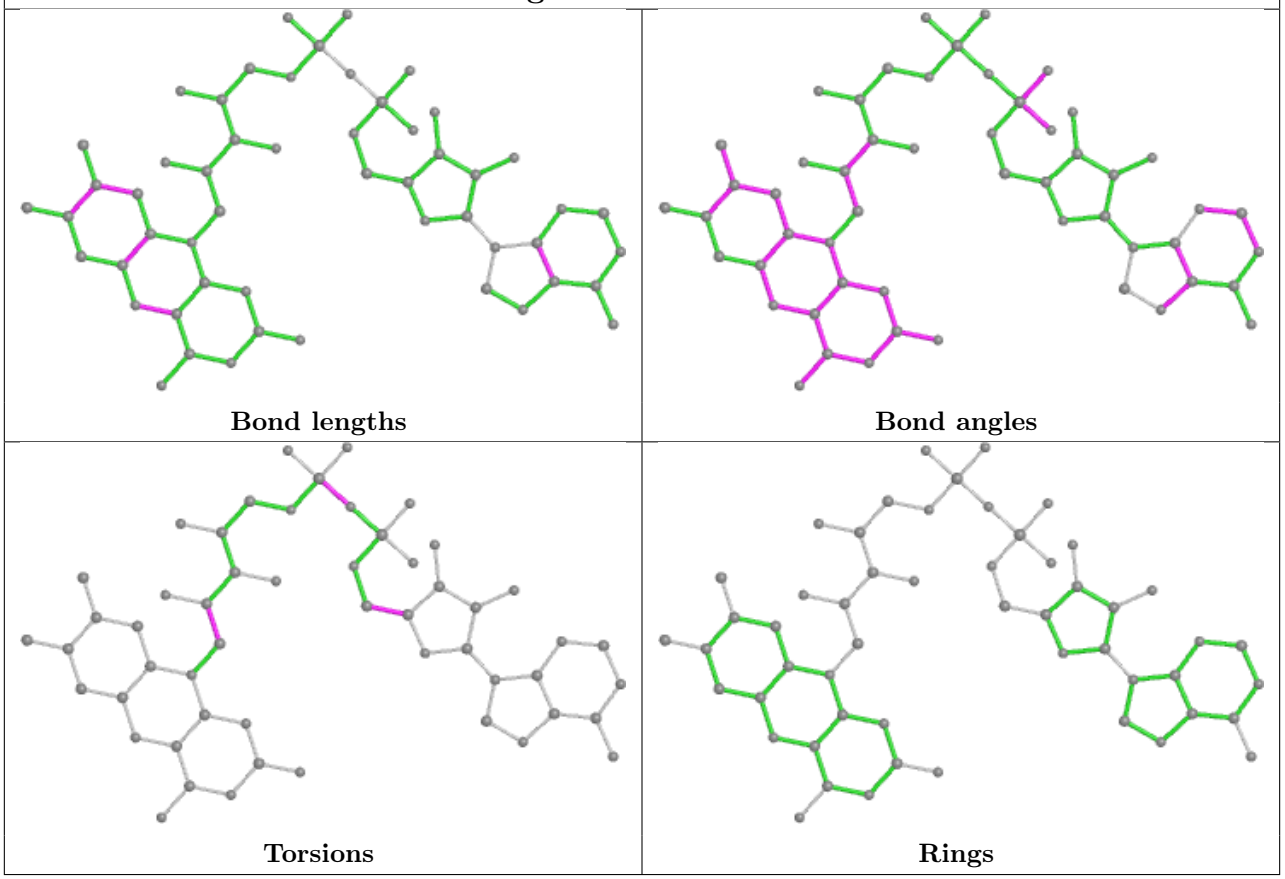
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

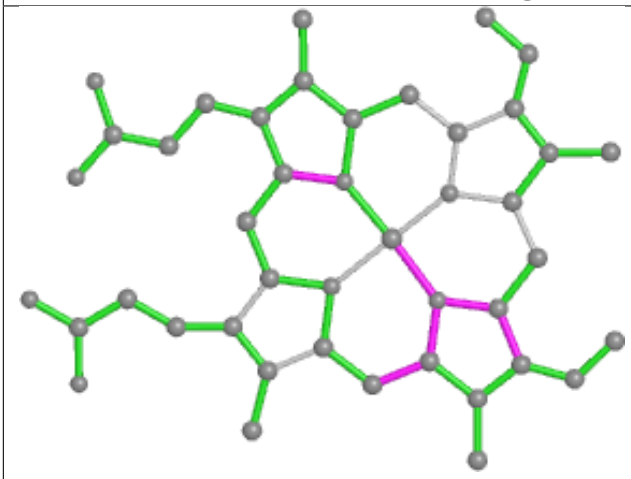
Ligand EPH D 201



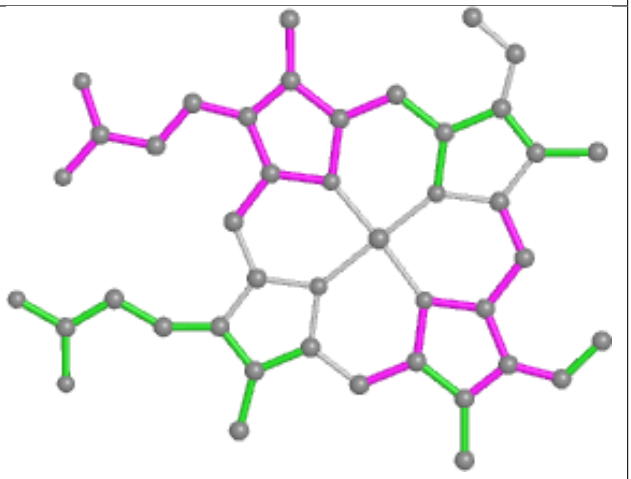
Ligand FAD E 702



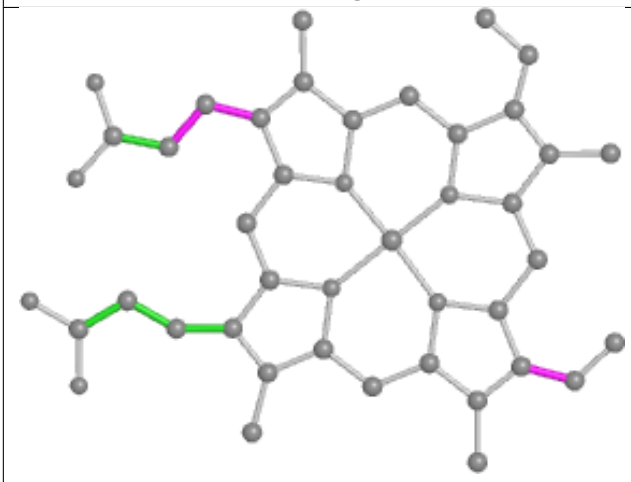
Ligand HEM C 201



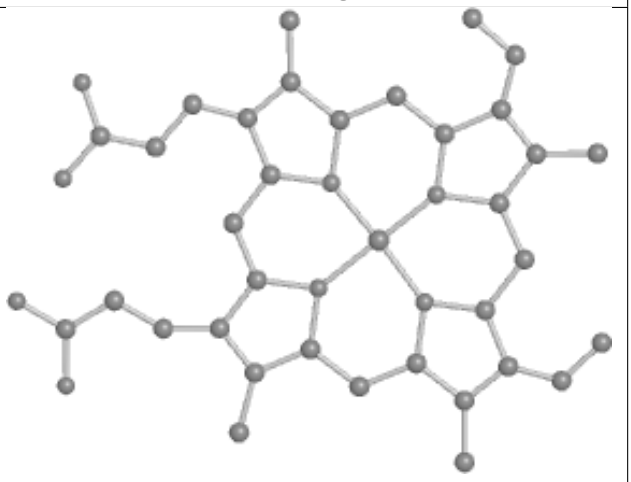
Bond lengths



Bond angles

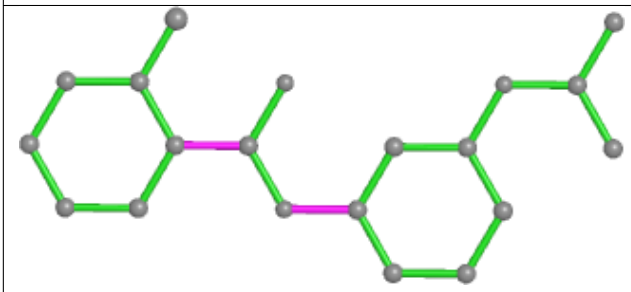


Torsions



Rings

Ligand 12J C 202



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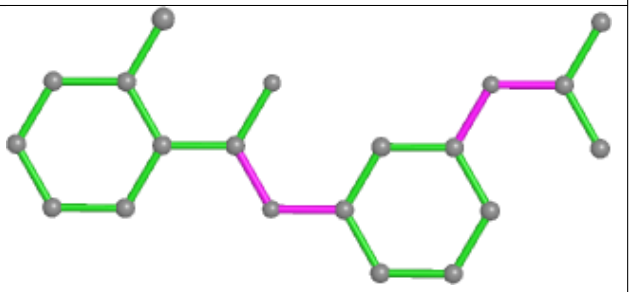
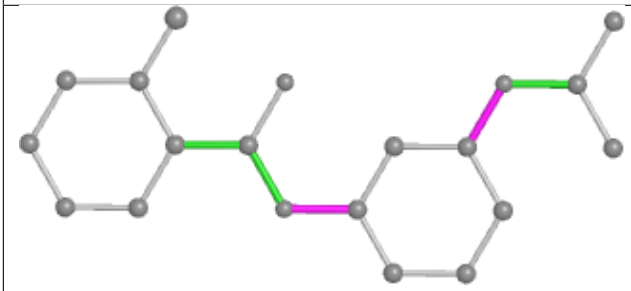
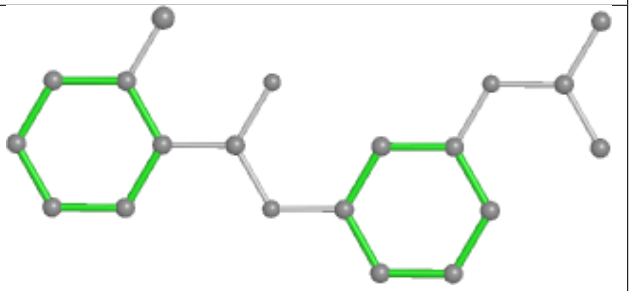


Bond angles

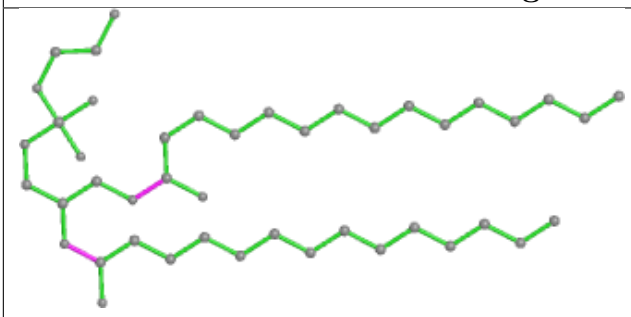


Torsions

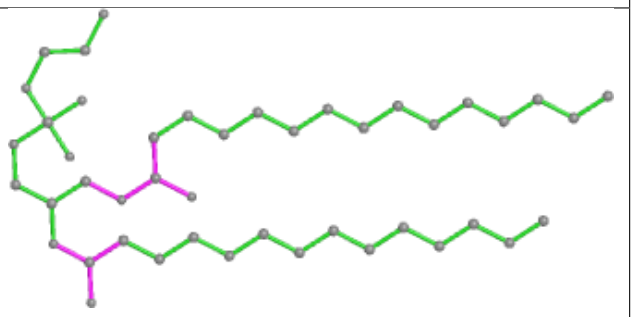


Rings

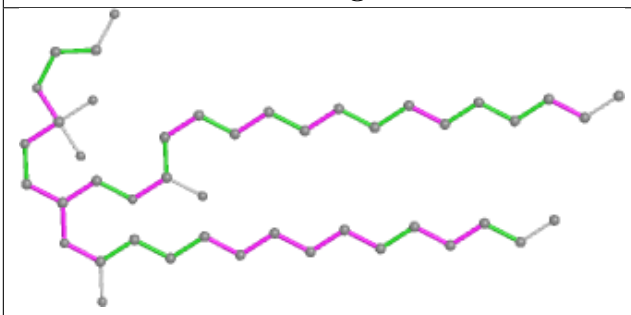
Ligand EPH H 201



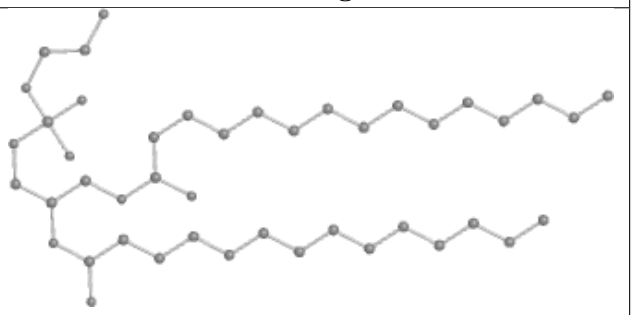
Bond lengths



Bond angles

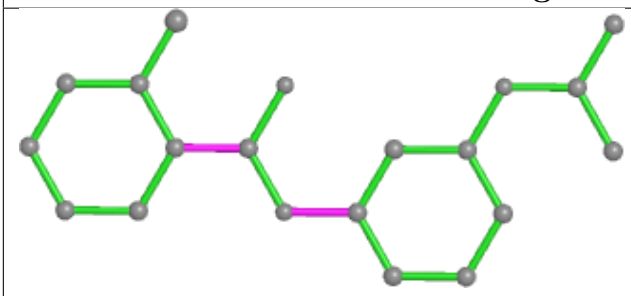


Torsions

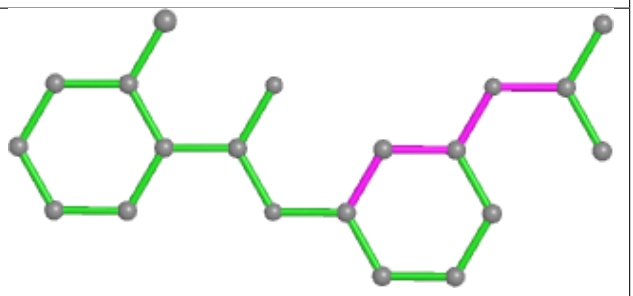


Rings

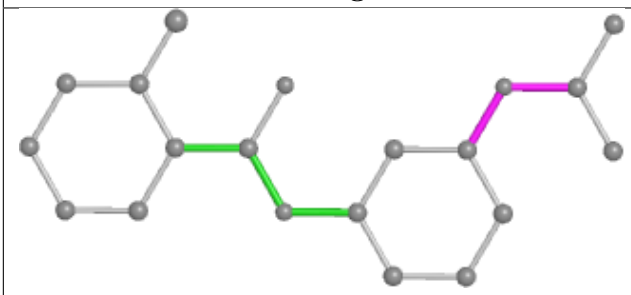
Ligand 12J G 202



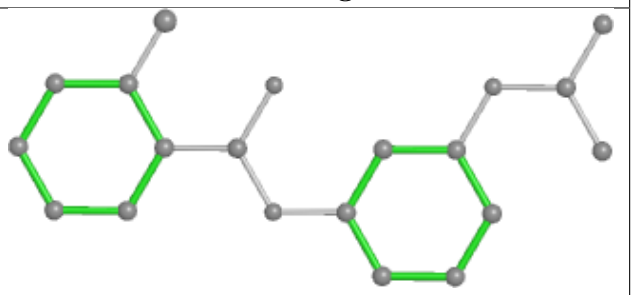
Bond lengths



Bond angles

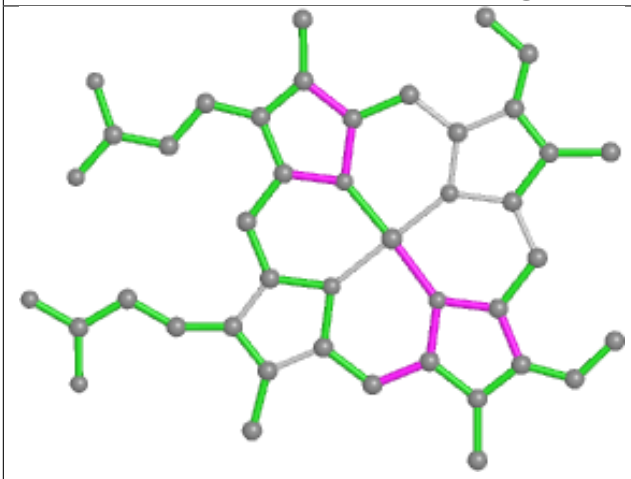


Torsions

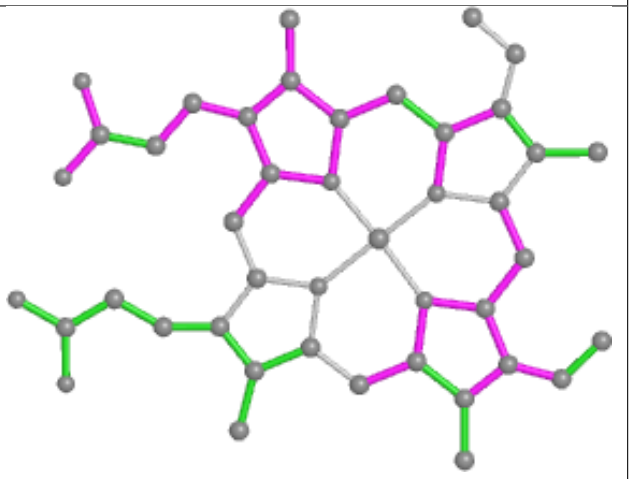


Rings

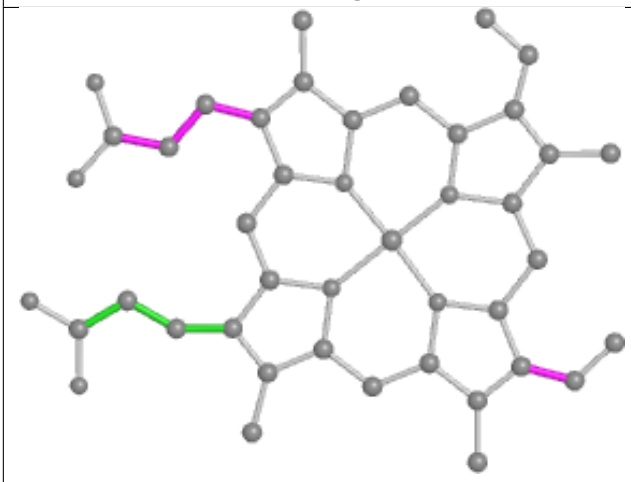
Ligand HEM G 201



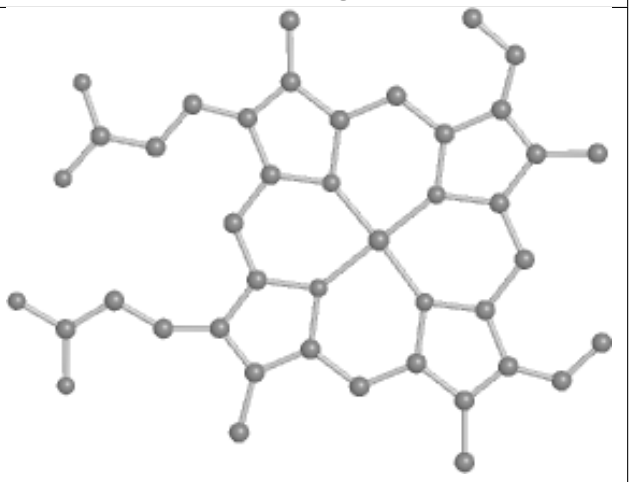
Bond lengths



Bond angles

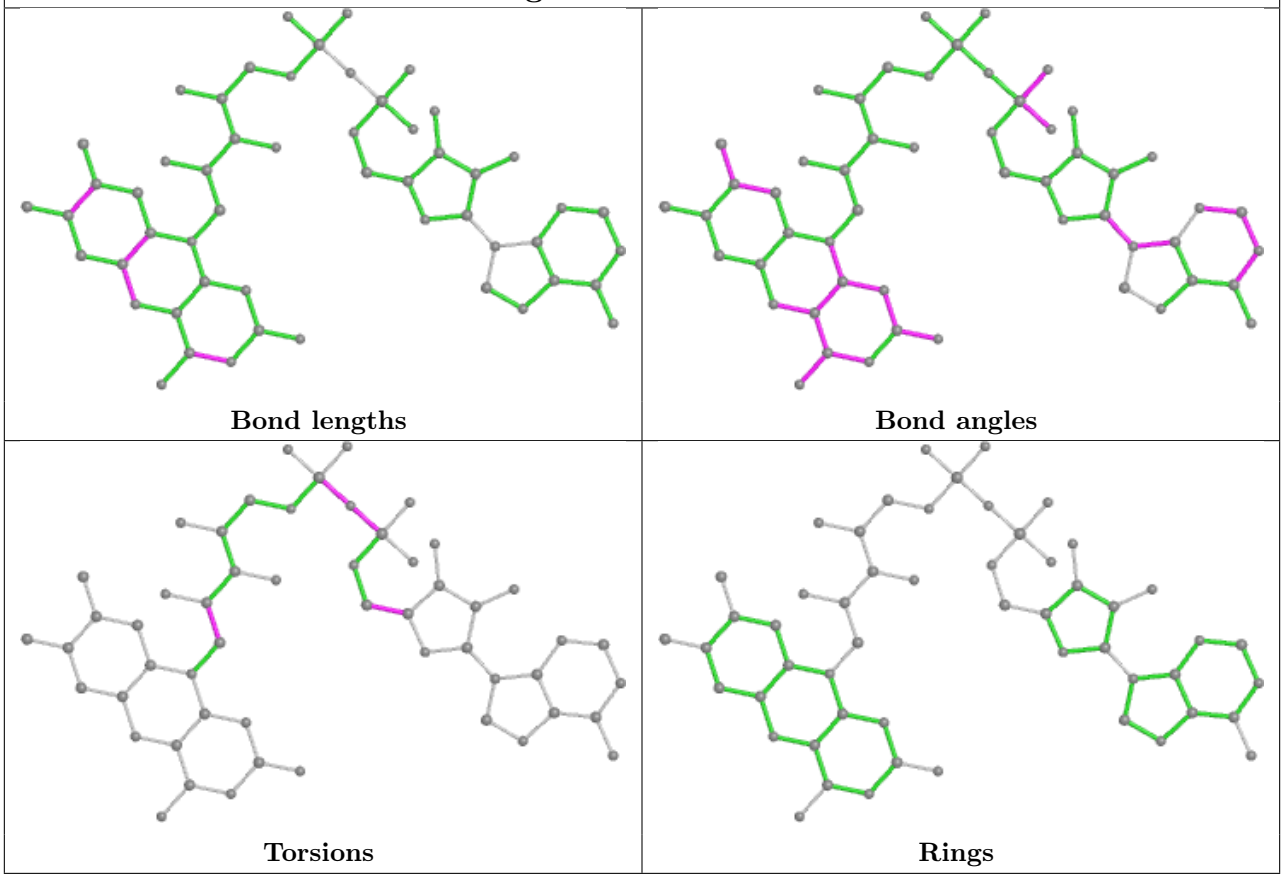


Torsions



Rings

Ligand FAD A 702



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	616/645 (95%)	-0.65	1 (0%) 92 88	18, 55, 80, 108	1 (0%)
1	E	616/645 (95%)	-0.61	1 (0%) 92 88	19, 57, 83, 112	1 (0%)
2	B	250/282 (88%)	-0.62	0 100 100	35, 52, 78, 94	0
2	F	250/282 (88%)	-0.57	0 100 100	39, 55, 79, 109	0
3	C	153/188 (81%)	-0.41	2 (1%) 74 61	46, 62, 104, 151	0
3	G	153/188 (81%)	-0.15	4 (2%) 57 42	48, 68, 136, 211	0
4	D	129/156 (82%)	-0.40	1 (0%) 82 72	54, 66, 104, 141	0
4	H	129/156 (82%)	-0.23	5 (3%) 44 33	52, 72, 120, 154	0
All	All	2296/2542 (90%)	-0.54	14 (0%) 85 78	18, 58, 93, 211	2 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	THR	4.7
1	E	499	THR	4.1
4	H	52	LEU	3.6
3	G	185	PRO	3.6
3	G	107	ILE	3.2

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

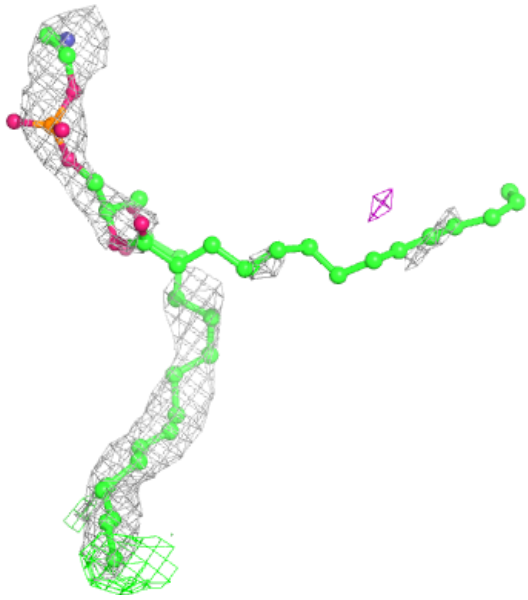
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

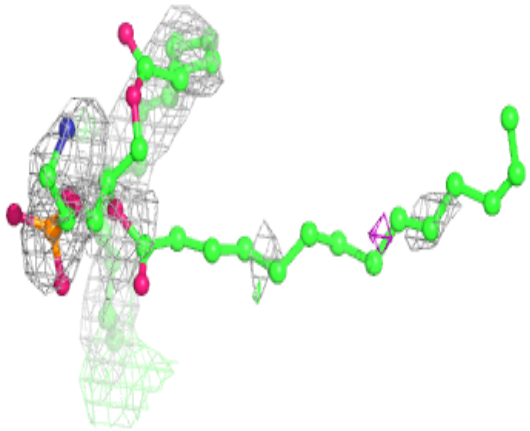
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	EPH	H	201	44/49	0.85	0.28	72,121,165,169	0
12	EPH	D	201	44/49	0.90	0.21	66,95,128,141	0
6	FAD	E	702	53/53	0.96	0.07	37,45,51,53	0
10	HEM	G	201	43/43	0.97	0.09	49,68,81,85	0
6	FAD	A	702	53/53	0.97	0.07	33,40,43,44	0
10	HEM	C	201	43/43	0.97	0.09	56,68,77,89	0
5	MLI	A	701	7/7	0.98	0.11	46,48,51,51	0
5	MLI	E	701	7/7	0.98	0.07	51,54,55,55	0
9	F3S	B	303	7/7	0.99	0.05	40,47,53,56	0
9	F3S	F	303	7/7	0.99	0.04	46,55,57,58	0
7	FES	B	301	4/4	0.99	0.03	44,46,48,49	0
7	FES	F	301	4/4	0.99	0.04	42,45,45,50	0
11	12J	C	202	20/20	0.99	0.08	61,70,76,77	0
11	12J	G	202	20/20	0.99	0.07	56,59,66,70	0
8	SF4	B	302	8/8	0.99	0.04	35,38,43,44	0
8	SF4	F	302	8/8	0.99	0.03	36,40,41,41	0

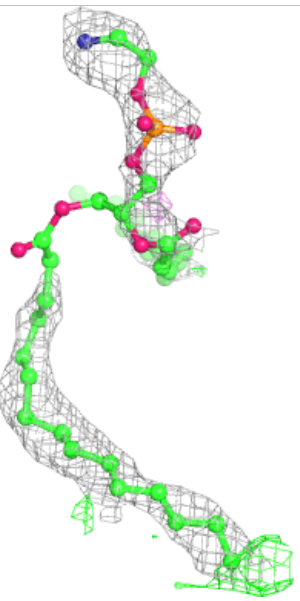
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

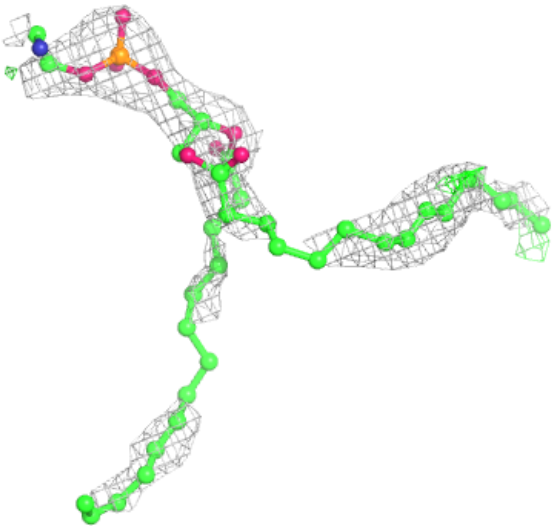


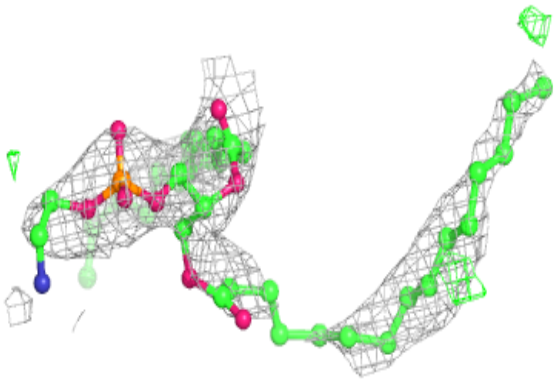


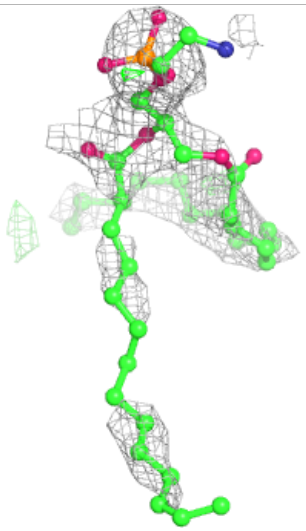


Electron density around EPH D 201:

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

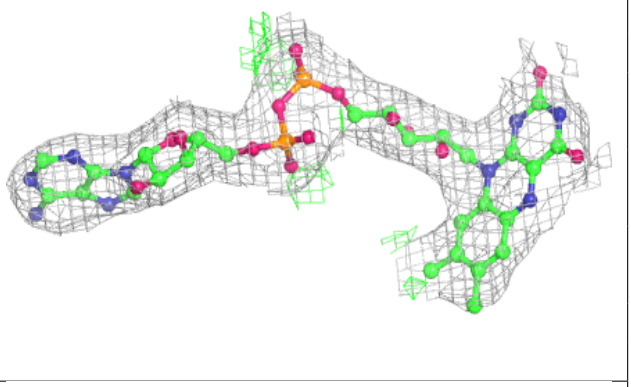


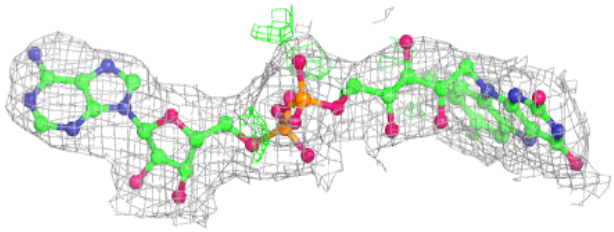


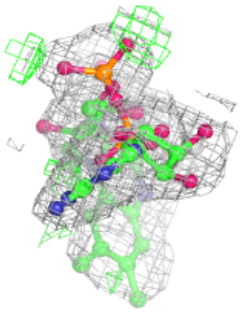


Electron density around FAD E 702:

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

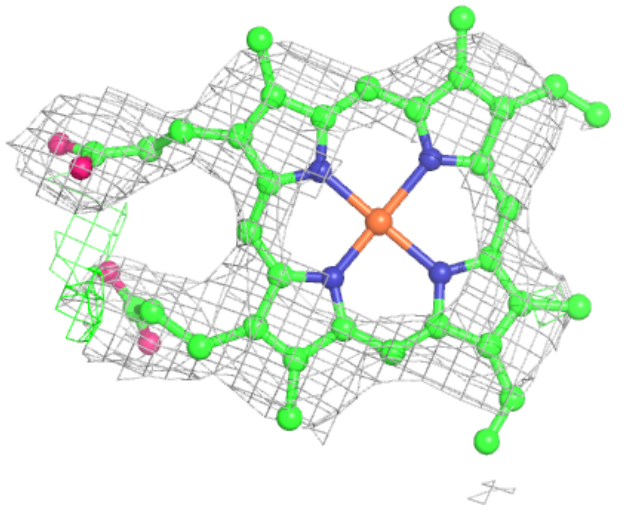


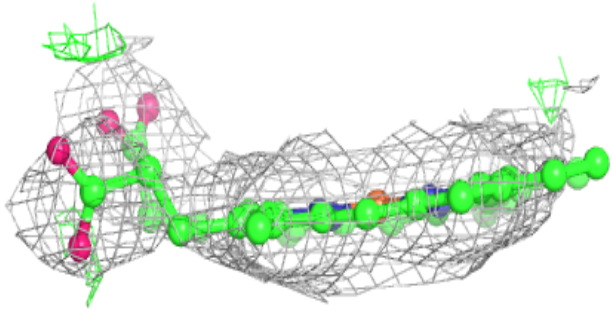


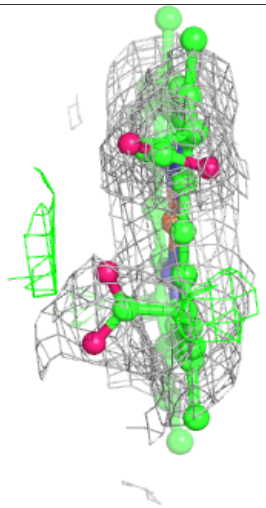


Electron density around HEM G 201:

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

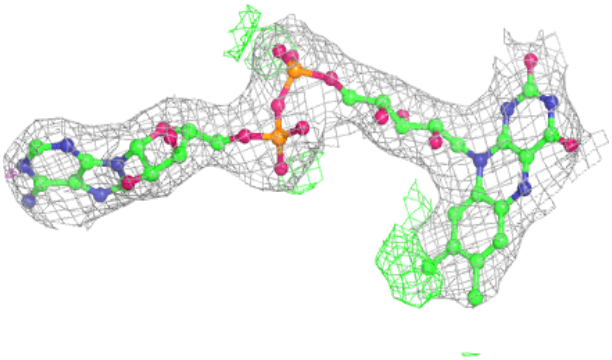


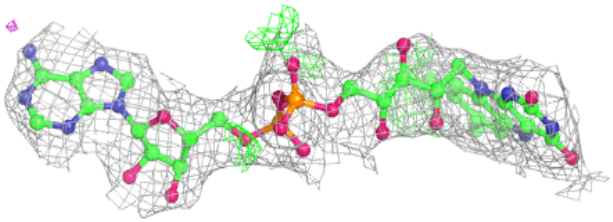


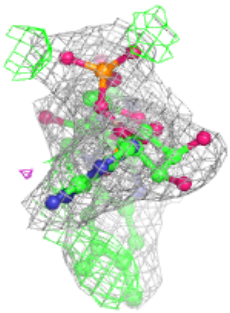


Electron density around FAD A 702:

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

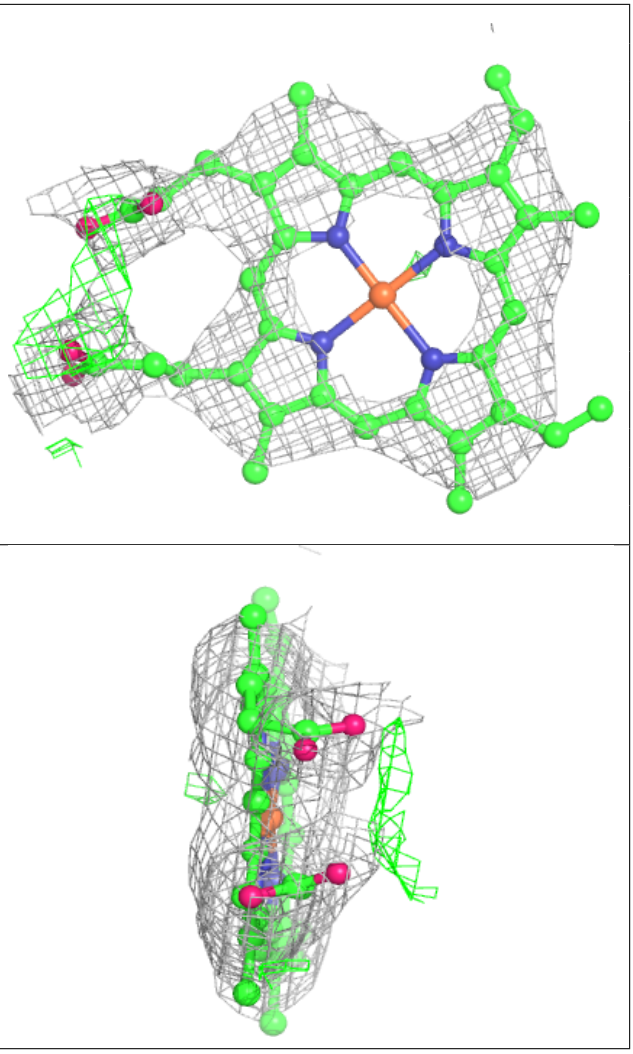






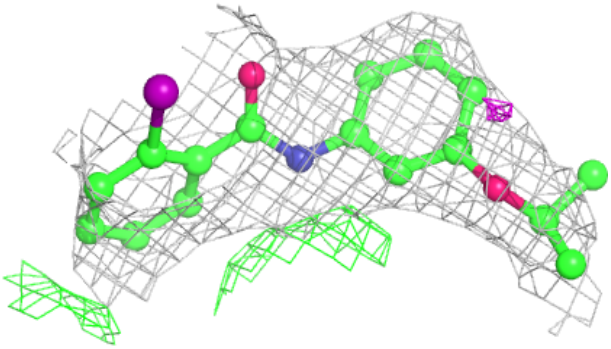
Electron density around HEM C 201:

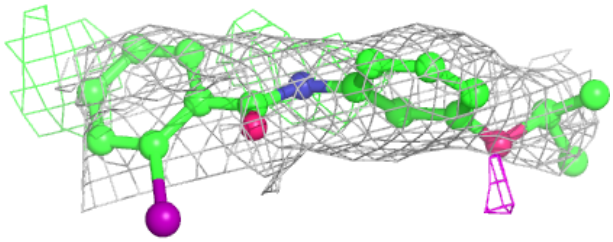
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

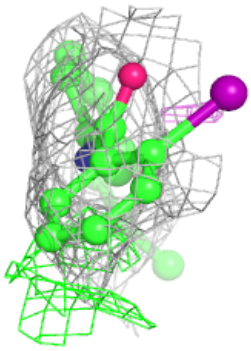


Electron density around 12J C 202:

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

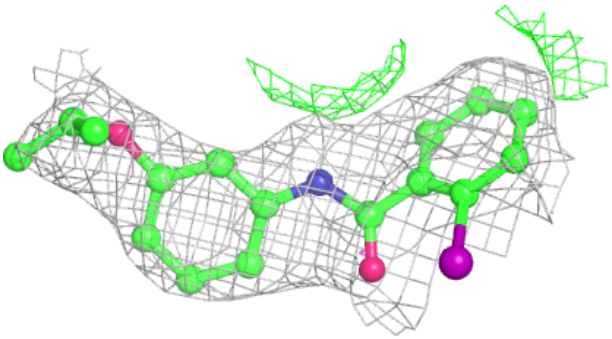


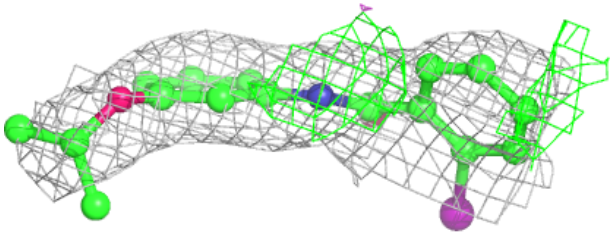


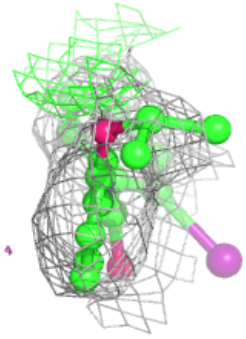


Electron density around 12J G 202:

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







6.5 Other polymers (i)

There are no such residues in this entry.