wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2026 – 04:22 pm BST

PDB ID	:	2BS4 / pdb_00002bs4
Title	:	GLU C180 -> ILE VARIANT QUINOL:FUMARATE REDUCTASE FROM-WOLINELLA SUCCINOGENES
Authors	:	Lancaster, C.R.D.
Deposited on	:	2005-05-14
Resolution	:	2.76 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:

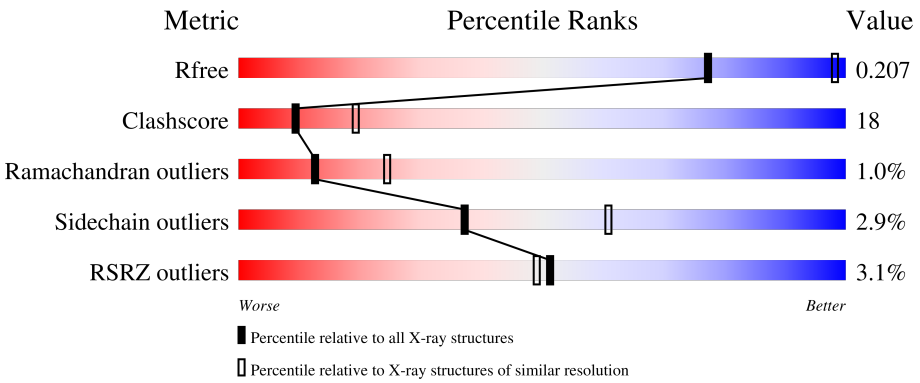
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	656	4% 67% 30% •
1	D	656	4% 66% 31% •
2	B	239	% 68% 31% •
2	E	239	% 67% 32% •
3	C	256	3% 61% 34% •

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Mol	Chain	Length	Quality of chain
3	F	256	4% 59% 36%

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	CIT	A	1657	-	-	X	-
5	CIT	D	1657	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 19050 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 QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	656	5094	3190	911	961	32	36	0	1
1	D	656	5094	3190	911	961	32	36	0	1

- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	1894	1194	322	355	23	6	0	0
2	E	239	1894	1194	322	355	23	6	0	0

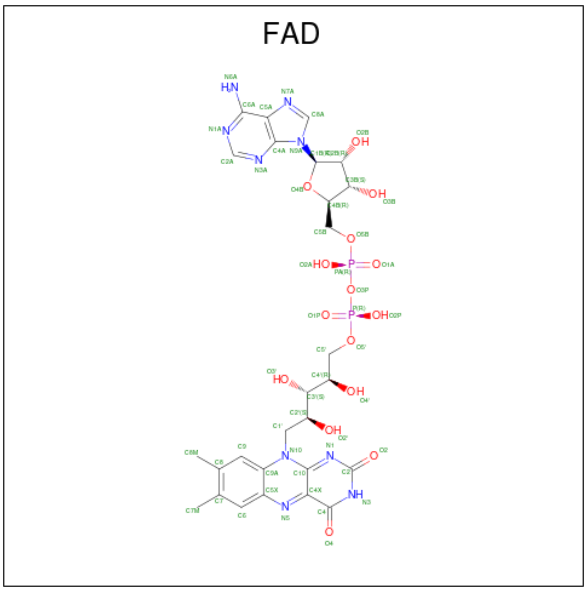
- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	255	2080	1389	334	343	14	15	0	1
3	F	255	2080	1389	334	343	14	15	0	1

There are 2 discrepancies between the modelled and reference sequences:

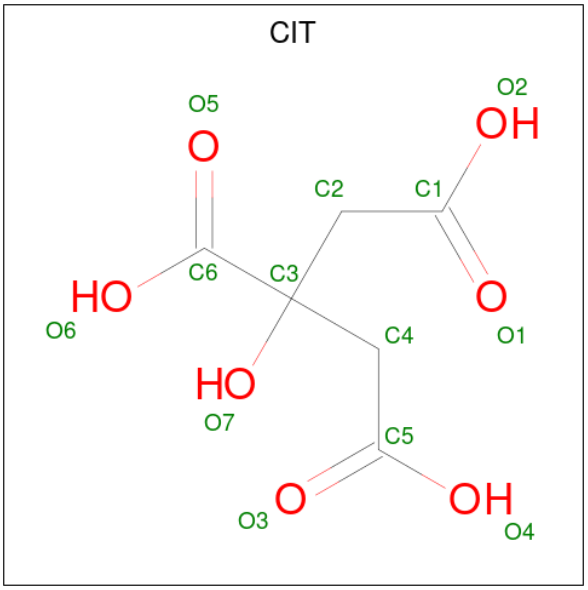
Chain	Residue	Modelled	Actual	Comment	Reference
C	180	ILE	GLU	conflict	UNP P17413
F	180	ILE	GLU	conflict	UNP P17413

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



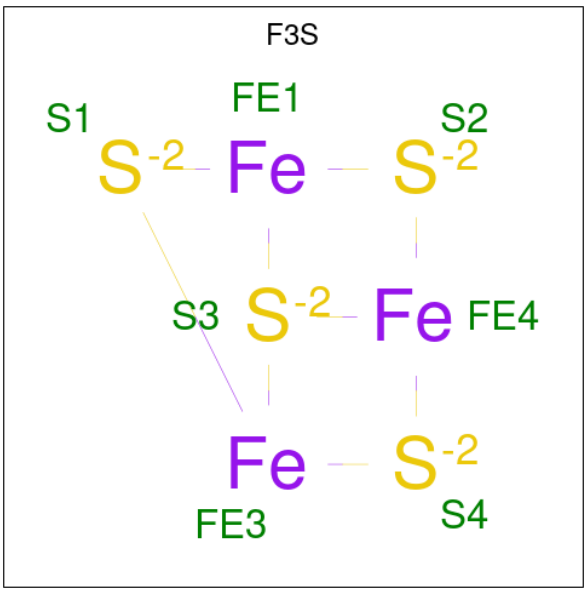
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
4	D	1	53	27	9	15	2	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



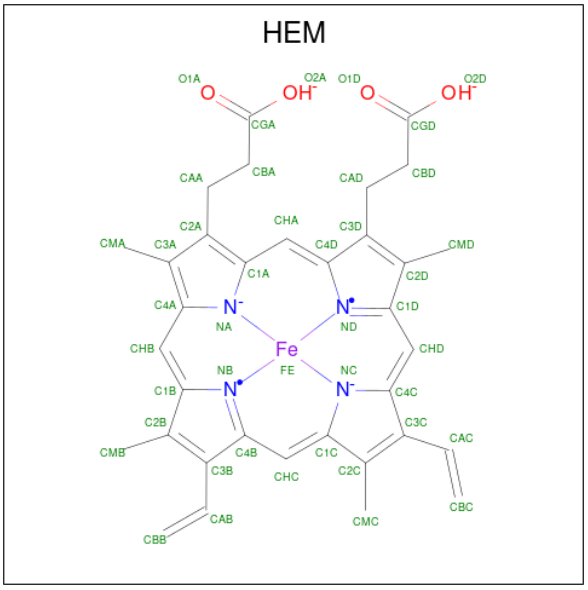
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	13	6	7	0	0
			Total	C	O		
5	D	1	13	6	7	0	0

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	7	3	4	0	0
			Total	Fe	S		
6	E	1	7	3	4	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

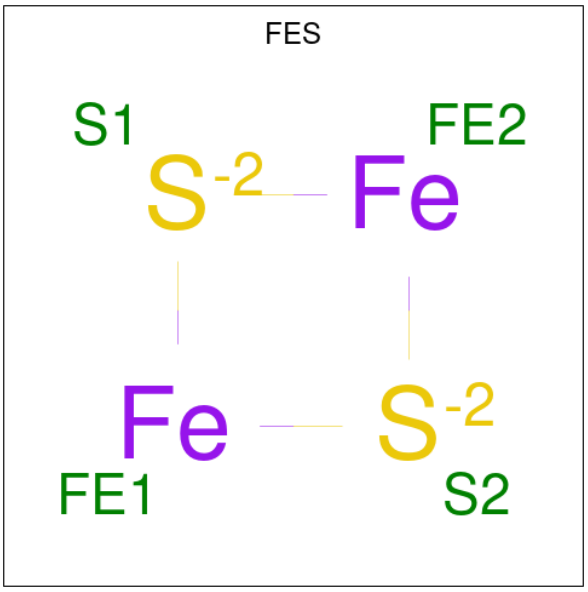


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
7	C	1	43	34	1	4	4	0	0
7	F	1	43	34	1	4	4	0	0
7	F	1	43	34	1	4	4	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

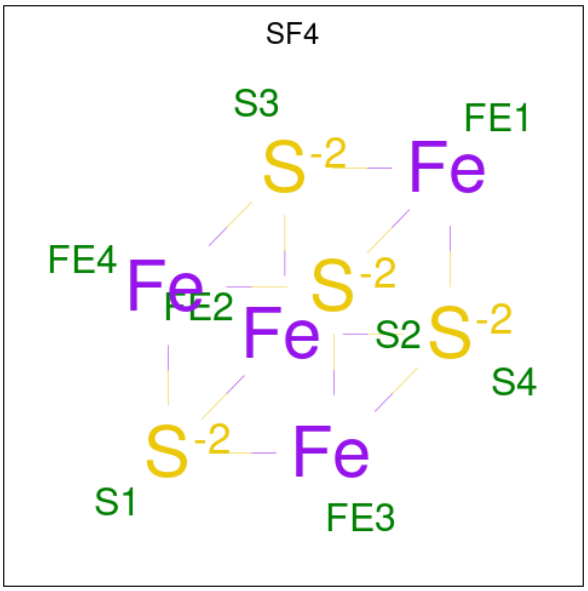
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	D	1	1	1	0	0
8	E	1	1	1	0	0

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



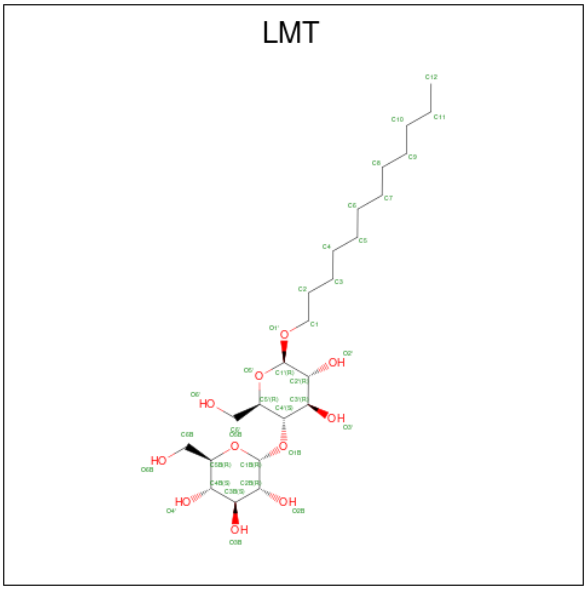
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



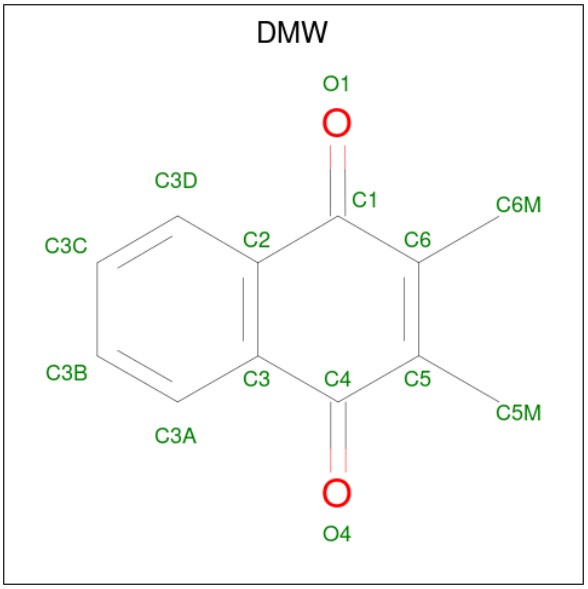
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	E	1	8	4	4	0	0
			Total	Fe	S		
10	E	1	8	4	4	0	0

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	E	1	35	24	11	16	0
			Total	C	O		
11	F	1	35	24	11	16	0

- Molecule 12 is 2,3-DIMETHYL-1,4-NAPHTHOQUINONE (CCD ID: DMW) (formula: $C_{12}H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	1	Total C O 14 12 2	0	0
12	F	1	Total C O 14 12 2	0	0

- Molecule 13 is water.

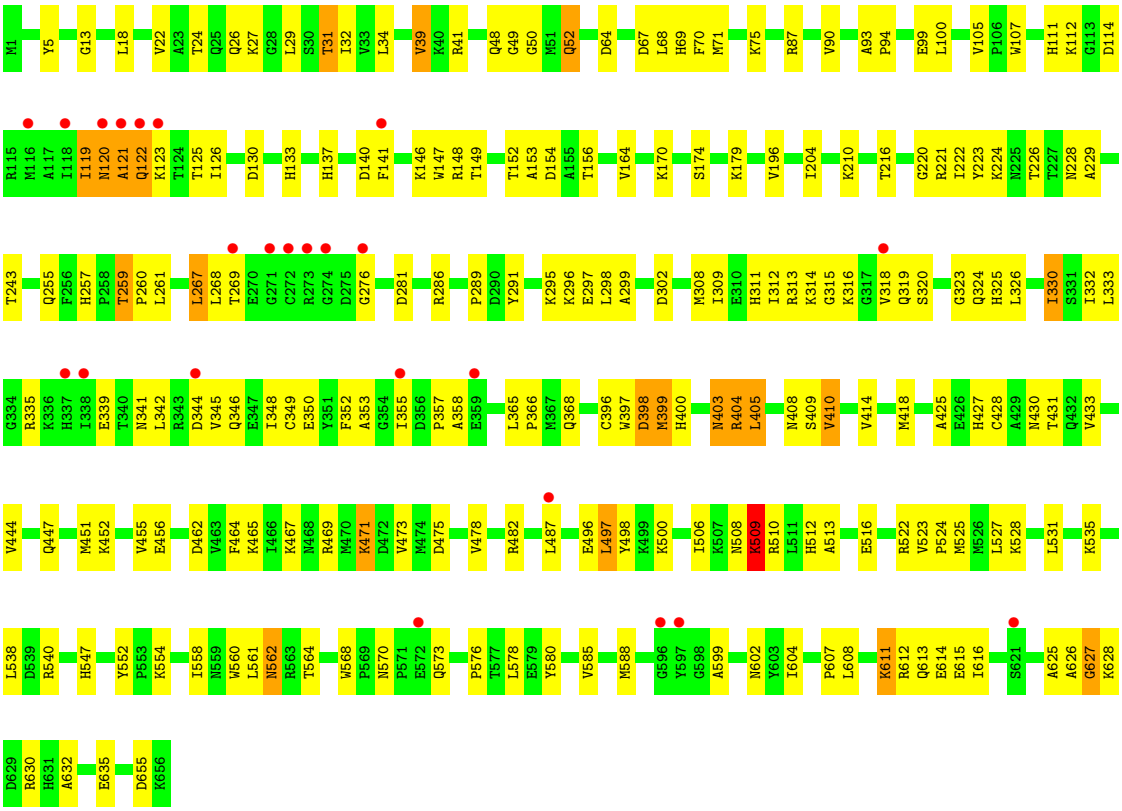
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	136	Total O 136 136	0	0
13	B	73	Total O 73 73	0	0
13	C	24	Total O 24 24	0	0
13	D	137	Total O 137 137	0	0
13	E	76	Total O 76 76	0	0
13	F	26	Total O 26 26	0	0

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.

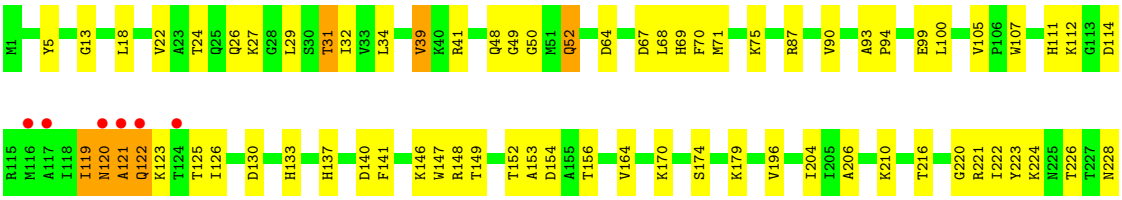
• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

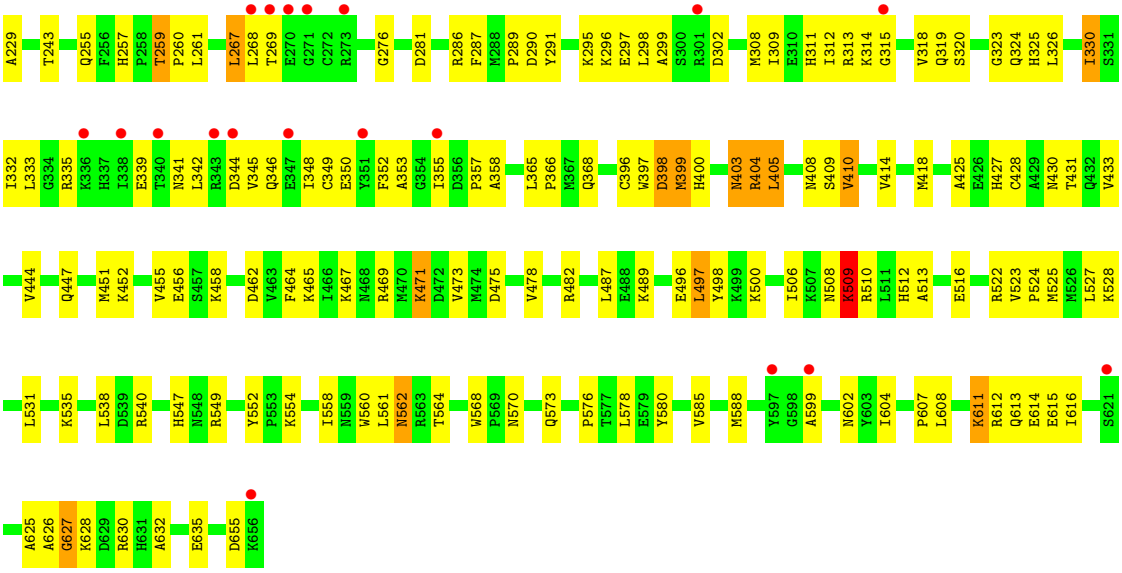
Chain A:



• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

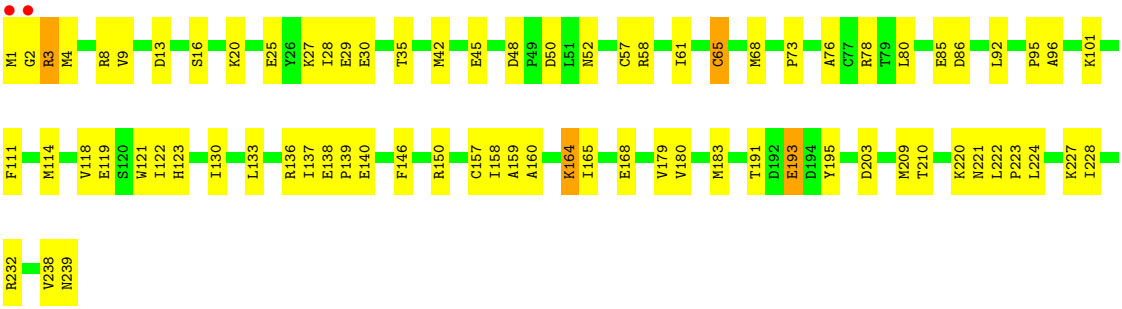
Chain D:





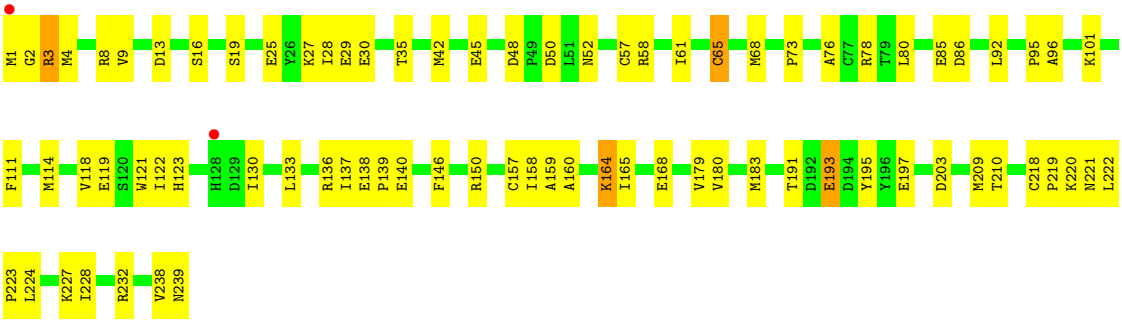
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

Chain B:



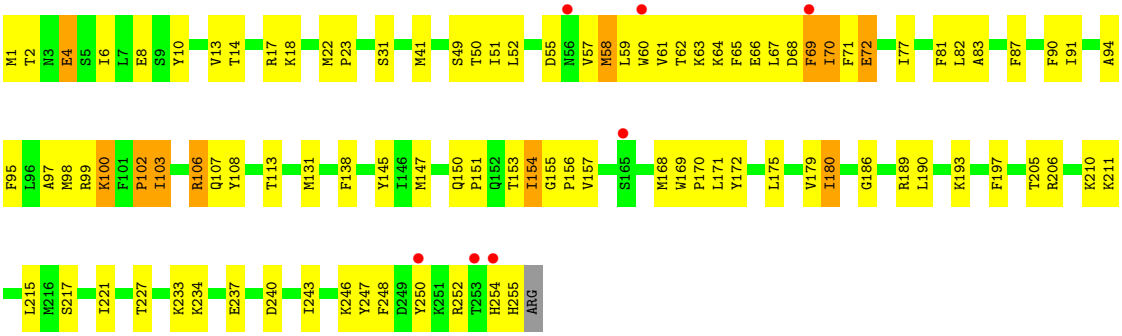
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

Chain E:



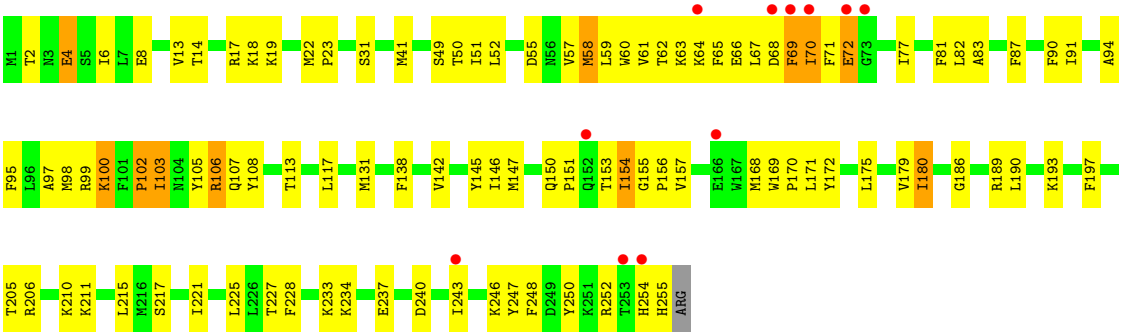
• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C

Chain C:



• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	29.65 – 2.76 29.65 – 2.76	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.65-2.76) 86.0 (29.65-2.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.216 0.191 , 0.207	Depositor DCC
R_{free} test set	1000 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19050	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: NA, FES, SF4, CIT, F3S, DMW, FAD, LMT, 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	0.43	1/5190 (0.0%)	0.96	21/6998 (0.3%)
1	D	0.43	1/5190 (0.0%)	0.96	21/6998 (0.3%)
2	B	0.45	0/1931	0.95	5/2604 (0.2%)
2	E	0.45	0/1931	0.95	5/2604 (0.2%)
3	C	0.42	1/2146 (0.0%)	0.90	4/2905 (0.1%)
3	F	0.42	1/2146 (0.0%)	0.90	4/2905 (0.1%)
All	All	0.43	4/18534 (0.0%)	0.95	60/25014 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	254	HIS	C-N	-5.59	1.25	1.33
3	C	254	HIS	C-N	-5.58	1.25	1.33
1	A	655	ASP	C-N	-5.24	1.26	1.33
1	D	655	ASP	C-N	-5.22	1.26	1.33

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	397	TRP	N-CA-C	-11.25	98.78	111.71
1	A	397	TRP	N-CA-C	-11.23	98.80	111.71
1	D	121	ALA	N-CA-C	-10.39	98.03	113.61
1	A	121	ALA	N-CA-C	-10.36	98.06	113.61
3	C	102	PRO	N-CA-C	-9.58	96.14	111.38

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	5094	0	5069	177	0
1	D	5094	0	5069	177	0
2	B	1894	0	1861	65	0
2	E	1894	0	1861	70	0
3	C	2080	0	2106	104	0
3	F	2080	0	2106	104	0
4	A	53	0	29	5	0
4	D	53	0	29	5	0
5	A	13	0	5	10	0
5	D	13	0	5	9	0
6	B	7	0	0	0	0
6	E	7	0	0	0	0
7	C	86	0	60	7	0
7	F	86	0	60	7	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
9	E	8	0	0	0	0
10	E	16	0	0	0	0
11	E	35	0	46	8	0
11	F	35	0	46	10	0
12	E	14	0	10	0	0
12	F	14	0	10	0	0
13	A	136	0	0	1	0
13	B	73	0	0	1	0
13	C	24	0	0	2	0
13	D	137	0	0	1	0
13	E	76	0	0	1	0
13	F	26	0	0	2	0
All	All	19050	0	18372	659	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 18.

The worst 5 of 659 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:ILE:HD12	3:F:103:ILE:CD1	1.70	1.22
3:C:103:ILE:CD1	3:F:103:ILE:HD12	1.70	1.21
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.56	0.87
1:A:289:PRO:HG3	1:A:296:LYS:HG2	1.55	0.86
1:D:289:PRO:HG3	1:D:296:LYS:HG2	1.55	0.86

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	654/656 (100%)	613 (94%)	34 (5%)	7 (1%)	11	22
1	D	654/656 (100%)	613 (94%)	34 (5%)	7 (1%)	11	22
2	B	237/239 (99%)	220 (93%)	15 (6%)	2 (1%)	16	30
2	E	237/239 (99%)	220 (93%)	15 (6%)	2 (1%)	16	30
3	C	253/256 (99%)	239 (94%)	11 (4%)	3 (1%)	10	20
3	F	253/256 (99%)	239 (94%)	11 (4%)	3 (1%)	10	20
All	All	2288/2302 (99%)	2144 (94%)	120 (5%)	24 (1%)	12	24

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
2	B	3	ARG
3	C	72	GLU
1	D	122	GLN
2	E	3	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	532/533 (100%)	515 (97%)	17 (3%)	34	58
1	D	532/533 (100%)	515 (97%)	17 (3%)	34	58
2	B	211/211 (100%)	207 (98%)	4 (2%)	50	70
2	E	211/211 (100%)	207 (98%)	4 (2%)	50	70
3	C	221/223 (99%)	214 (97%)	7 (3%)	34	58
3	F	221/223 (99%)	214 (97%)	7 (3%)	34	58
All	All	1928/1934 (100%)	1872 (97%)	56 (3%)	37	61

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	THR
3	F	180	ILE
1	D	403	ASN
3	F	154	ILE
3	F	4	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	48	GLN
1	D	319	GLN
2	E	116	GLN
1	D	57	ASN
1	D	225	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)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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	$\#\|Z\| > 2$
7	HEM	F	1255	3	50,50,50	1.35	8 (16%)	66,82,82	0.83	1 (1%)
5	CIT	A	1657	-	12,12,12	0.77	0	17,17,17	1.45	1 (5%)
4	FAD	A	1656	1	56,58,58	1.71	13 (23%)	81,89,89	1.22	5 (6%)
7	HEM	C	1255	3	50,50,50	1.35	8 (16%)	66,82,82	0.83	1 (1%)
9	FES	E	1245	2	0,4,4	-	-	-		
7	HEM	F	1256	3	50,50,50	1.31	8 (16%)	66,82,82	0.92	3 (4%)
4	FAD	D	1656	1	56,58,58	1.71	13 (23%)	81,89,89	1.22	5 (6%)
10	SF4	E	1241	2	0,12,12	-	-	-		
10	SF4	E	1247	2	0,12,12	-	-	-		
11	LMT	F	1257	-	36,36,36	1.14	2 (5%)	47,47,47	1.21	4 (8%)
7	HEM	C	1256	3	50,50,50	1.31	8 (16%)	66,82,82	0.91	3 (4%)
6	F3S	B	1240	2	0,9,9	-	-	-		
11	LMT	E	1242	-	36,36,36	1.14	2 (5%)	47,47,47	1.21	4 (8%)
9	FES	E	1240	2	0,4,4	-	-	-		
6	F3S	E	1246	2	0,9,9	-	-	-		
5	CIT	D	1657	-	12,12,12	0.77	0	17,17,17	1.45	1 (5%)
12	DMW	F	1258	-	15,15,15	2.28	5 (33%)	22,22,22	0.78	0
12	DMW	E	1244	-	15,15,15	2.29	5 (33%)	22,22,22	0.77	0

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
7	HEM	F	1255	3	-	6/14/54/54	-
5	CIT	A	1657	-	-	0/16/16/16	-
4	FAD	A	1656	1	-	4/34/50/50	0/6/6/6
7	HEM	C	1255	3	-	6/14/54/54	-
9	FES	E	1245	2	-	-	0/1/1/1
10	SF4	E	1241	2	-	-	0/6/5/5
4	FAD	D	1656	1	-	4/34/50/50	0/6/6/6
6	F3S	E	1246	2	-	-	0/3/3/3
10	SF4	E	1247	2	-	-	0/6/5/5
11	LMT	F	1257	-	-	14/21/61/61	0/2/2/2
7	HEM	C	1256	3	-	4/14/54/54	-
6	F3S	B	1240	2	-	-	0/3/3/3
11	LMT	E	1242	-	-	14/21/61/61	0/2/2/2
9	FES	E	1240	2	-	-	0/1/1/1
7	HEM	F	1256	3	-	4/14/54/54	-
5	CIT	D	1657	-	-	0/16/16/16	-
12	DMW	F	1258	-	-	-	0/2/2/2
12	DMW	E	1244	-	-	-	0/2/2/2

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1656	FAD	C1'-C2'	4.76	1.59	1.52
4	A	1656	FAD	C1'-C2'	4.72	1.59	1.52
12	E	1244	DMW	C3A-C3	4.54	1.47	1.39
12	F	1258	DMW	C3A-C3	4.51	1.47	1.39
4	D	1656	FAD	PA-O2A	-4.12	1.36	1.55

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	1242	LMT	C1-O1'-C1'	4.47	121.26	113.84
11	F	1257	LMT	C1-O1'-C1'	4.47	121.26	113.84
5	A	1657	CIT	O6-C6-C3	4.24	120.41	113.05
5	D	1657	CIT	O6-C6-C3	4.22	120.38	113.05
4	D	1656	FAD	C1'-N10-C9A	-4.19	113.52	120.51

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1656	FAD	PA-O3P-P-O5'
4	D	1656	FAD	PA-O3P-P-O5'
7	C	1256	HEM	C2C-C3C-CAC-CBC
7	F	1256	HEM	C2C-C3C-CAC-CBC
11	E	1242	LMT	O5'-C5'-C6'-O6'

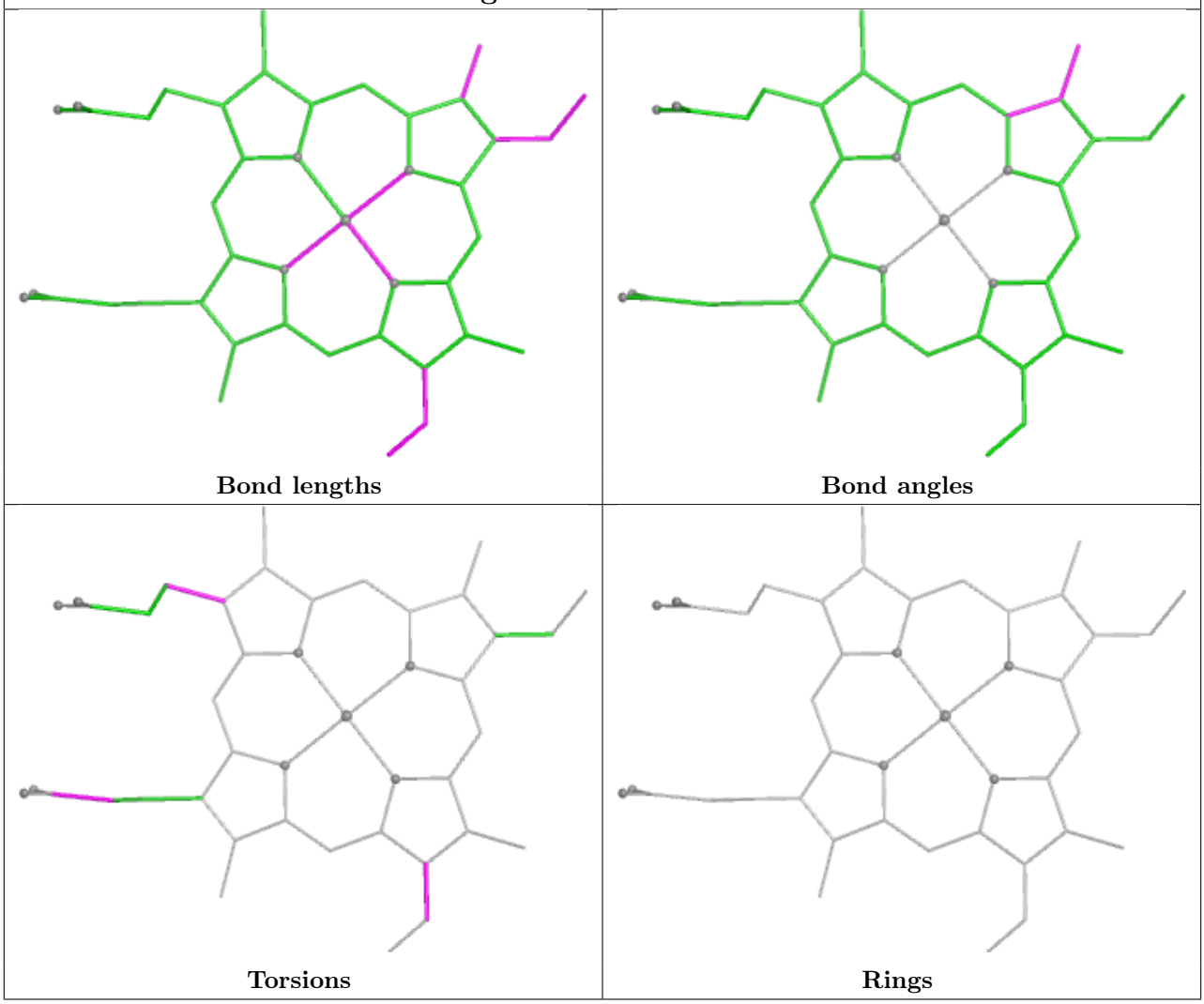
There are no ring outliers.

10 monomers are involved in 57 short contacts:

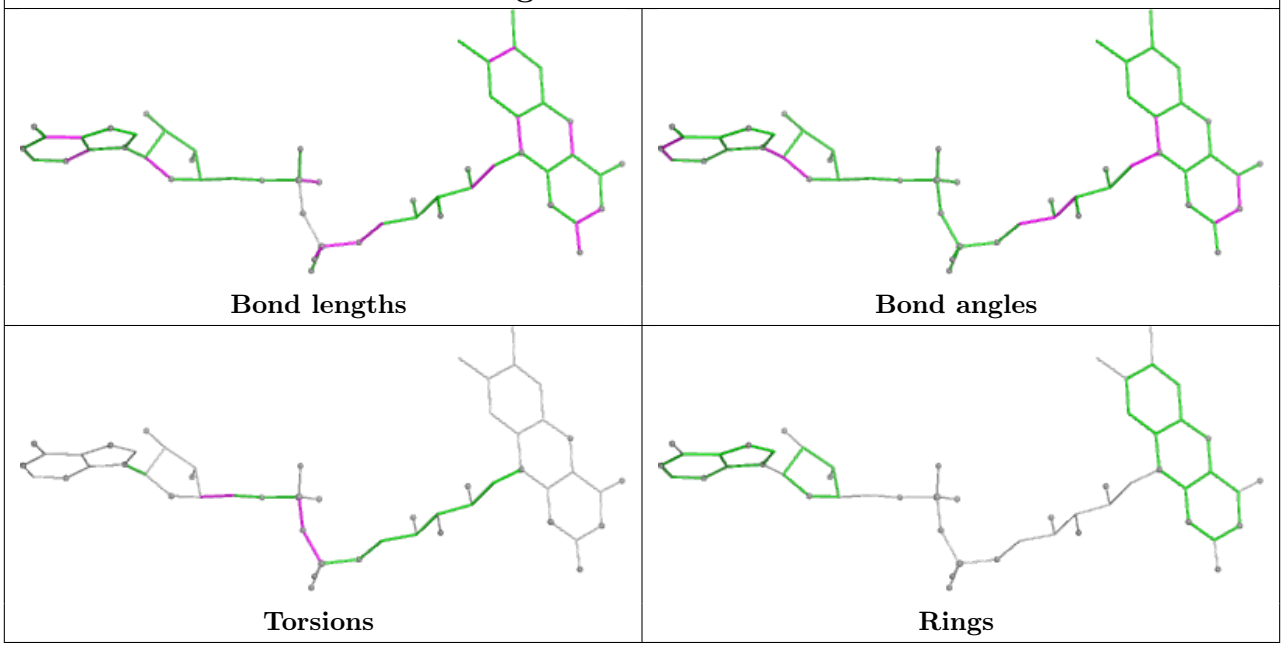
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1255	HEM	3	0
5	A	1657	CIT	10	0
4	A	1656	FAD	5	0
7	C	1255	HEM	3	0
7	F	1256	HEM	4	0
4	D	1656	FAD	5	0
11	F	1257	LMT	10	0
7	C	1256	HEM	4	0
11	E	1242	LMT	8	0
5	D	1657	CIT	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

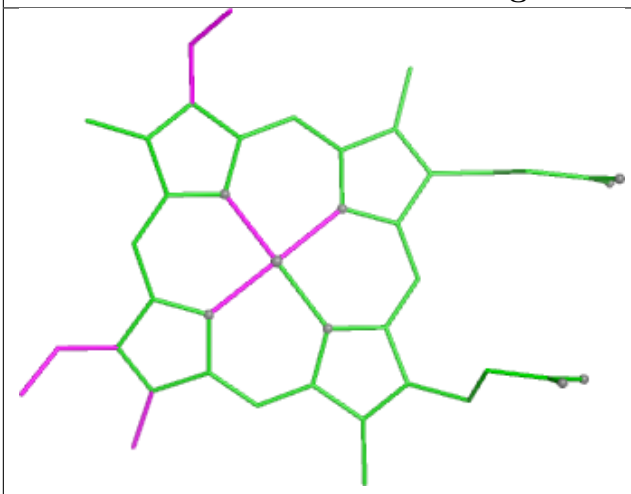
Ligand HEM F 1255



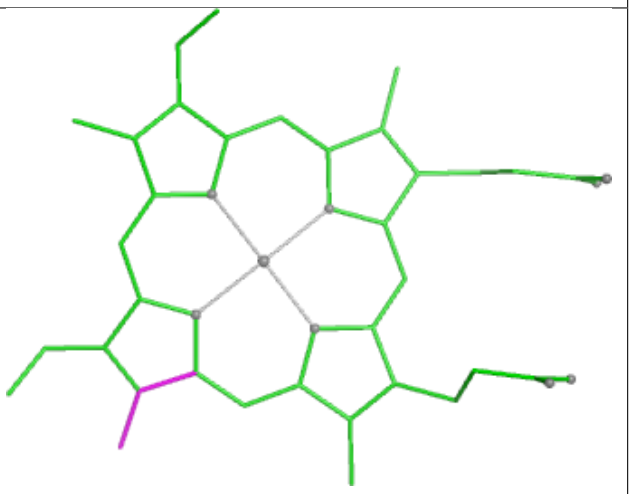
Ligand FAD A 1656



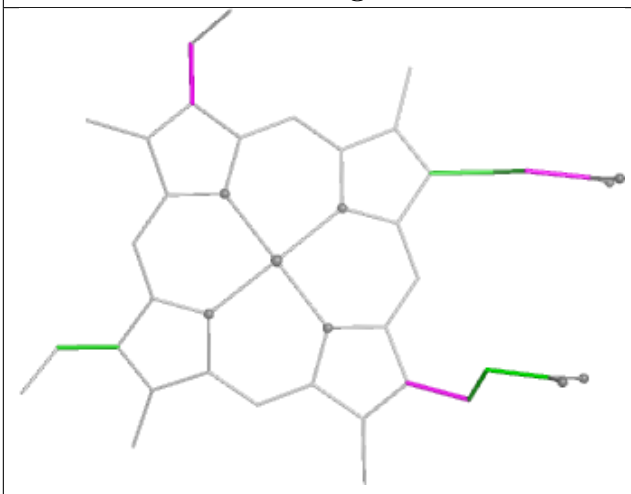
Ligand HEM C 1255



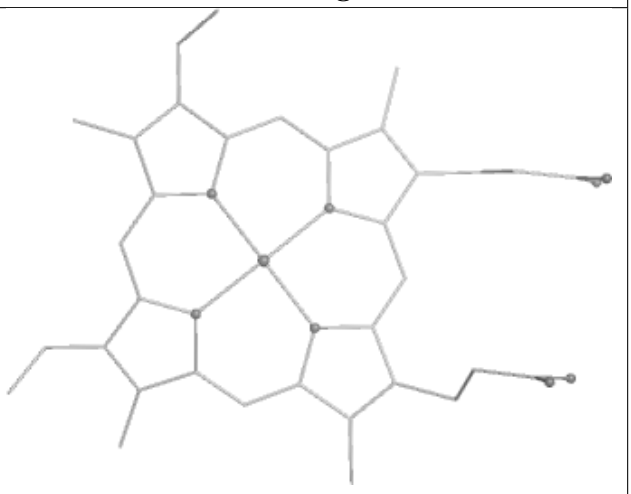
Bond lengths



Bond angles

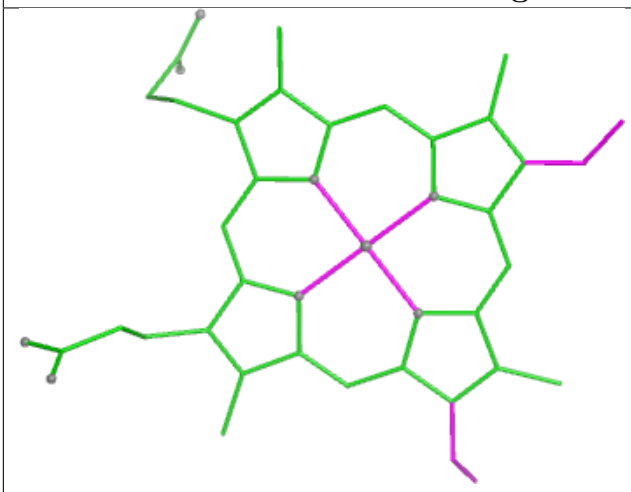


Torsions

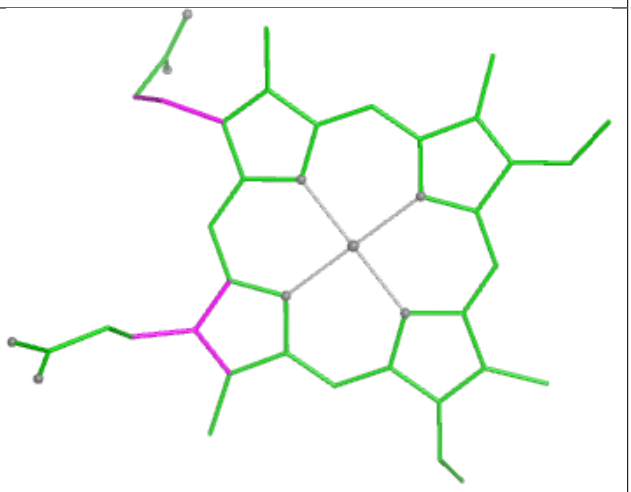


Rings

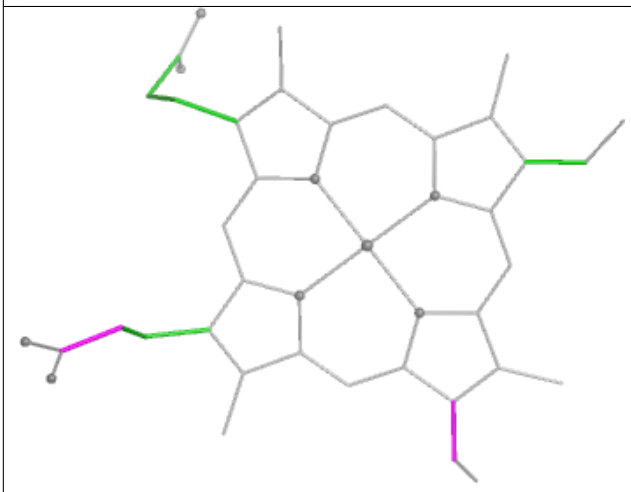
Ligand HEM F 1256



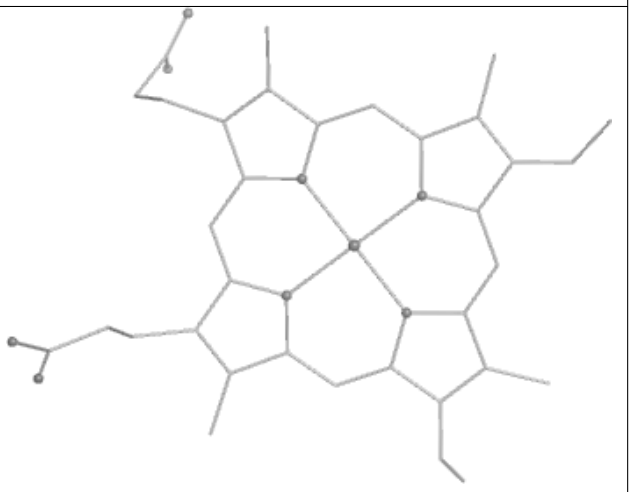
Bond lengths



Bond angles

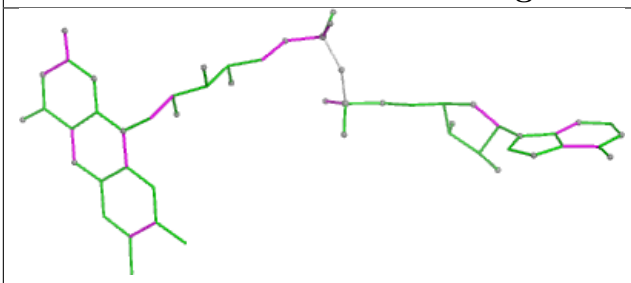


Torsions

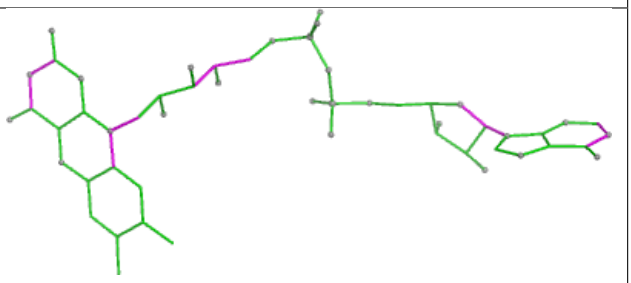


Rings

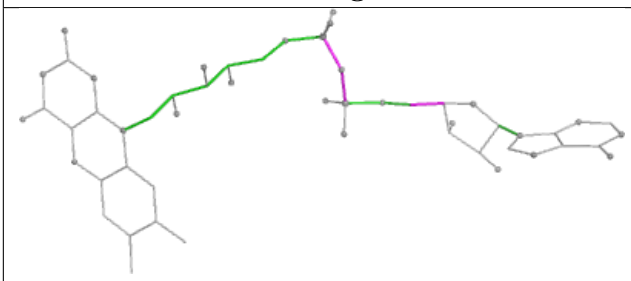
Ligand FAD D 1656



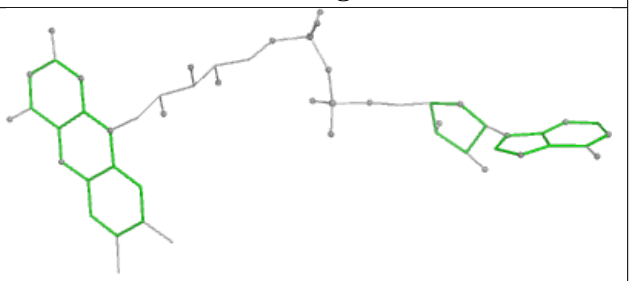
Bond lengths



Bond angles

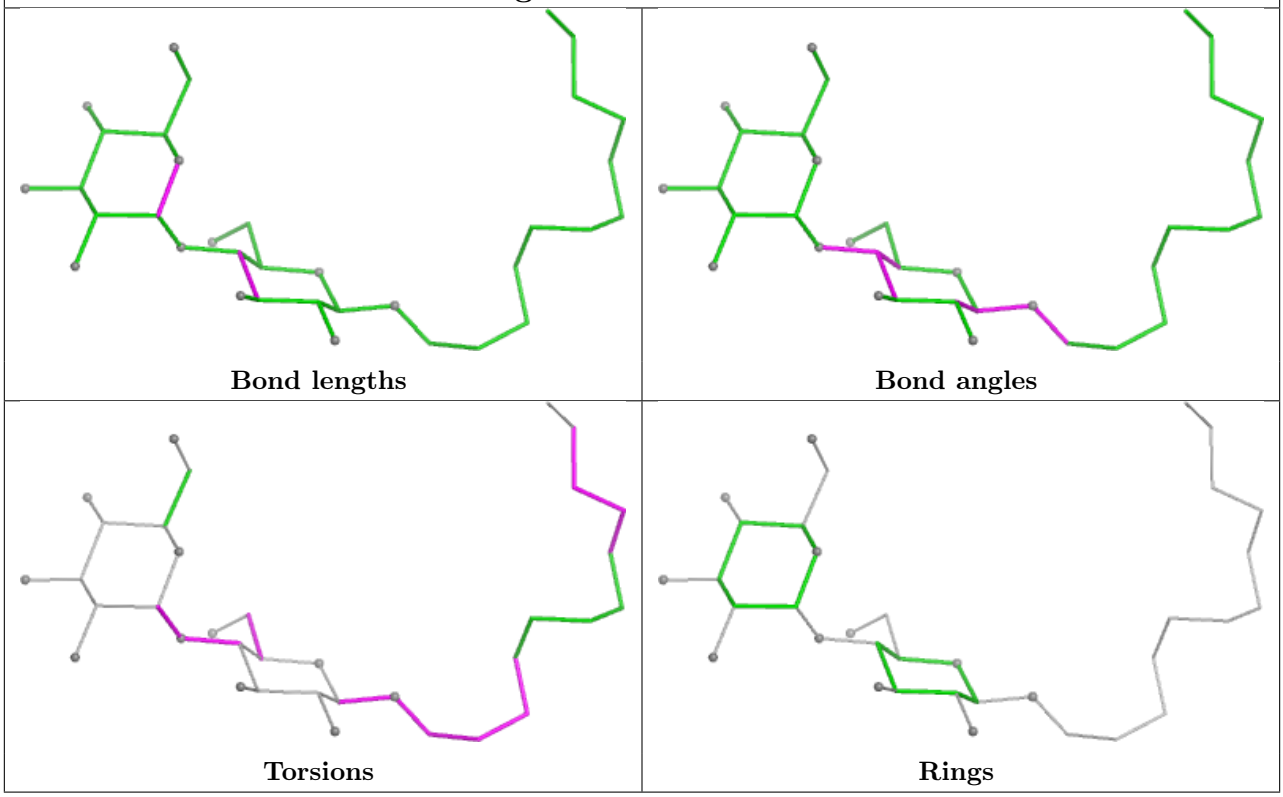


Torsions

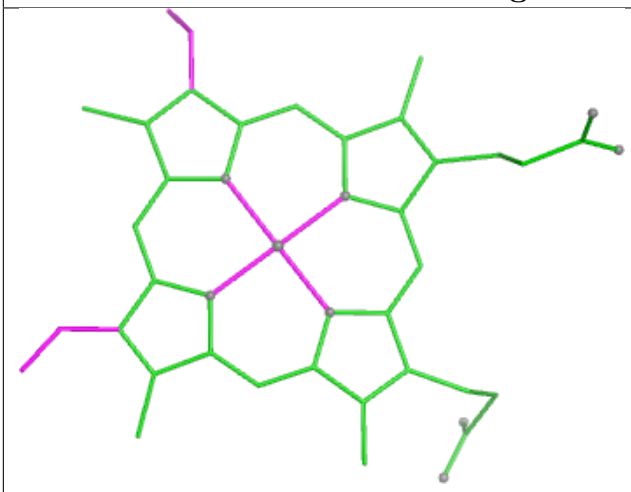


Rings

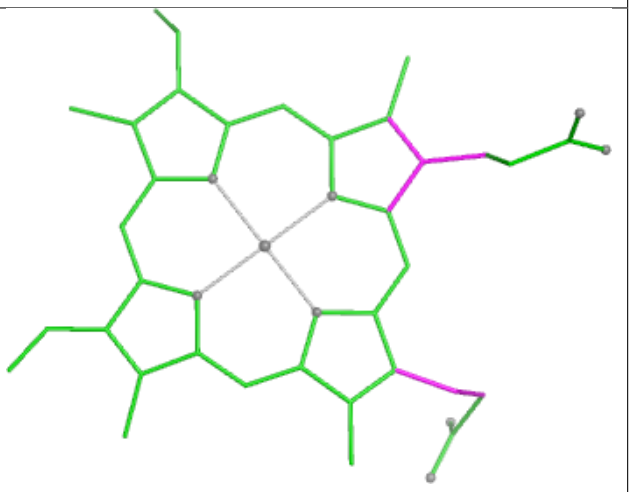
Ligand LMT F 1257



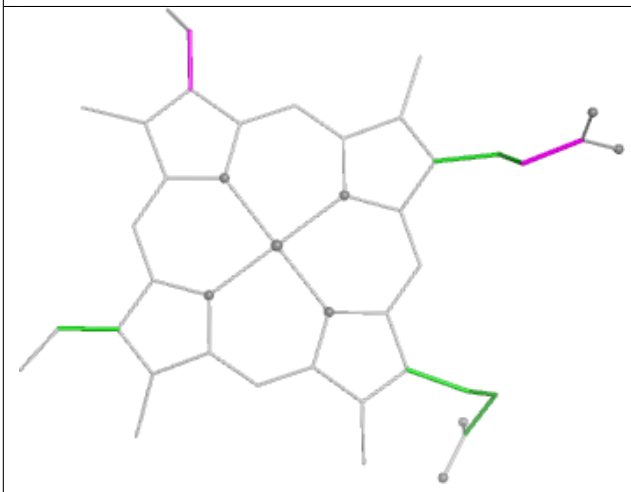
Ligand HEM C 1256



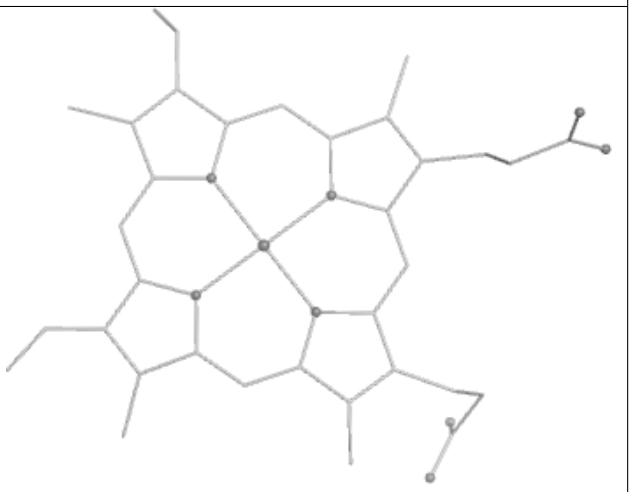
Bond lengths



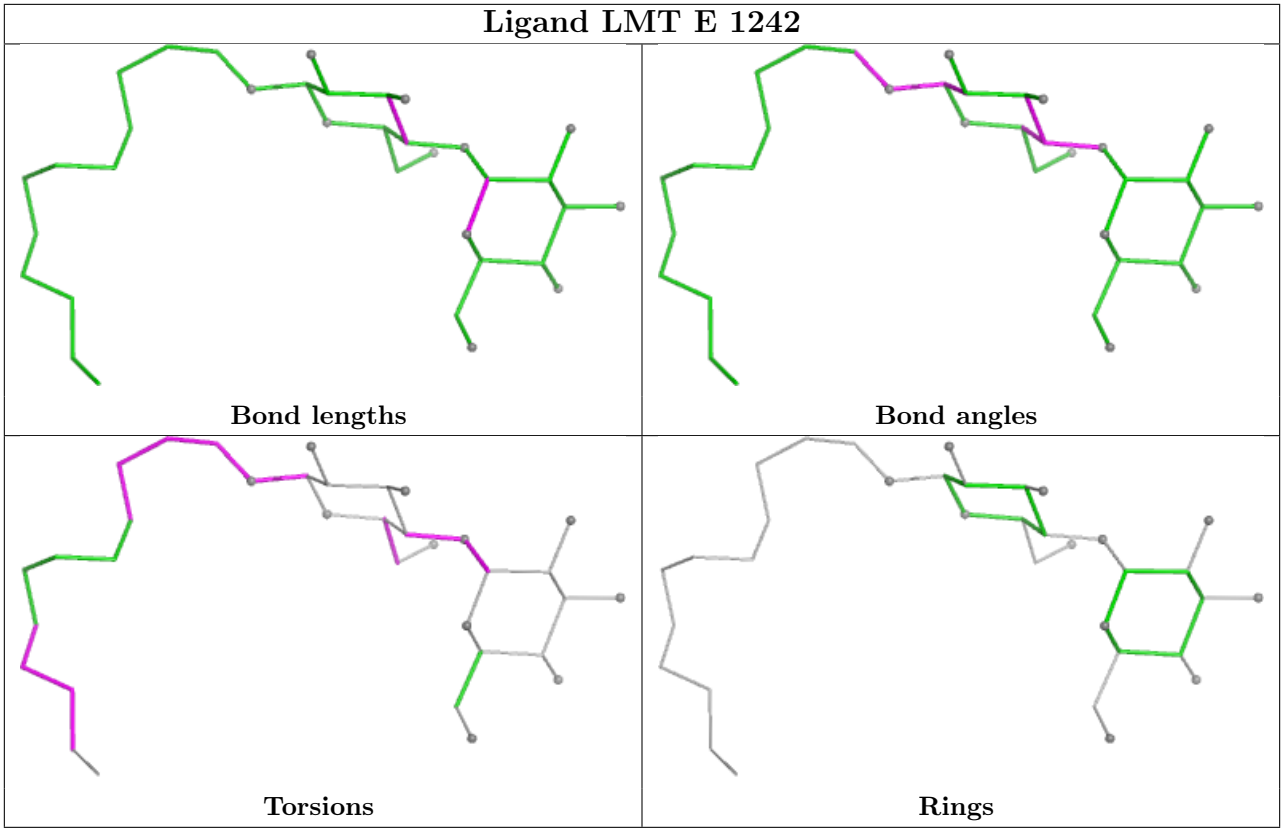
Bond angles



Torsions



Rings



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	656/656 (100%)	0.01	24 (3%)	45	42	16, 33, 70, 91	15 (2%)
1	D	656/656 (100%)	0.07	25 (3%)	44	41	16, 33, 70, 91	15 (2%)
2	B	239/239 (100%)	-0.26	2 (0%)	82	82	17, 27, 49, 88	2 (0%)
2	E	239/239 (100%)	-0.20	2 (0%)	82	82	17, 27, 49, 88	2 (0%)
3	C	255/256 (99%)	0.35	7 (2%)	56	54	22, 44, 76, 100	10 (3%)
3	F	255/256 (99%)	0.27	11 (4%)	40	38	22, 44, 76, 100	10 (3%)
All	All	2300/2302 (99%)	0.04	71 (3%)	51	49	16, 34, 70, 100	54 (2%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	GLU	4.5
1	D	271	GLY	4.2
1	A	271	GLY	3.9
1	D	338	ILE	3.5
1	D	121	ALA	3.5

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)

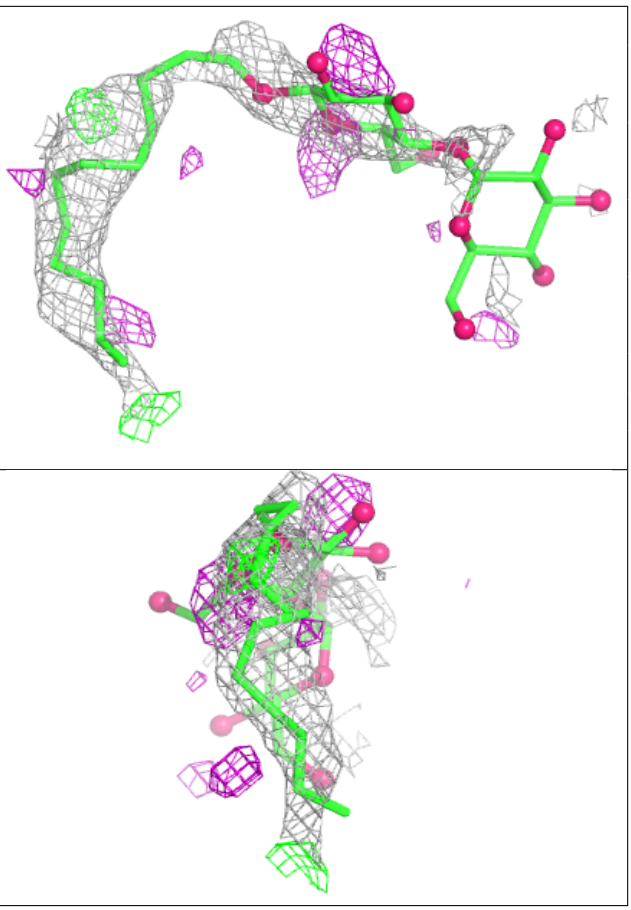
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

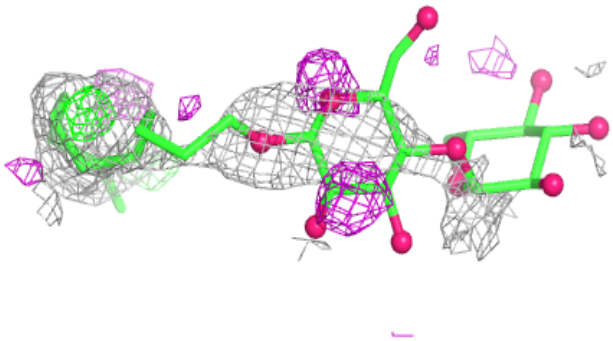
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	LMT	E	1242	35/35	0.80	0.21	60,65,68,68	16
12	DMW	E	1244	14/14	0.82	0.29	27,28,29,30	14
5	CIT	A	1657	13/13	0.83	0.30	24,28,34,35	13
5	CIT	D	1657	13/13	0.84	0.30	24,28,34,35	13
11	LMT	F	1257	35/35	0.86	0.19	60,65,68,68	16
12	DMW	F	1258	14/14	0.86	0.28	27,28,29,30	14
8	NA	E	1243	1/1	0.95	0.07	17,17,17,17	0
7	HEM	C	1256	43/43	0.96	0.09	39,44,45,46	0
7	HEM	F	1255	43/43	0.96	0.09	29,36,39,44	0
8	NA	D	1658	1/1	0.96	0.04	17,17,17,17	0
7	HEM	C	1255	43/43	0.96	0.10	29,36,39,44	0
6	F3S	E	1246	7/7	0.97	0.06	22,23,24,26	0
7	HEM	F	1256	43/43	0.97	0.08	39,44,45,46	0
4	FAD	A	1656	53/53	0.97	0.06	12,20,23,26	0
4	FAD	D	1656	53/53	0.97	0.07	12,20,23,26	0
10	SF4	E	1247	8/8	0.99	0.04	18,21,22,22	0
6	F3S	B	1240	7/7	0.99	0.04	22,23,24,26	0
9	FES	E	1240	4/4	0.99	0.04	19,20,21,21	0
9	FES	E	1245	4/4	0.99	0.03	19,20,21,21	0
10	SF4	E	1241	8/8	0.99	0.03	18,21,22,22	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 LMT E 1242:

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





Electron density around LMT F 1257:

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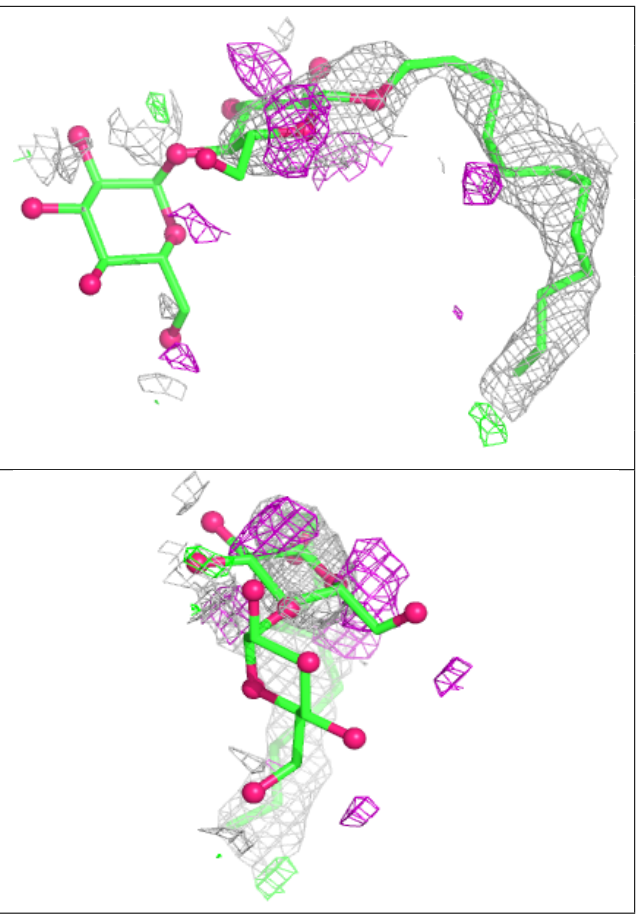
and green (positive)



Electron density around HEM C 1256:

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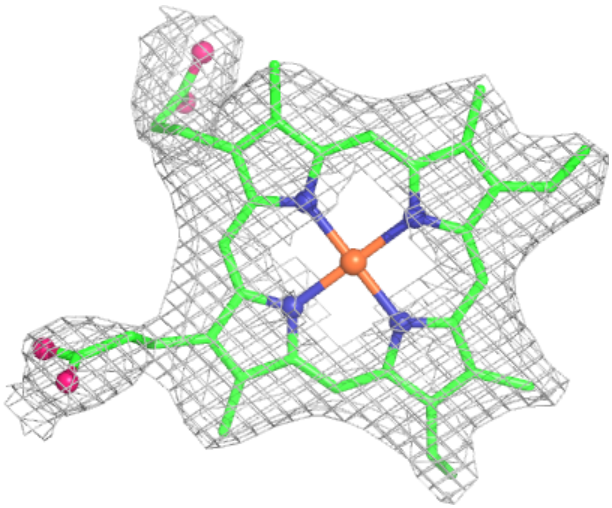
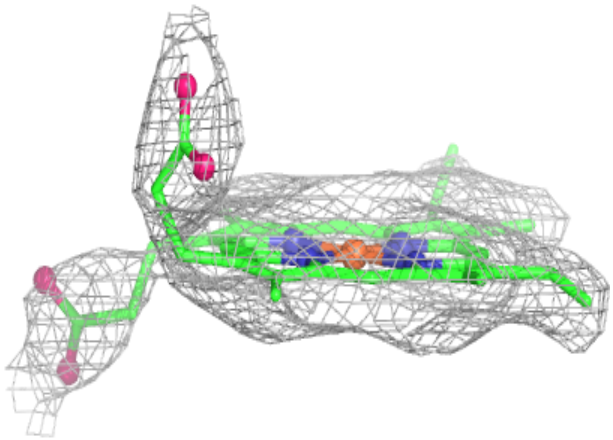
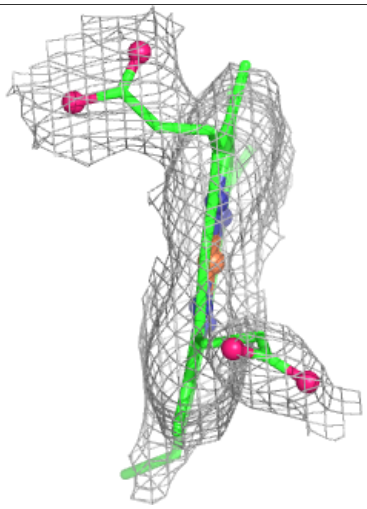
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

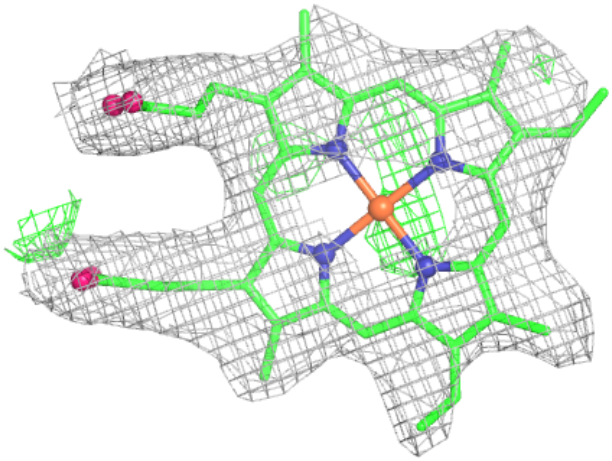


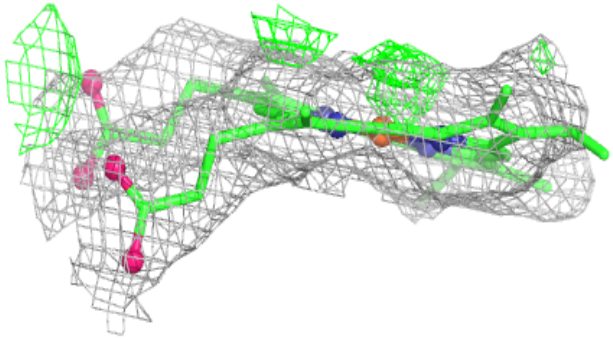


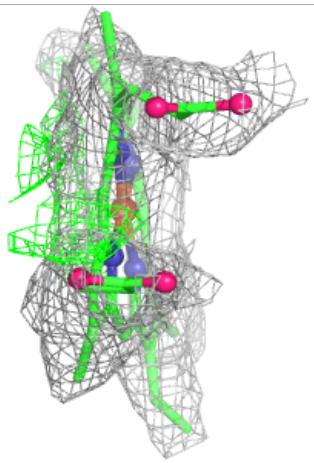


Electron density around HEM F 1255:

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

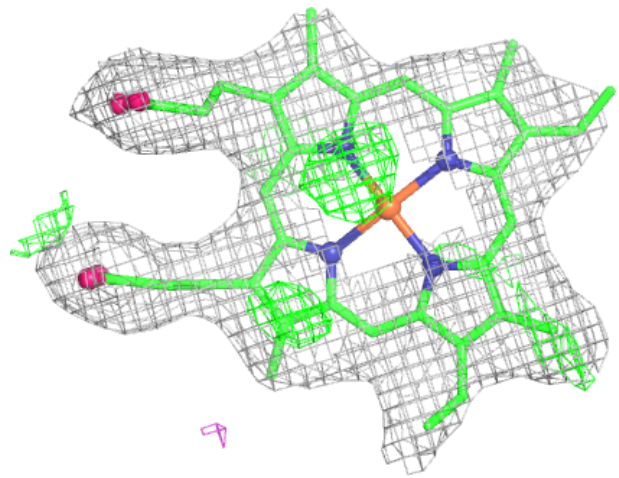


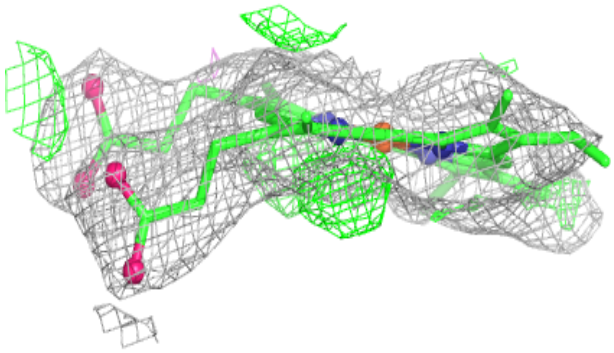


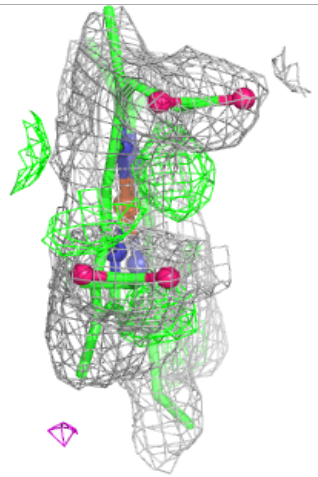


Electron density around HEM C 1255:

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

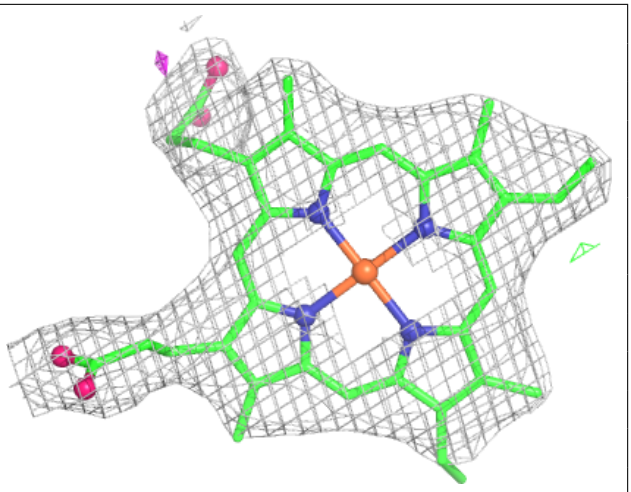


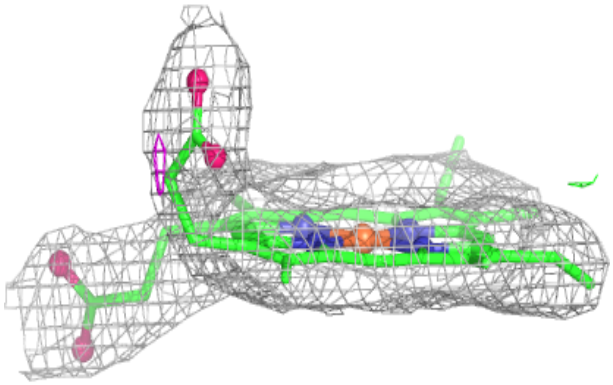


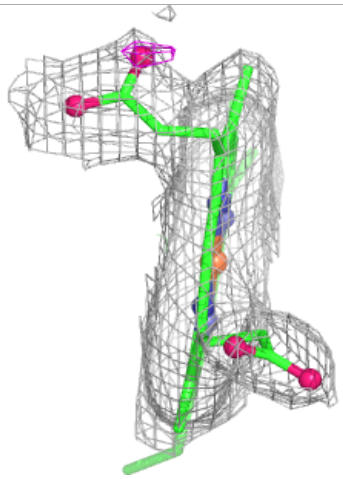


Electron density around HEM F 1256:

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

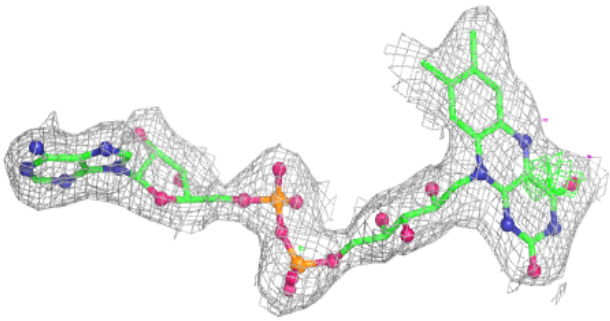


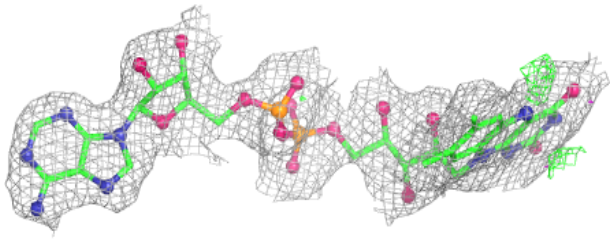


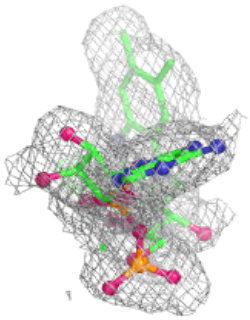


Electron density around FAD A 1656:

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

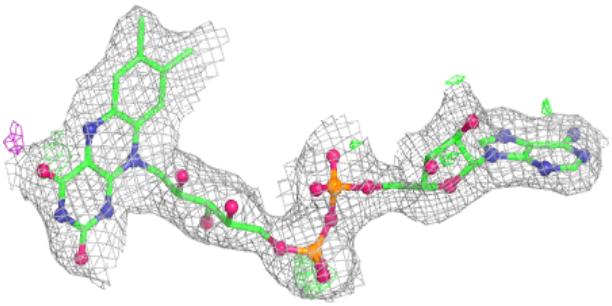


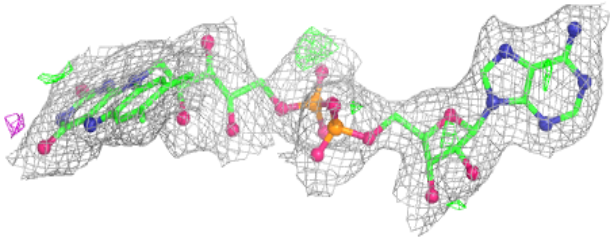


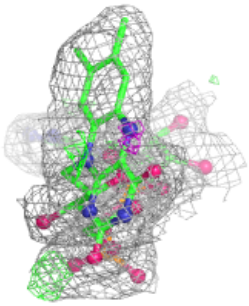


Electron density around FAD D 1656:

$2mF_o$-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.