Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 05:17 PM EDT

PDB ID	:	6MYP
Title	:	Avian mitochondrial complex II with TTFA (thenoyltrifluoroacetone) bound
Authors	:	Berry, E.A.; Huang, L.-S.
Deposited on	:	2018-11-02
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

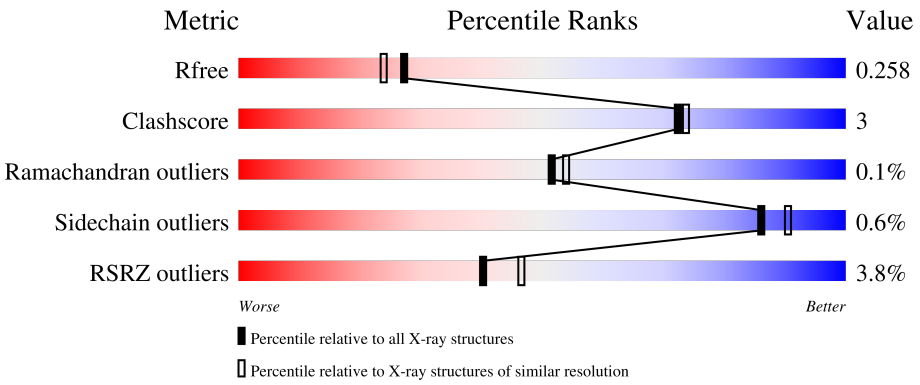
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	621	3% 88% 10% •
2	B	252	7% 88% 7% 5%
3	C	140	% 95% • ••
4	D	103	3% 95% • •

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
10	PEG	A	1006	-	-	-	X
11	UNL	A	1020	-	-	-	X
11	UNL	A	1023	-	-	X	-
11	UNL	A	1030[A]	-	-	-	X
11	UNL	A	1030[B]	-	-	-	X
11	UNL	A	1032	-	-	-	X
11	UNL	C	206	-	-	-	X
11	UNL	C	210	-	-	-	X
18	3PE	D	201	-	-	-	X
6	OAA	A	1002	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 9421 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	612	4737	2965	845	898	29	0	2	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	240	1928	1219	326	361	22	0	0	0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	139	1076	707	178	186	5	0	0	0

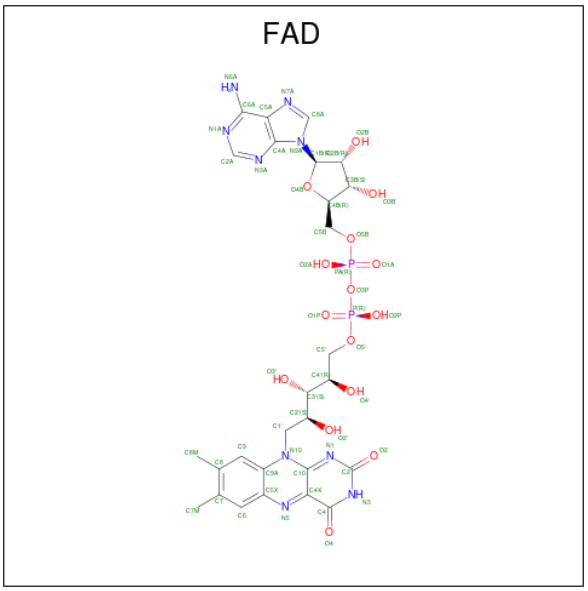
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	ALA	SER	conflict	UNP D0VWW3
C	140	MET	GLU	conflict	UNP D0VWW3

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

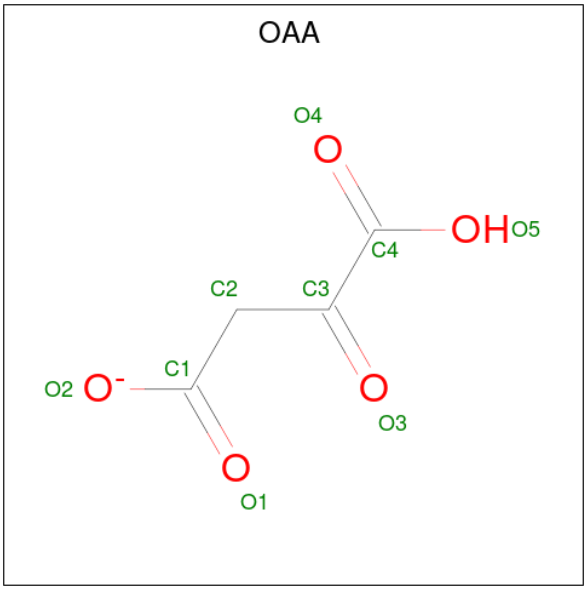
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	771	508	122	138	3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	9	4	5	0	0

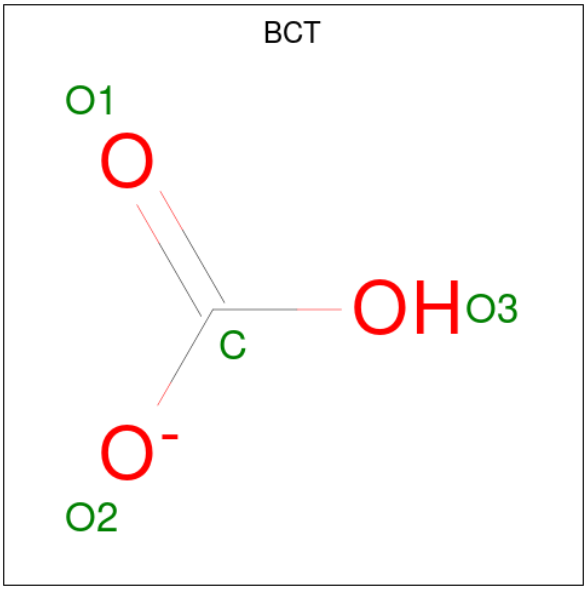
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

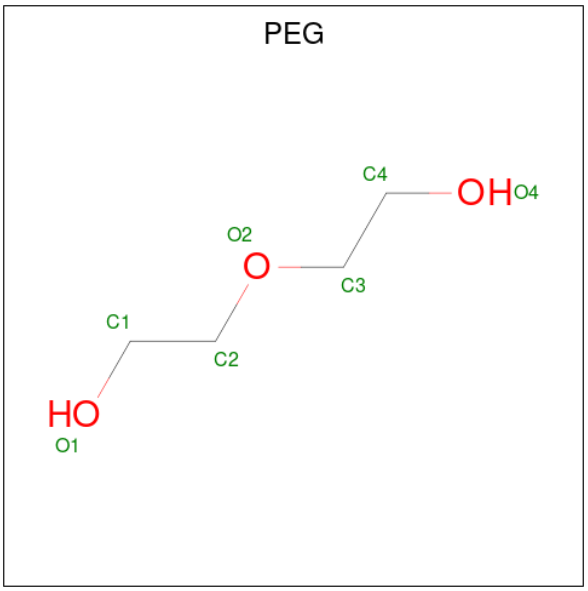
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 1 3	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

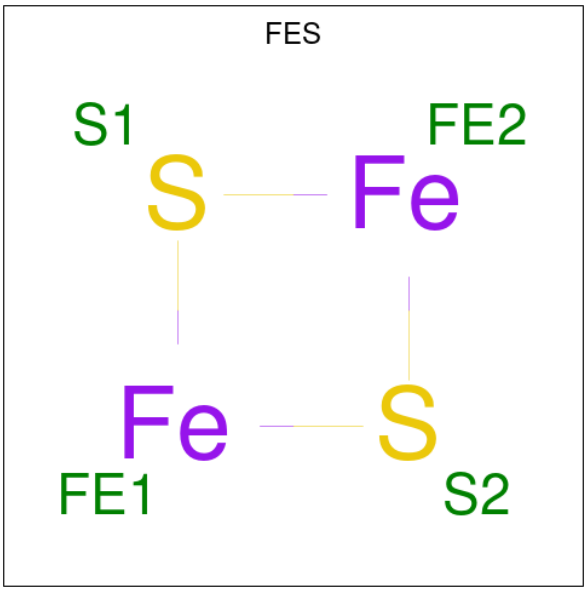


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 5 3 2	0	0

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

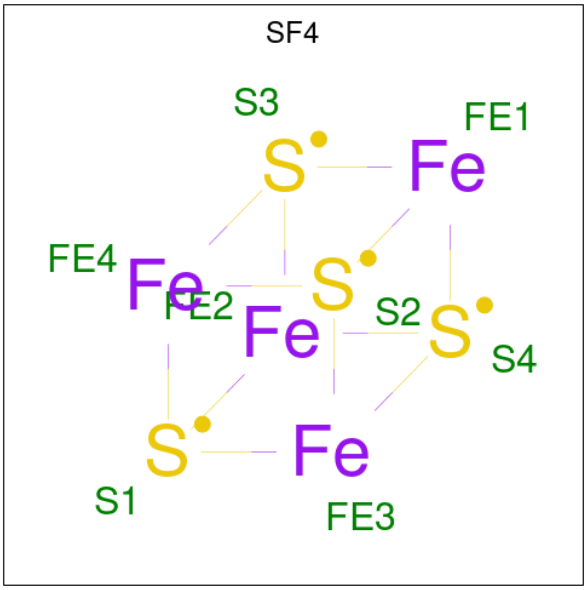
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	26	Total C N O S 82 27 20 33 2	0	1
11	B	15	Total C N O S 43 6 30 6 1	0	0
11	C	8	Total C N O S 52 27 6 18 1	0	0
11	D	14	Total C N O 71 41 5 25	0	0

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



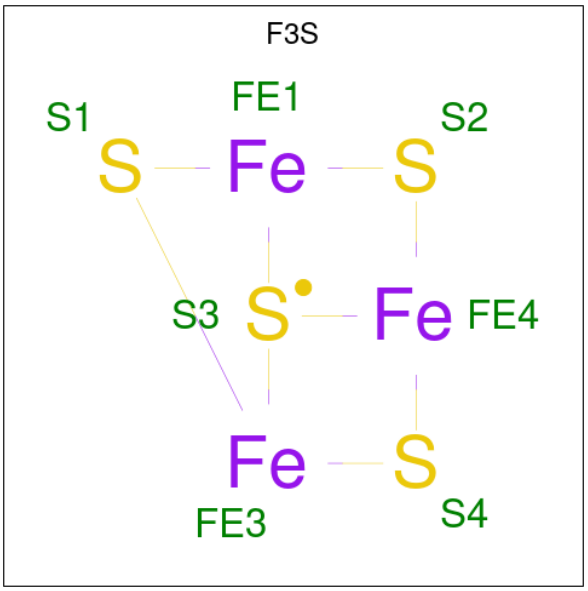
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
12	B	1	4	2	2	0	0

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



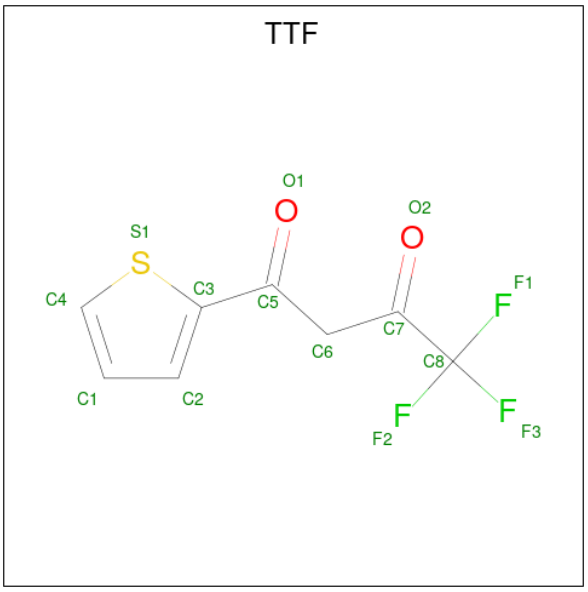
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
13	B	1	8	4	4	0	0

- Molecule 14 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



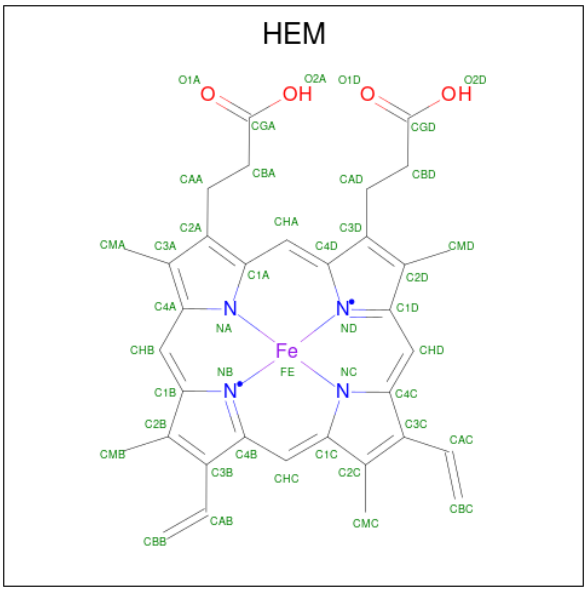
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	B	1	7	3	4	0	0

- Molecule 15 is 4,4,4-TRIFLUORO-1-THIEN-2-YLBUTANE-1,3-DIONE (three-letter code: TTF) (formula: $C_8H_5F_3O_2S$).



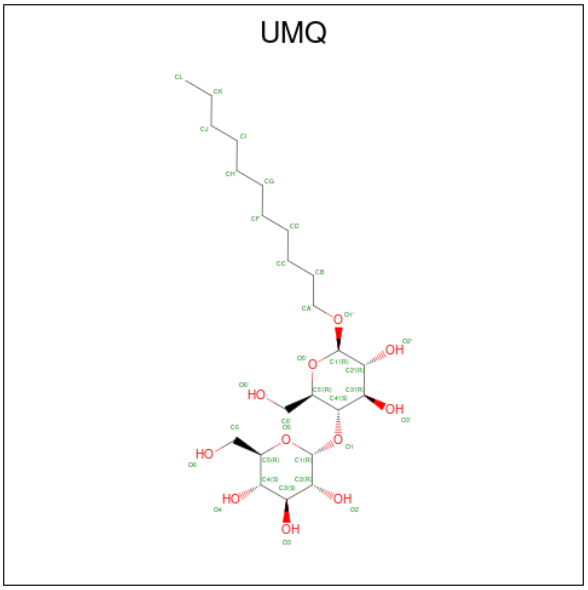
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	O	S		
15	C	1	14	8	3	2	1	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



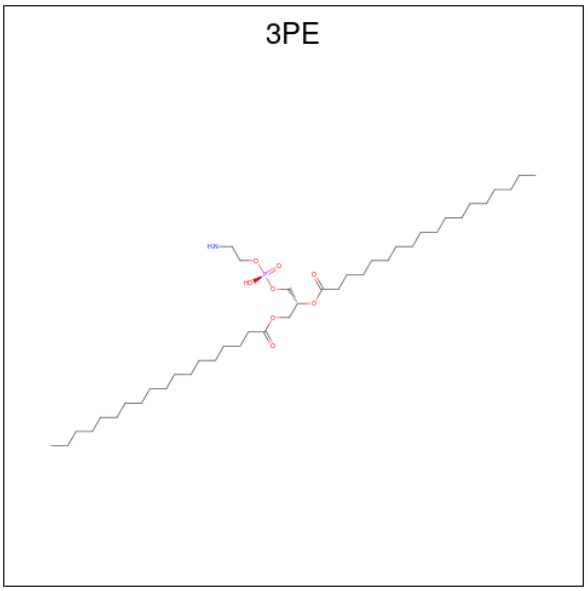
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
16	C	1	41	32	1	4	4	0	0

- Molecule 17 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



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

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
18	D	1	42	32	1	8	1	0	0

- Molecule 19 is water.

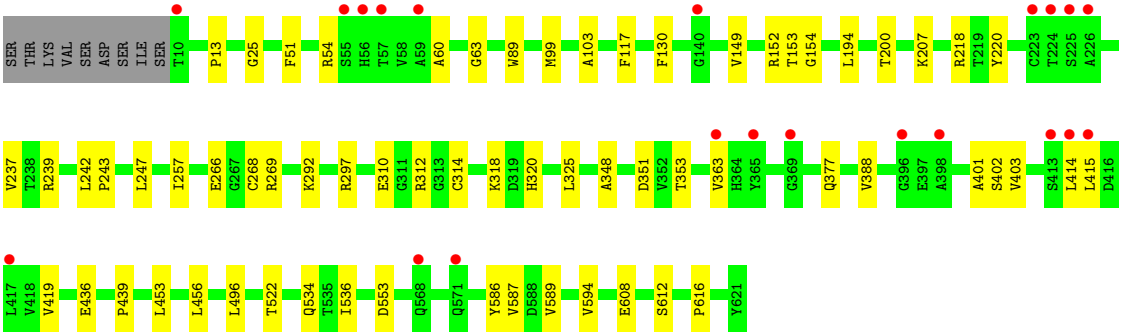
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	214	214	214	0	0
			Total	O		
19	B	143	144	144	0	1
			Total	O		
19	C	54	54	54	0	0
			Total	O		
19	D	26	26	26	0	0

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.

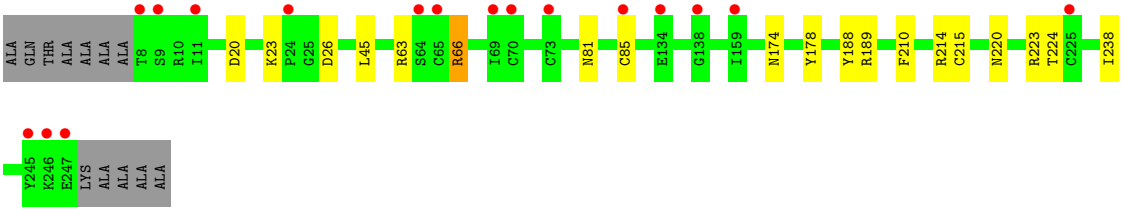
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A:



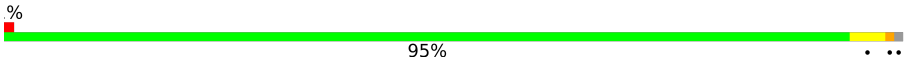
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

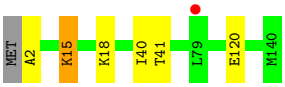
Chain B:



• Molecule 3: Succinate dehydrogenase cytochrome b, large subunit

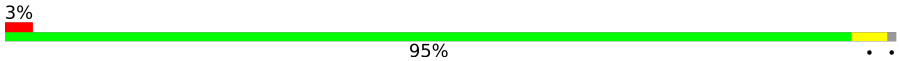
Chain C:





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

Chain D:



GLY
S2
L29
Y30
T44
D57
F80
W101
S102
I103

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.95Å 84.30Å 290.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.36 – 2.10 50.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.36-2.10) 93.2 (50.36-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.10Å)	Xtriage
Refinement program	PHENIX (DEV_3150: ???)	Depositor
R, R_{free}	0.235 , 0.259 0.235 , 0.258	Depositor DCC
R_{free} test set	2048 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: MLZ, TTF, PEG, OAA, F3S, FES, UMQ, FAD, K, UNL, BCT, MG, SF4, 3PE, 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	0.23	0/4841	0.42	0/6554
2	B	0.23	0/1970	0.40	0/2656
3	C	0.23	0/1094	0.36	0/1486
4	D	0.23	0/794	0.35	0/1089
All	All	0.23	0/8699	0.40	0/11785

There are no bond length outliers.

There are no bond angle outliers.

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	4737	0	4625	43	0
2	B	1928	0	1921	11	0
3	C	1076	0	1115	5	0
4	D	771	0	763	2	0
5	A	53	0	29	2	0
6	A	9	0	2	5	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	4	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	5	0	5	0	0
11	A	82	0	0	3	0
11	B	43	0	0	1	0
11	C	52	0	0	0	0
11	D	71	0	0	0	0
12	B	4	0	0	0	0
13	B	8	0	0	0	0
14	B	7	0	0	1	0
15	C	14	0	5	1	0
16	C	41	0	24	0	0
17	C	34	0	44	1	0
18	D	42	0	61	0	0
19	A	214	0	0	3	0
19	B	144	0	0	0	0
19	C	54	0	0	1	0
19	D	26	0	0	0	0
All	All	9421	0	8595	59	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 3.

All (59) 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:297:ARG:HH22	6:A:1002:OAA:C2	1.20	1.49
1:A:297:ARG:NH2	6:A:1002:OAA:H22	1.04	1.35
1:A:297:ARG:HH22	6:A:1002:OAA:C1	1.83	0.92
1:A:297:ARG:NH2	6:A:1002:OAA:C2	1.97	0.91
1:A:297:ARG:HH21	6:A:1002:OAA:H22	1.33	0.89
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.70	0.73
2:B:20:ASP:OD2	2:B:23:LYS:NZ	2.30	0.64
2:B:174:ASN:HD21	4:D:57:ASP:HA	1.64	0.61
1:A:207:LYS:HG2	1:A:439:PRO:HD3	1.81	0.61
1:A:401:ALA:N	1:A:402:SER:HA	2.16	0.60
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.85	0.58
3:C:41:THR:HG21	17:C:203:UMQ:HK1	1.87	0.56
1:A:194:LEU:HD22	1:A:453:LEU:HD11	1.88	0.54
1:A:310:GLU:OE1	1:A:312:ARG:NH2	2.39	0.54
1:A:553:ASP:OD1	1:A:553:ASP:N	2.40	0.54
1:A:207:LYS:NZ	1:A:436:GLU:OE1	2.36	0.53
1:A:218:ARG:NH1	19:A:1120:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.91	0.53
1:A:239:ARG:HG2	1:A:589:VAL:HG11	1.91	0.53
1:A:257:ILE:HD11	1:A:348:ALA:HB2	1.91	0.52
2:B:188:TYR:HB2	2:B:238:ILE:HD11	1.90	0.52
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.92	0.51
3:C:2:ALA:N	19:C:305:HOH:O	2.43	0.51
2:B:223:ARG:NH2	3:C:120:GLU:OE2	2.40	0.50
1:A:13:PRO:HG2	1:A:200:THR:HG22	1.94	0.49
2:B:220:ASN:OD1	11:B:1018:UNL:O	2.31	0.49
3:C:15:MLZ:HA	3:C:18:LYS:HE2	1.93	0.49
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.48	0.48
1:A:103:ALA:HA	1:A:415:LEU:HD11	1.95	0.48
1:A:63:GLY:HA2	1:A:153:THR:HG21	1.94	0.48
1:A:608:GLU:O	11:A:1023:UNL:O	2.32	0.48
1:A:99:MET:HA	1:A:419:VAL:HG11	1.96	0.47
2:B:210:PHE:HA	2:B:214:ARG:HG2	1.98	0.46
1:A:612:SER:OG	11:A:1023:UNL:O	2.27	0.46
1:A:237:VAL:HG13	1:A:242:LEU:HB2	1.98	0.45
1:A:247:LEU:HD12	1:A:534:GLN:HB2	1.99	0.45
2:B:81:ASN:O	2:B:224:THR:OG1	2.35	0.45
1:A:587:VAL:HG22	1:A:594:VAL:HG22	1.99	0.44
1:A:314:CYS:N	1:A:320:HIS:O	2.42	0.44
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.53	0.44
3:C:40:ILE:HD13	15:C:202:TTF:H61	2.01	0.43
2:B:215:CYS:HA	14:B:1003:F3S:S2	2.58	0.43
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.99	0.43
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.33	0.43
1:A:292:LYS:NZ	19:A:1137:HOH:O	2.47	0.42
1:A:152:ARG:NH2	19:A:1116:HOH:O	2.39	0.42
1:A:496:LEU:HD12	1:A:536:ILE:HG21	2.00	0.42
1:A:534:GLN:O	11:A:1015:UNL:O	2.38	0.42
1:A:401:ALA:HB3	1:A:403:VAL:N	2.36	0.41
1:A:414:LEU:HG	5:A:1001:FAD:C2	2.50	0.41
1:A:377:GLN:HB3	1:A:388:VAL:HG13	2.02	0.41
1:A:351:ASP:OD2	1:A:353:THR:OG1	2.36	0.41
1:A:51:PHE:HB3	1:A:54:ARG:HG2	2.01	0.41
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.56	0.41
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.56	0.41
1:A:318:LYS:HE3	1:A:318:LYS:HB3	1.97	0.40
2:B:23:LYS:HB2	2:B:26:ASP:HB2	2.03	0.40
2:B:45:LEU:HD22	2:B:85:CYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD13	1:A:522:THR:HG22	2.04	0.40

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	612/621 (99%)	589 (96%)	23 (4%)	0	100	100
2	B	238/252 (94%)	229 (96%)	8 (3%)	1 (0%)	34	32
3	C	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
4	D	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
All	All	1086/1116 (97%)	1051 (97%)	34 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	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	498/506 (98%)	497 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	216/219 (99%)	213 (99%)	3 (1%)	67	73
3	C	116/117 (99%)	116 (100%)	0	100	100
4	D	78/79 (99%)	77 (99%)	1 (1%)	69	75
All	All	908/921 (99%)	903 (99%)	5 (1%)	86	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	PHE
2	B	63	ARG
2	B	66	ARG
2	B	189	ARG
4	D	101	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	MLZ	C	15	3	8,9,10	0.65	0	4,9,11	1.51	1 (25%)

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
3	MLZ	C	15	3	-	0/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	15	MLZ	CM-NZ-CE	2.86	120.21	111.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	15	MLZ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 2 are monoatomic and 64 are unknown - leaving 11 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	$\#\|Z\| > 2$
6	OAA	A	1002	-	8,8,8	2.18	1 (12%)	9,10,10	1.14	1 (11%)
15	TTF	C	202	-	13,14,14	0.67	0	13,20,20	1.42	2 (15%)
16	HEM	C	201	3,4	40,48,50	1.25	1 (2%)	46,80,82	1.43	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	UMQ	C	203	-	35,35,35	0.40	0	46,46,46	0.64	1 (2%)
18	3PE	D	201	-	41,41,50	1.03	2 (4%)	44,46,55	1.07	2 (4%)
5	FAD	A	1001	1	53,58,58	0.85	1 (1%)	68,89,89	1.22	6 (8%)
14	F3S	B	1003	2	0,9,9	-	-	-		
12	FES	B	1001	2	0,4,4	-	-	-		
13	SF4	B	1002	2	0,12,12	-	-	-		
10	PEG	A	1006	-	4,4,6	0.41	0	3,3,5	0.32	0
9	BCT	A	1005	-	2,3,3	1.16	0	2,3,3	4.51	2 (100%)

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
6	OAA	A	1002	-	-	5/8/8/8	-
16	HEM	C	201	3,4	-	3/10/50/54	-
15	TTF	C	202	-	-	1/10/14/14	0/1/1/1
17	UMQ	C	203	-	-	1/20/60/60	0/2/2/2
18	3PE	D	201	-	-	6/45/45/54	-
5	FAD	A	1001	1	-	6/30/50/50	0/6/6/6
14	F3S	B	1003	2	-	-	0/3/3/3
12	FES	B	1001	2	-	-	0/1/1/1
13	SF4	B	1002	2	-	-	0/6/5/5
10	PEG	A	1006	-	-	0/2/2/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	OAA	C3-C4	-5.49	1.46	1.53
18	D	201	3PE	O31-C31	4.29	1.45	1.33
18	D	201	3PE	O21-C21	4.22	1.46	1.34
5	A	1001	FAD	C4-N3	-2.74	1.33	1.38
16	C	201	HEM	C2C-C3C	-2.26	1.34	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1005	BCT	O2-C-O1	5.56	133.96	119.55
5	A	1001	FAD	C4-N3-C2	-4.09	118.09	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	202	TTF	C1-C4-S1	-3.96	109.77	112.98
18	D	201	3PE	O21-C21-C22	3.75	119.59	111.50
5	A	1001	FAD	C4X-C4-N3	3.42	121.88	113.19
16	C	201	HEM	C1B-NB-C4B	3.24	108.42	105.07
9	A	1005	BCT	O3-C-O1	-3.13	111.43	119.55
16	C	201	HEM	C4D-ND-C1D	3.02	108.19	105.07
18	D	201	3PE	O31-C31-C32	2.81	120.72	111.91
5	A	1001	FAD	P-O3P-PA	-2.81	123.20	132.83
5	A	1001	FAD	O4-C4-C4X	-2.72	119.38	126.60
16	C	201	HEM	C4B-CHC-C1C	2.49	125.84	122.56
5	A	1001	FAD	C4X-C10-N1	-2.45	119.05	124.73
16	C	201	HEM	C4C-CHD-C1D	2.42	125.76	122.56
15	C	202	TTF	O1-C5-C6	2.29	123.14	120.56
17	C	203	UMQ	C1-O1-C4'	-2.13	112.68	117.96
16	C	201	HEM	C3D-C4D-ND	-2.08	107.84	110.17
5	A	1001	FAD	C10-N1-C2	2.07	121.03	116.90
6	A	1002	OAA	O4-C4-C3	-2.05	118.99	121.72

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
6	A	1002	OAA	O2-C1-C2-C3
6	A	1002	OAA	O3-C3-C4-O4
6	A	1002	OAA	O3-C3-C4-O5
6	A	1002	OAA	C2-C3-C4-O5
18	D	201	3PE	O22-C21-O21-C2
18	D	201	3PE	C22-C21-O21-C2
18	D	201	3PE	C21-C22-C23-C24
17	C	203	UMQ	CA-CB-CC-CD
5	A	1001	FAD	PA-O3P-P-O5'
6	A	1002	OAA	C2-C3-C4-O4
5	A	1001	FAD	P-O3P-PA-O2A
5	A	1001	FAD	O4B-C4B-C5B-O5B
15	C	202	TTF	C6-C7-C8-F1
16	C	201	HEM	C2A-CAA-CBA-CGA
16	C	201	HEM	CAA-CBA-CGA-O2A
5	A	1001	FAD	C5B-O5B-PA-O1A
18	D	201	3PE	C1-O11-P-O14
18	D	201	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
16	C	201	HEM	CAA-CBA-CGA-O1A
18	D	201	3PE	O22-C21-C22-C23

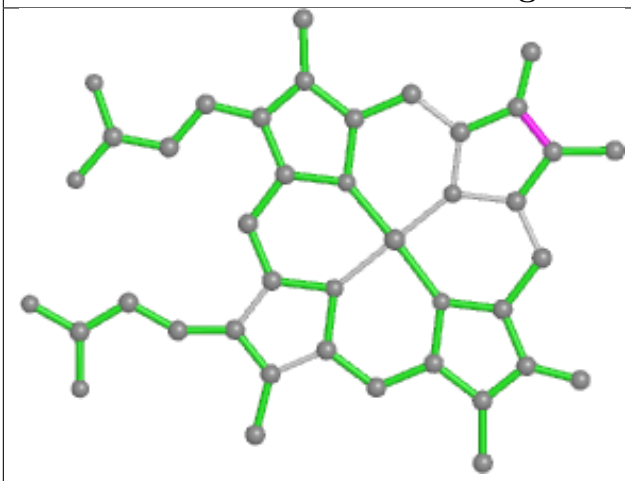
There are no ring outliers.

5 monomers are involved in 10 short contacts:

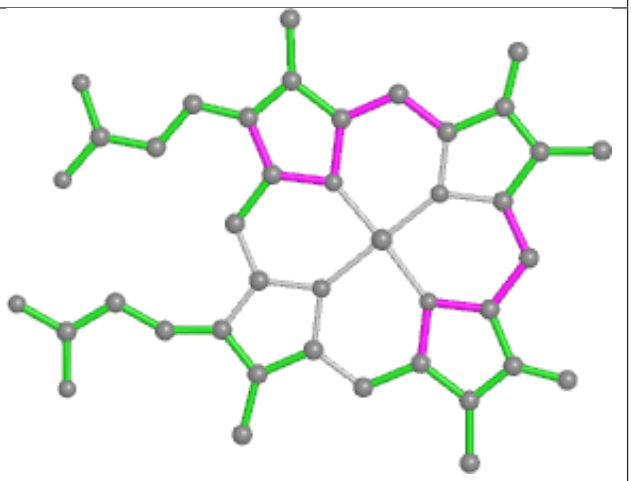
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	OAA	5	0
15	C	202	TTF	1	0
17	C	203	UMQ	1	0
5	A	1001	FAD	2	0
14	B	1003	F3S	1	0

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.

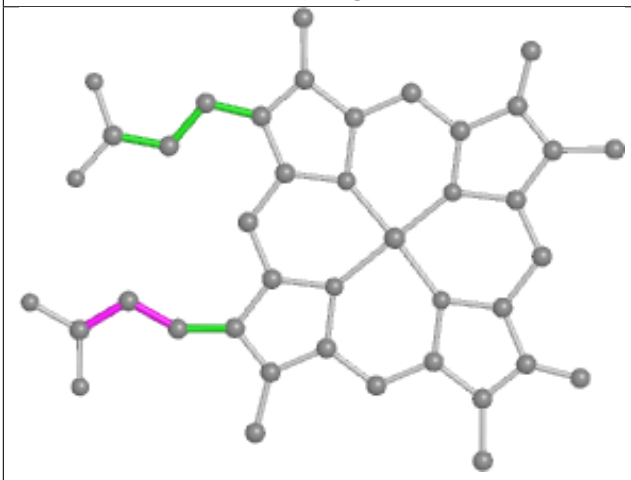
Ligand HEM C 201



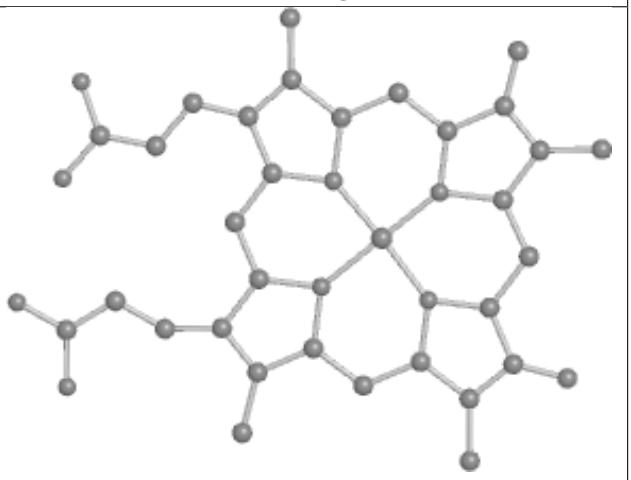
Bond lengths



Bond angles

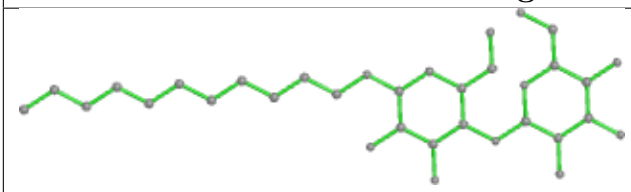


Torsions

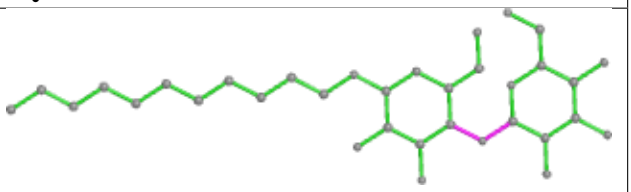


Rings

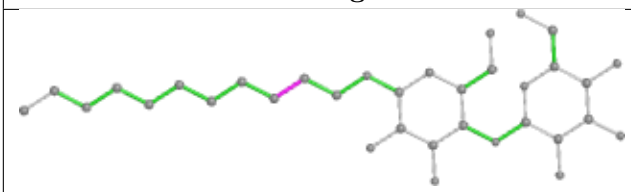
Ligand UMQ C 203



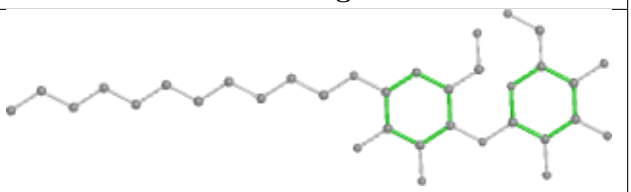
Bond lengths



Bond angles

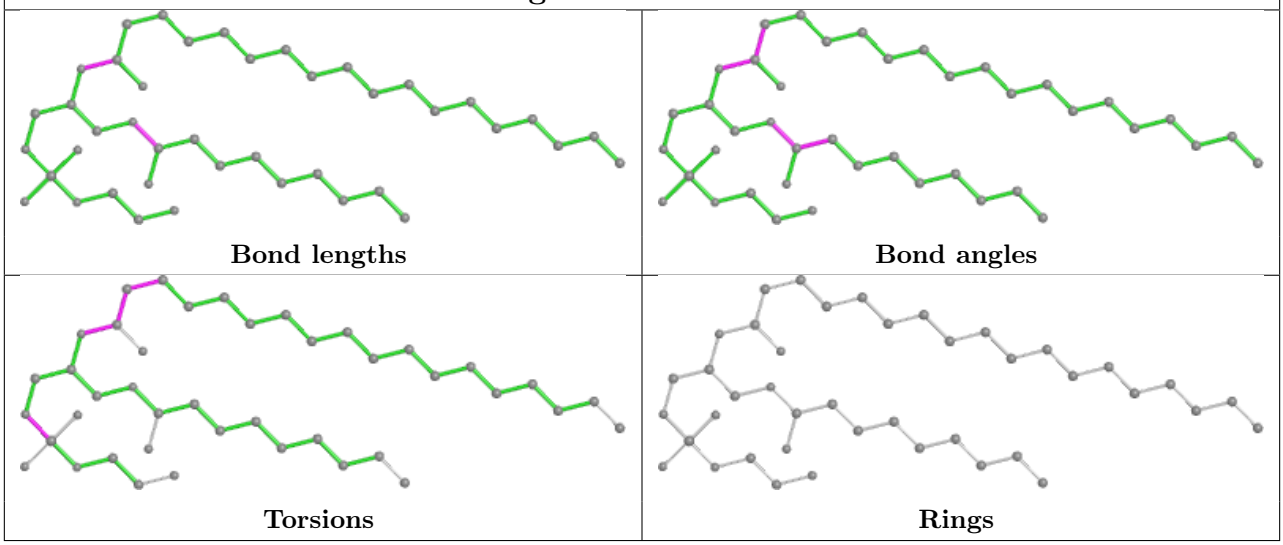


Torsions

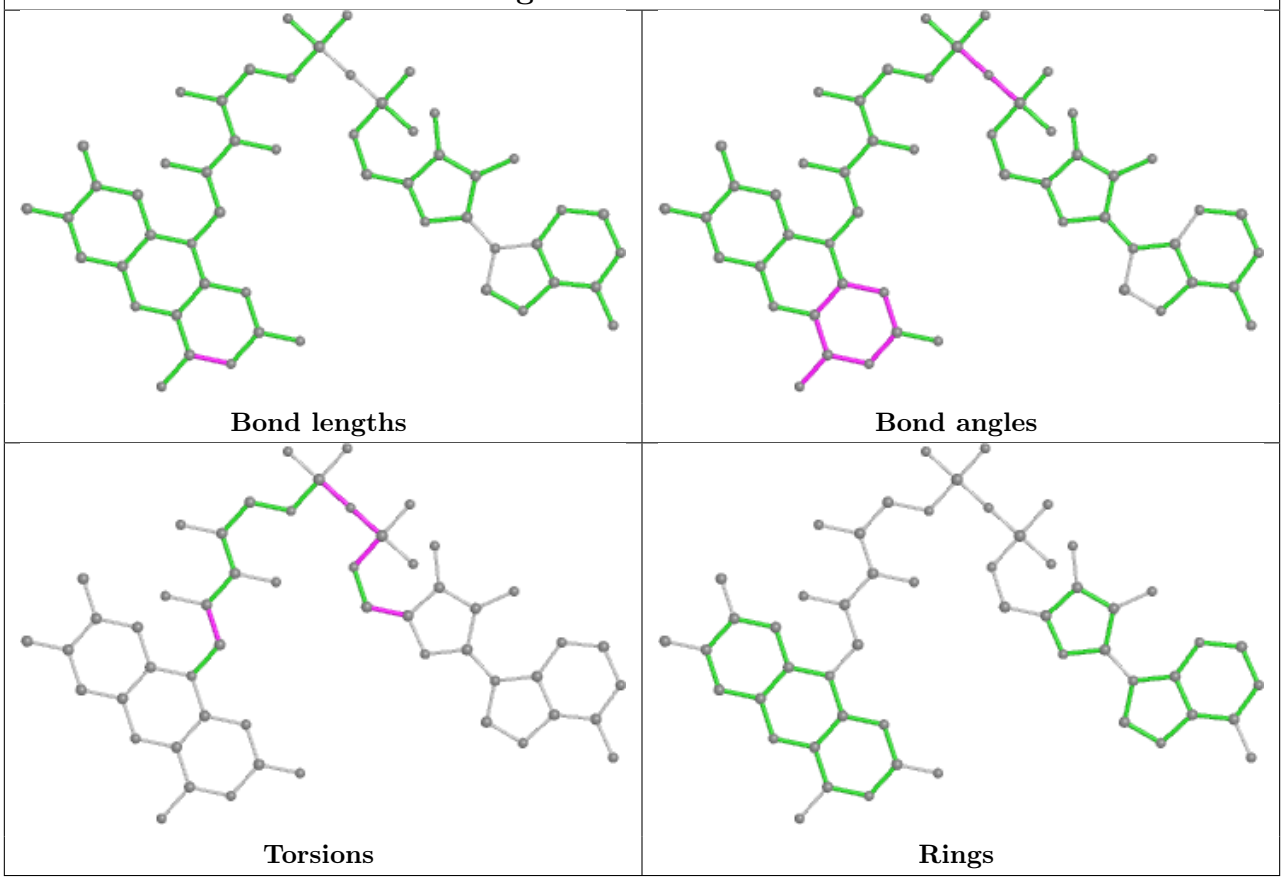


Rings

Ligand 3PE D 201



Ligand FAD A 1001



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	612/621 (98%)	0.21	21 (3%)	45	51	30, 50, 78, 106	1 (0%)
2	B	240/252 (95%)	0.21	17 (7%)	16	20	30, 41, 78, 108	0
3	C	138/140 (98%)	0.01	1 (0%)	87	89	35, 46, 79, 92	0
4	D	102/103 (99%)	0.04	3 (2%)	51	57	35, 46, 71, 91	0
All	All	1092/1116 (97%)	0.17	42 (3%)	40	46	30, 48, 78, 108	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	TYR	4.1
1	A	226	ALA	4.0
2	B	65	CYS	3.5
1	A	140	GLY	3.5
1	A	225	SER	3.5
4	D	30	TYR	3.3
2	B	134	GLU	3.2
2	B	247	GLU	3.1
2	B	70	CYS	3.1
1	A	224	THR	3.1
1	A	417	LEU	3.1
2	B	138	GLY	2.9
1	A	10	THR	2.9
1	A	223	CYS	2.8
1	A	56	HIS	2.8
2	B	8	THR	2.8
2	B	24	PRO	2.8
2	B	246	LYS	2.7
2	B	9	SER	2.6
4	D	2	SER	2.6
1	A	571	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	365	TYR	2.5
2	B	225	CYS	2.5
4	D	29	LEU	2.5
1	A	55	SER	2.5
1	A	57	THR	2.5
1	A	568	GLN	2.5
2	B	64	SER	2.5
1	A	59	ALA	2.3
1	A	363	VAL	2.3
3	C	79	LEU	2.3
2	B	11	ILE	2.3
1	A	414	LEU	2.1
1	A	415	LEU	2.1
1	A	398	ALA	2.1
2	B	69	ILE	2.1
2	B	159	ILE	2.1
2	B	85	CYS	2.1
1	A	413	SER	2.1
1	A	396	GLY	2.0
2	B	73	CYS	2.0
1	A	369	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	MLZ	C	15	10/11	0.90	0.15	54,55,58,61	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	UNL	A	1030[A]	1/-	0.51	0.48	53,53,53,53	1
11	UNL	A	1030[B]	1/-	0.51	0.48	51,51,51,51	1
11	UNL	D	210	13/-	0.53	0.31	83,90,95,96	0
11	UNL	B	1008	3/-	0.54	0.24	75,75,77,77	0
11	UNL	C	210	2/-	0.56	0.40	42,42,42,45	0
11	UNL	A	1020	6/-	0.57	0.46	80,82,87,87	0
11	UNL	A	1032	1/-	0.59	0.47	71,71,71,71	0
11	UNL	C	206	23/-	0.61	0.82	65,72,76,78	23
11	UNL	A	1015	3/-	0.66	0.38	50,50,53,53	0
11	UNL	A	1011	4/-	0.67	0.15	60,61,63,67	0
11	UNL	D	215	1/-	0.67	0.33	57,57,57,57	0
11	UNL	A	1031	1/-	0.68	0.19	62,62,62,62	0
11	UNL	D	209	5/-	0.68	0.26	72,73,76,76	0
11	UNL	D	202	11/-	0.70	0.20	77,83,85,85	0
18	3PE	D	201	42/51	0.70	0.48	89,101,126,127	0
11	UNL	A	1008	4/-	0.72	0.34	87,88,88,88	0
11	UNL	D	208	4/-	0.72	0.18	77,78,78,78	0
11	UNL	B	1013	3/-	0.72	0.25	64,64,67,68	0
11	UNL	D	212	10/-	0.74	0.23	57,65,69,71	0
11	UNL	C	208	3/-	0.75	0.16	68,68,69,70	0
11	UNL	D	205	3/-	0.75	0.31	44,44,44,46	3
11	UNL	A	1012	3/-	0.76	0.28	38,38,39,52	3
11	UNL	A	1024	2/-	0.77	0.26	59,59,59,60	0
11	UNL	B	1007	3/-	0.78	0.25	68,68,69,69	0
11	UNL	A	1019	3/-	0.78	0.21	56,56,57,59	0
11	UNL	A	1016	3/-	0.79	0.22	48,48,52,52	0
11	UNL	D	214	1/-	0.79	0.18	64,64,64,64	0
10	PEG	A	1006	5/7	0.80	0.43	68,68,70,71	0
11	UNL	D	211	10/-	0.81	0.21	82,88,90,91	0
11	UNL	A	1014	10/-	0.82	0.29	89,92,94,94	0
11	UNL	B	1014	3/-	0.82	0.45	47,47,48,50	0
11	UNL	D	213	1/-	0.82	0.19	64,64,64,64	0
11	UNL	B	1011	3/-	0.83	0.20	69,69,72,73	0
11	UNL	D	206	3/-	0.84	0.10	68,68,68,69	0
9	BCT	A	1005	4/4	0.84	0.22	72,72,74,74	0
11	UNL	A	1029	1/-	0.85	0.31	50,50,50,50	0
11	UNL	C	209	1/-	0.85	0.26	41,41,41,41	0
11	UNL	B	1016	3/-	0.85	0.31	55,55,56,59	3
11	UNL	B	1006	3/-	0.85	0.15	63,63,63,65	0
11	UNL	C	207	12/-	0.85	0.24	70,75,77,78	0

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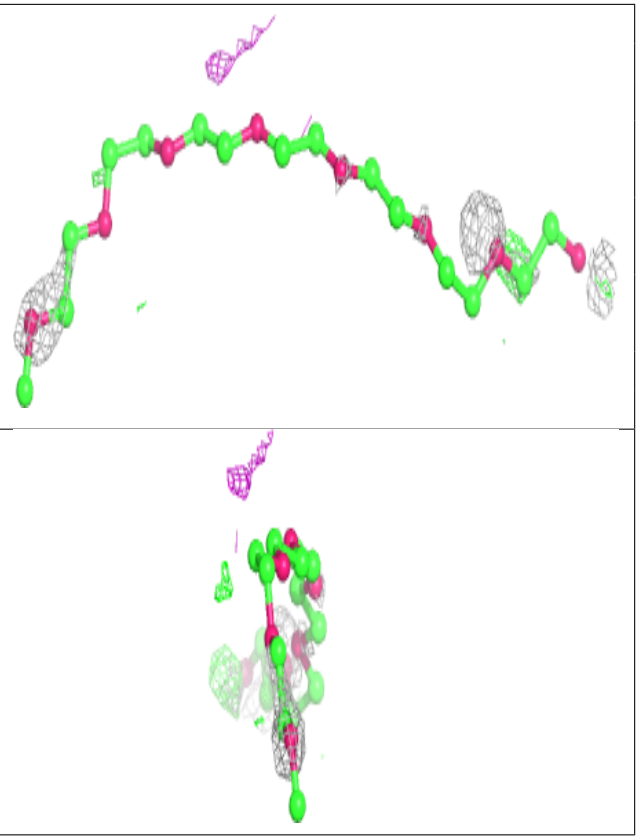
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	UNL	A	1028	1/-	0.87	0.38	56,56,56,56	0
11	UNL	B	1015	3/-	0.88	0.24	55,55,59,59	0
11	UNL	A	1007	8/-	0.88	0.26	54,56,57,57	6
11	UNL	C	205	4/-	0.88	0.15	66,70,70,72	0
11	UNL	A	1021	3/-	0.88	0.50	44,44,45,46	3
11	UNL	A	1010	4/-	0.88	0.14	65,67,69,72	0
11	UNL	A	1017	3/-	0.89	0.12	54,54,55,56	0
11	UNL	B	1012	3/-	0.89	0.18	68,68,70,71	0
11	UNL	C	204	4/-	0.89	0.17	66,67,69,73	0
17	UMQ	C	203	34/34	0.90	0.17	39,65,77,80	0
11	UNL	A	1018	3/-	0.90	0.19	42,42,52,54	0
11	UNL	A	1022	3/-	0.91	0.13	53,53,56,56	3
14	F3S	B	1003	7/7	0.91	0.17	32,34,59,59	0
11	UNL	C	211	3/-	0.91	0.30	48,48,48,49	3
11	UNL	B	1009	3/-	0.91	0.24	56,56,61,62	0
11	UNL	A	1026	2/-	0.92	0.19	62,62,62,64	0
13	SF4	B	1002	8/8	0.92	0.16	32,34,37,37	0
6	OAA	A	1002	9/9	0.92	0.19	35,43,47,48	0
11	UNL	D	204	3/-	0.92	0.32	44,44,46,52	0
11	UNL	A	1013	3/-	0.92	0.45	66,66,67,68	3
11	UNL	B	1004	4/-	0.93	0.11	47,51,56,60	0
15	TTF	C	202	14/14	0.93	0.09	36,44,51,51	0
11	UNL	A	1027	1/-	0.94	0.39	46,46,46,46	0
11	UNL	D	207	3/-	0.94	0.10	54,54,54,55	0
11	UNL	D	203	3/-	0.94	0.14	44,44,46,50	0
11	UNL	A	1009	4/-	0.94	0.23	69,70,71,74	0
11	UNL	B	1005	3/-	0.94	0.14	45,45,49,50	0
8	MG	A	1004	1/1	0.95	0.11	71,71,71,71	0
11	UNL	B	1017	2/-	0.95	0.16	51,51,51,54	0
11	UNL	B	1018	1/-	0.95	0.11	48,48,48,48	0
5	FAD	A	1001	53/53	0.95	0.24	33,37,42,46	0
11	UNL	B	1010	3/-	0.95	0.24	39,39,44,51	0
11	UNL	A	1025	3/-	0.95	0.18	51,51,51,53	0
11	UNL	A	1023	1/-	0.96	0.12	53,53,53,53	0
7	K	A	1003	1/1	0.97	0.14	45,45,45,45	0
16	HEM	C	201	41/43	0.97	0.12	35,42,50,56	0
12	FES	B	1001	4/4	0.98	0.20	35,36,44,44	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.

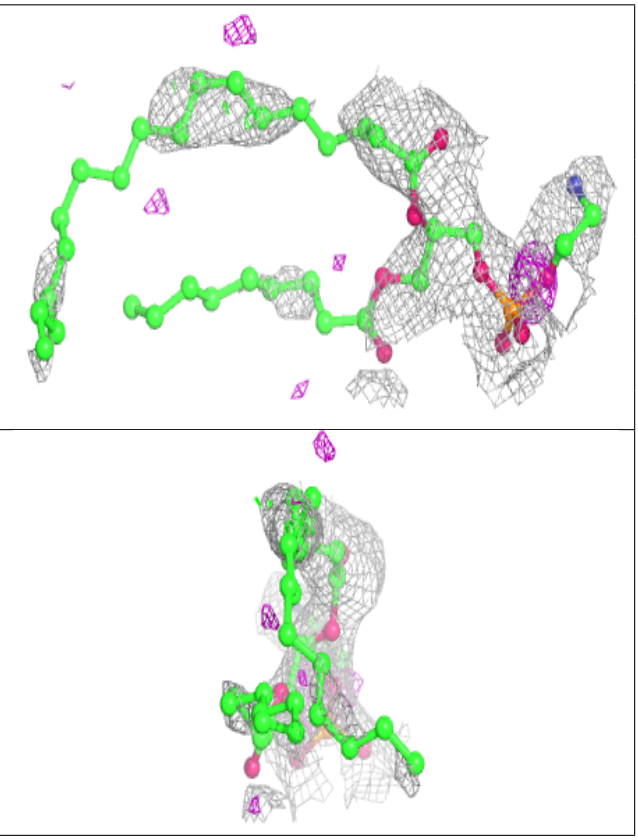
Electron density around UNL C 206:

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



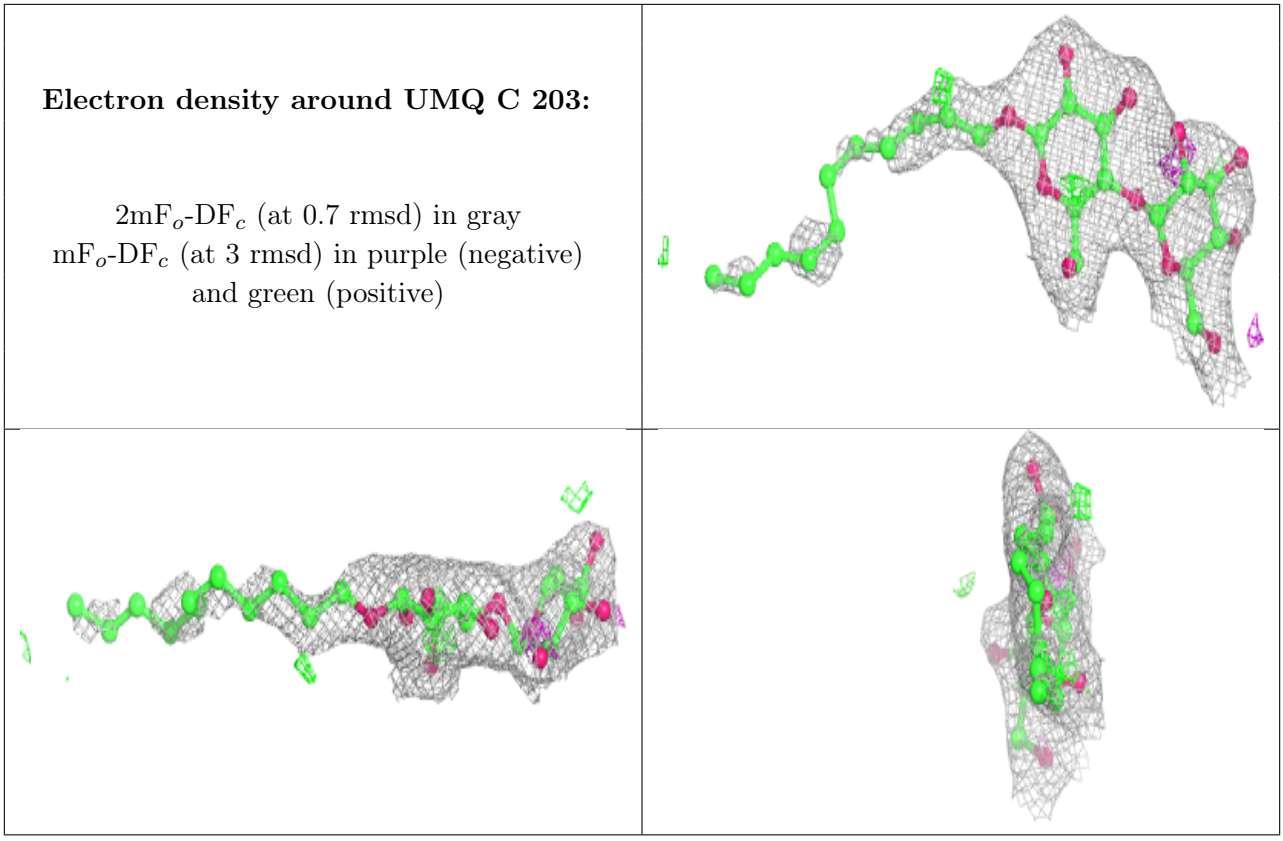
Electron density around 3PE D 201:

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



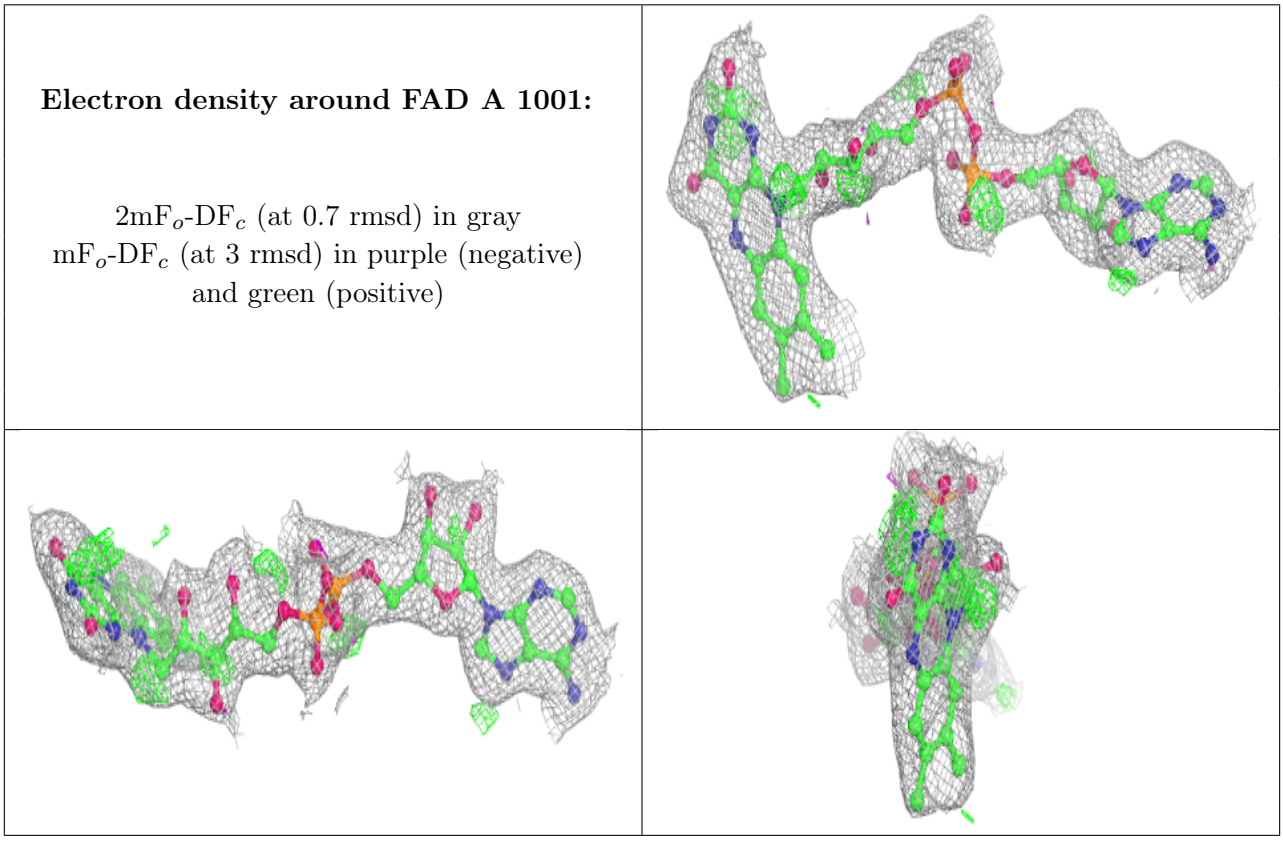
Electron density around UMQ C 203:

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



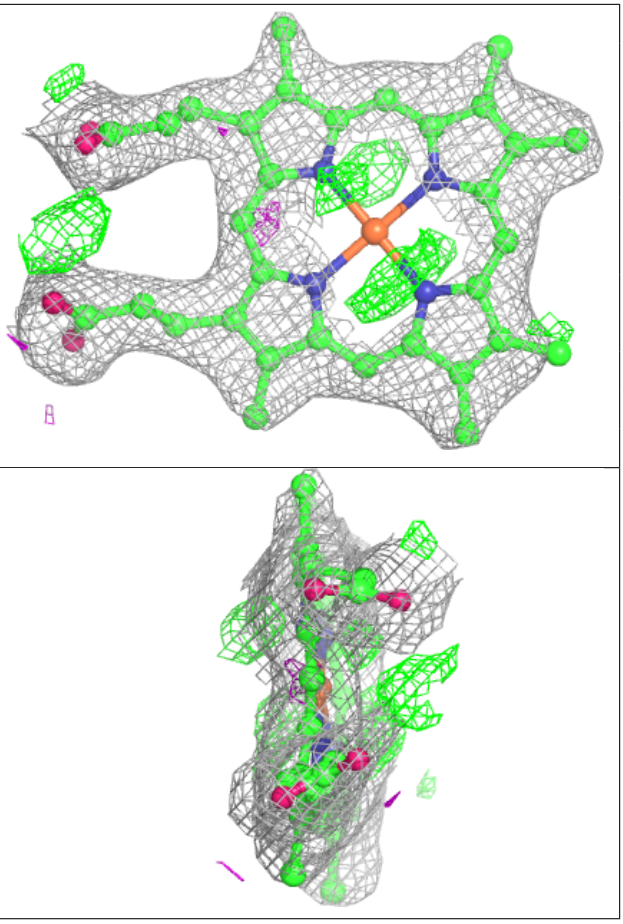
Electron density around FAD A 1001:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.