



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BS2
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-
GENES
Authors : Lancaster, C.R.D.
Deposited on : 2005-05-14
Resolution : 1.78 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

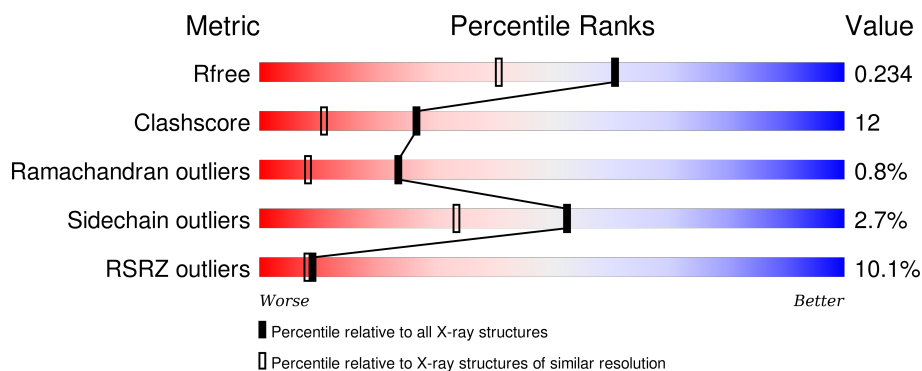
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	660	<div> <div>8%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	660	<div> <div>10%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	B	241	<div> <div>6%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
2	E	241	<div> <div>5%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
3	C	256	<div> <div>18%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	256	

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
11	LMT	C	1257	-	-	-	X
11	LMT	F	1257	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19666 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
1	A	656	Total	C	N	O	S	27	5	1
			5145	3219	927	967	32			
1	D	656	Total	C	N	O	S	32	3	1
			5125	3207	921	965	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			
2	E	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			

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

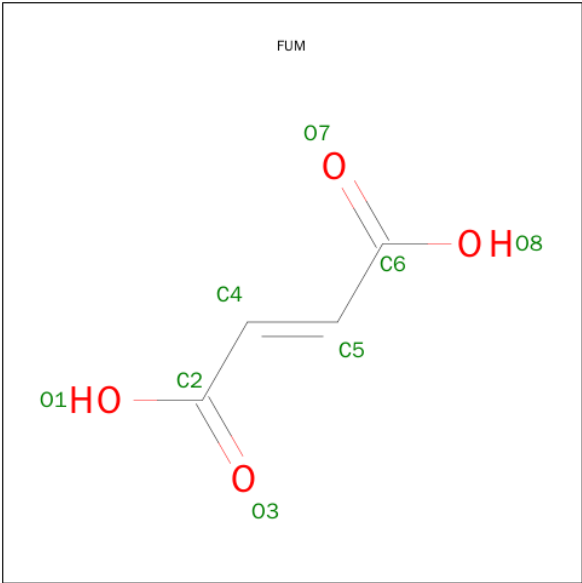
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	16	2	1
			2099	1398	336	351	14			
3	F	255	Total	C	N	O	S	12	2	1
			2099	1398	336	351	14			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).

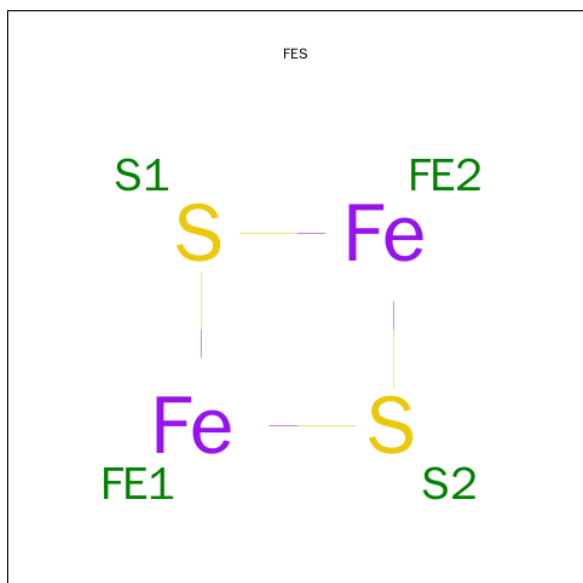


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

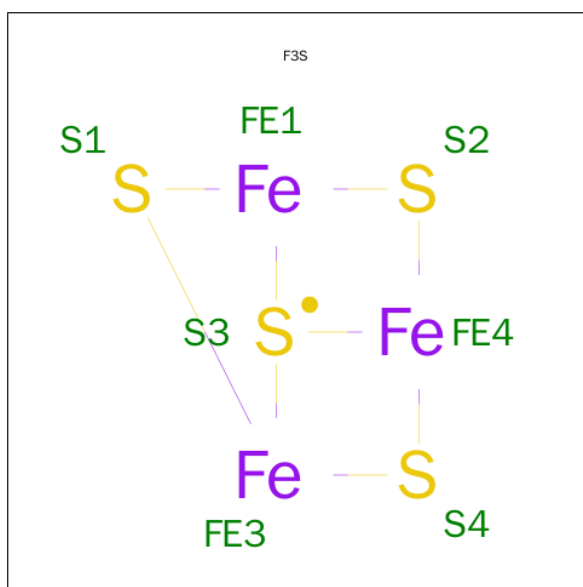
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



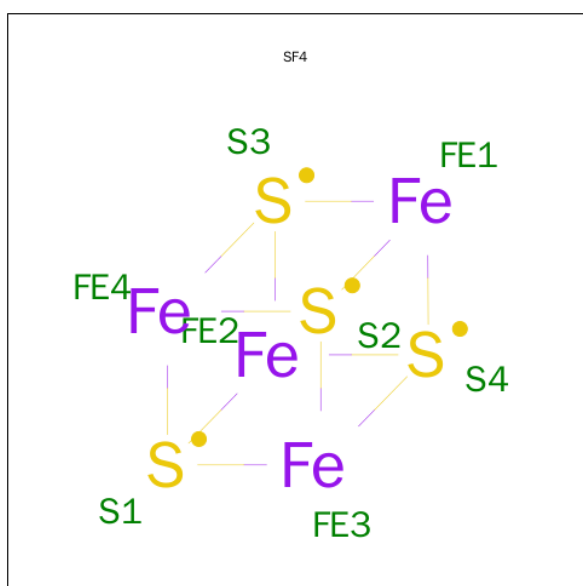
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



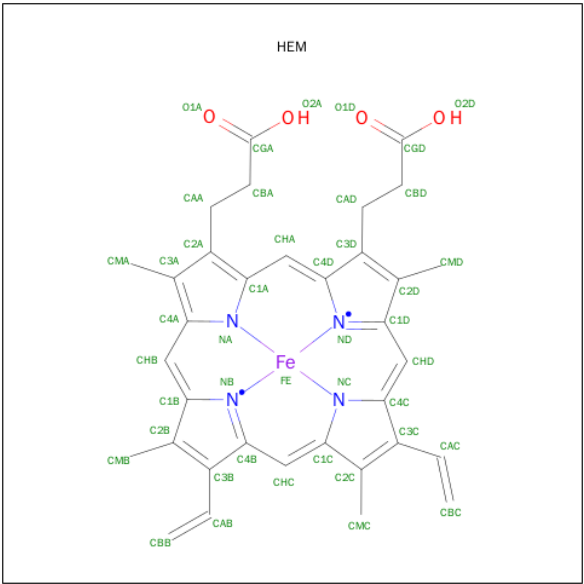
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



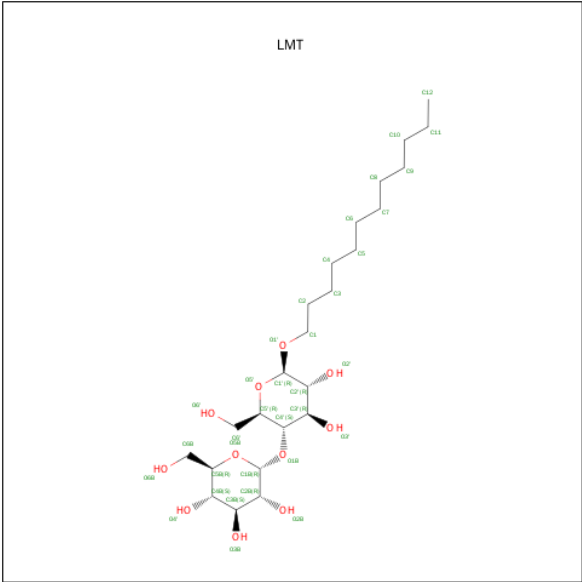
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		

- 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	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

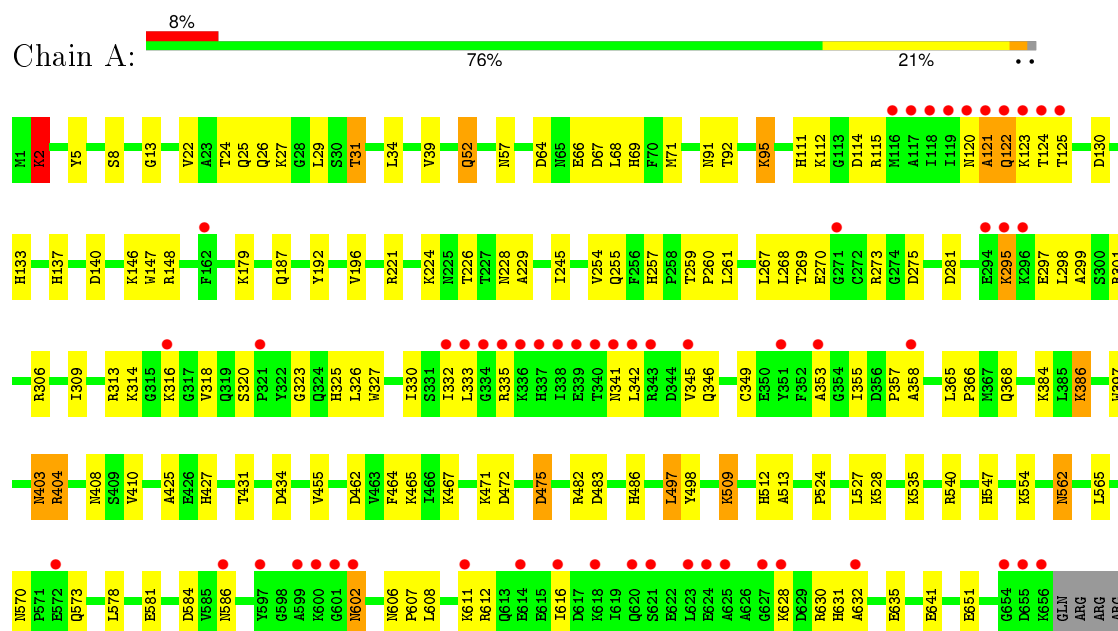
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	273	Total	O	1	0
			273	273		
12	B	155	Total	O	0	0
			155	155		
12	C	55	Total	O	0	0
			55	55		
12	D	287	Total	O	4	0
			287	287		
12	E	164	Total	O	0	0
			164	164		
12	F	56	Total	O	0	0
			56	56		

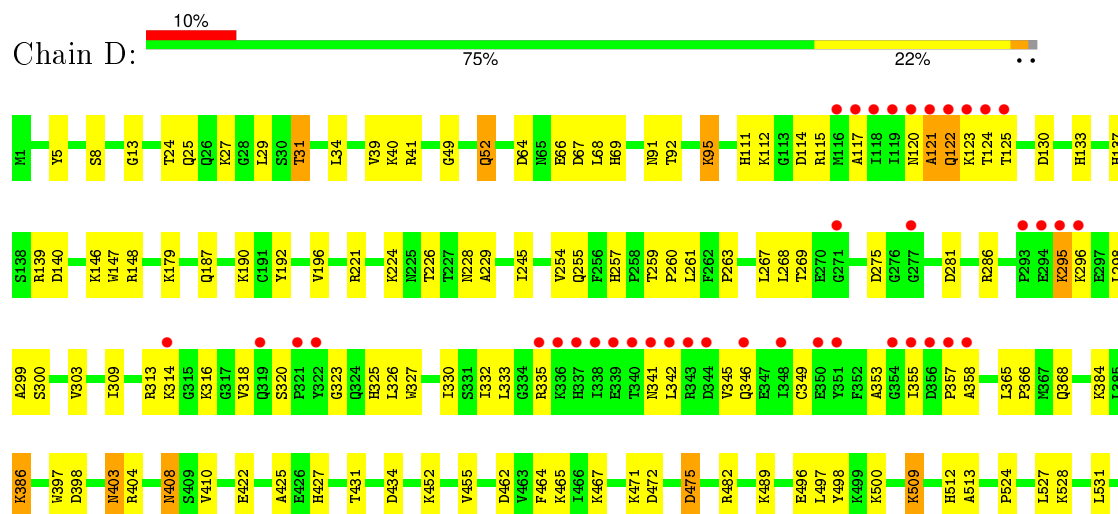
3 Residue-property plots

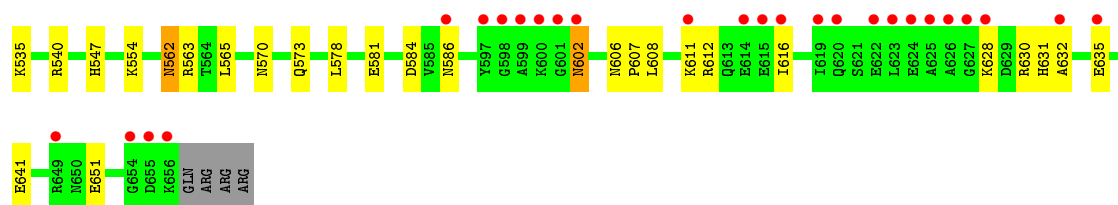
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

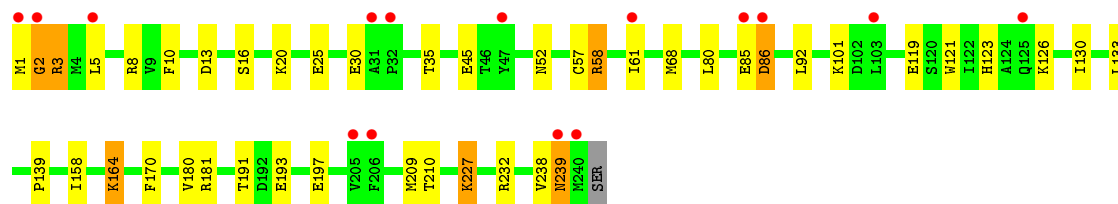
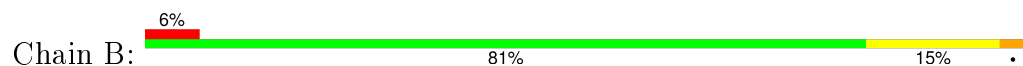


• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

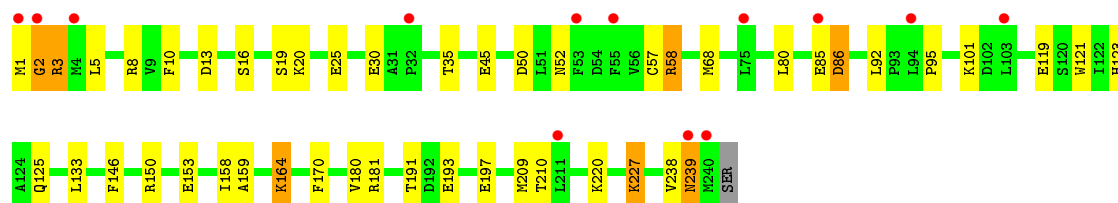
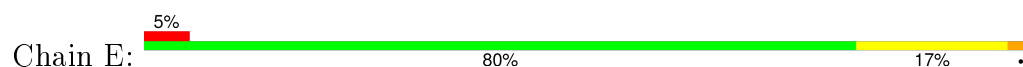




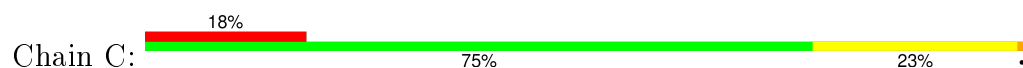
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B



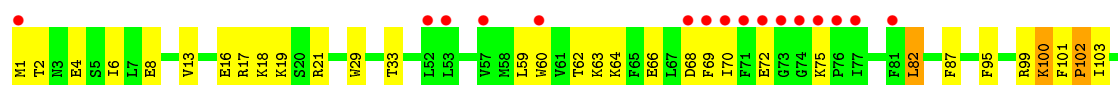
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

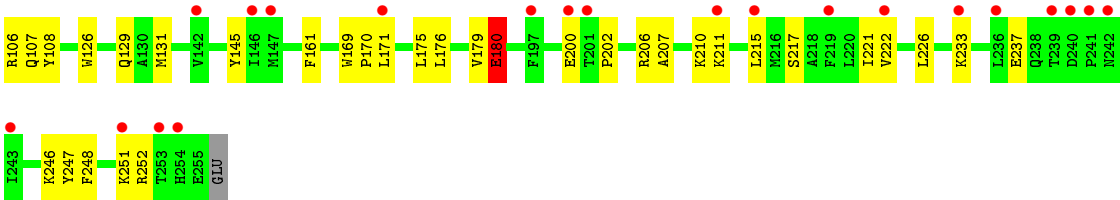


• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C



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





4 Data and refinement statistics

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)	28.70 – 1.78 28.70 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.70-1.78) 92.3 (28.70-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.237 0.226 , 0.234	Depositor DCC
R_{free} test set	4488 reflections (1.44%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 317966 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19666	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 12.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, SF4, LMT, F3S, FES, HEM, FUM, FAD

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	2.00	2/5241 (0.0%)	0.61	3/7063 (0.0%)
1	D	0.32	0/5221	0.59	1/7038 (0.0%)
2	B	0.34	0/1939	0.59	0/2616
2	E	0.35	0/1939	0.59	0/2616
3	C	2.35	2/2165 (0.1%)	2.34	3/2930 (0.1%)
3	F	7.27	6/2165 (0.3%)	2.64	9/2930 (0.3%)
All	All	2.82	10/18670 (0.1%)	1.31	16/25193 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	180[A]	GLU	CD-OE2	220.23	3.67	1.25
3	F	180[B]	GLU	CD-OE2	220.23	3.67	1.25
1	A	2[A]	LYS	CE-NZ	101.15	4.01	1.49
1	A	2[B]	LYS	CE-NZ	101.15	4.01	1.49
3	F	180[A]	GLU	CG-CD	83.46	2.77	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	180[A]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	C	180[B]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	F	180[A]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[B]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[A]	GLU	CG-CD-OE2	-38.95	40.40	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180[A]	GLU	Sidechain
3	F	180[A]	GLU	Sidechain

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	5145	0	5124	126	0
1	D	5125	0	5100	128	0
2	B	1902	0	1869	44	0
2	E	1902	0	1869	49	0
3	C	2099	0	2111	56	0
3	F	2099	0	2111	67	0
4	A	53	0	29	3	0
4	D	53	0	29	3	0
5	A	8	0	2	0	0
5	D	8	0	2	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	1	0
10	F	86	0	60	1	0
11	C	35	0	46	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	35	0	46	9	0
12	A	273	0	0	9	0
12	B	155	0	0	3	0
12	C	55	0	0	1	0
12	D	287	0	0	5	0
12	E	164	0	0	2	0
12	F	56	0	0	1	0
All	All	19666	0	18458	444	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 12.

The worst 5 of 444 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:F:180[B]:GLU:CG	3:F:180[B]:GLU:CD	1.80	1.47
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:OE1	1.70	1.31
3:F:180[B]:GLU:HG2	3:F:180[B]:GLU:OE1	1.47	1.11
2:B:1:MET:HG2	2:B:2:GLY:H	1.24	1.01
2:E:1:MET:HG2	2:E:2:GLY:H	1.24	0.98

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	659/660 (100%)	634 (96%)	21 (3%)	4 (1%)	30	13
1	D	657/660 (100%)	631 (96%)	22 (3%)	4 (1%)	30	13
2	B	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	11	2
2	E	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	11	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	39	22
3	F	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	39	22
All	All	2304/2314 (100%)	2213 (96%)	73 (3%)	18 (1%)	24	8

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
2	B	86	ASP
3	C	72	GLU
1	D	121	ALA
2	E	86	ASP

5.3.2 Protein sidechains ⓘ

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	537/537 (100%)	519 (97%)	18 (3%)	44	24
1	D	535/537 (100%)	518 (97%)	17 (3%)	46	26
2	B	212/213 (100%)	208 (98%)	4 (2%)	65	49
2	E	212/213 (100%)	208 (98%)	4 (2%)	65	49
3	C	223/223 (100%)	218 (98%)	5 (2%)	60	42
3	F	223/223 (100%)	218 (98%)	5 (2%)	60	42
All	All	1942/1946 (100%)	1889 (97%)	53 (3%)	52	34

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	82	LEU
1	D	95	LYS
3	F	18	LYS
3	C	87	PHE
3	C	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	123	HIS
1	D	57	ASN
2	E	116	GLN
2	B	177	ASN
1	D	26	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
4	FAD	A	1656	1	48,58,58	1.91	12 (25%)	54,89,89	2.05	11 (20%)
5	FUM	A	1657	-	1,7,7	1.50	0	0,8,8	0.00	-
7	FES	B	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	B	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	B	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
10	HEM	C	1255	3	30,50,50	2.91	12 (40%)	24,82,82	2.13	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEM	C	1256	3	30,50,50	2.98	11 (36%)	24,82,82	2.15	7 (29%)
11	LMT	C	1257	-	36,36,36	1.08	2 (5%)	47,47,47	1.28	4 (8%)
4	FAD	D	1656	1	48,58,58	1.75	11 (22%)	54,89,89	2.07	12 (22%)
5	FUM	D	1657	-	1,7,7	1.48	0	0,8,8	0.00	-
7	FES	E	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	E	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	E	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
10	HEM	F	1255	3	30,50,50	2.82	11 (36%)	24,82,82	2.14	7 (29%)
10	HEM	F	1256	3	30,50,50	2.94	10 (33%)	24,82,82	2.15	7 (29%)
11	LMT	F	1257	-	36,36,36	1.08	2 (5%)	47,47,47	1.28	4 (8%)

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
4	FAD	A	1656	1	-	0/30/50/50	0/6/6/6
5	FUM	A	1657	-	-	0/0/5/5	0/0/0/0
7	FES	B	1240	2	-	0/0/4/4	0/1/1/1
8	F3S	B	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	B	1242	2	-	0/0/48/48	0/6/5/5
10	HEM	C	1255	3	-	0/10/54/54	0/0/8/8
10	HEM	C	1256	3	-	0/10/54/54	0/0/8/8
11	LMT	C	1257	-	-	0/21/61/61	0/2/2/2
4	FAD	D	1656	1	-	0/30/50/50	0/6/6/6
5	FUM	D	1657	-	-	0/0/5/5	0/0/0/0
7	FES	E	1240	2	-	0/0/4/4	0/1/1/1
8	F3S	E	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	E	1242	2	-	0/0/48/48	0/6/5/5
10	HEM	F	1255	3	-	0/10/54/54	0/0/8/8
10	HEM	F	1256	3	-	0/10/54/54	0/0/8/8
11	LMT	F	1257	-	-	0/21/61/61	0/2/2/2

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1256	HEM	C3B-C4B	-8.01	1.44	1.51
10	F	1256	HEM	C3B-C4B	-7.87	1.44	1.51
10	C	1255	HEM	C3B-C4B	-7.55	1.45	1.51
10	F	1255	HEM	C3B-C4B	-7.11	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1256	HEM	C2D-C3D	-6.37	1.35	1.54

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1656	FAD	C1'-N10-C9A	-5.91	112.23	118.86
4	A	1656	FAD	C1'-N10-C9A	-5.87	112.27	118.86
4	D	1656	FAD	C4X-C4-N3	-4.75	117.10	123.59
4	A	1656	FAD	C4X-C4-N3	-4.73	117.12	123.59
4	A	1656	FAD	C4X-C10-N10	-4.71	117.75	120.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1656	FAD	3	0
10	C	1256	HEM	1	0
11	C	1257	LMT	8	0
4	D	1656	FAD	3	0
10	F	1256	HEM	1	0
11	F	1257	LMT	9	0

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	656/660 (99%)	0.51	55 (8%) 14 13	19, 33, 69, 80	14 (2%)
1	D	656/660 (99%)	0.59	65 (9%) 9 8	19, 33, 69, 80	16 (2%)
2	B	240/241 (99%)	0.35	15 (6%) 23 22	21, 29, 50, 74	2 (0%)
2	E	240/241 (99%)	0.40	13 (5%) 29 27	20, 28, 51, 74	2 (0%)
3	C	255/256 (99%)	1.05	47 (18%) 2 1	26, 44, 77, 91	11 (4%)
3	F	255/256 (99%)	0.88	37 (14%) 3 3	25, 43, 76, 90	10 (3%)
All	All	2302/2314 (99%)	0.61	232 (10%) 9 8	19, 34, 70, 91	55 (2%)

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	121	ALA	13.9
2	B	1	MET	11.8
3	C	254	HIS	11.3
1	A	121	ALA	10.5
1	A	122	GLN	10.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
11	LMT	C	1257	35/35	0.55	0.34	8.64	59,63,68,69	16
11	LMT	F	1257	35/35	0.73	0.25	7.51	59,63,69,69	16
5	FUM	D	1657	8/8	0.79	0.18	1.28	43,46,47,48	0
5	FUM	A	1657	8/8	0.76	0.17	1.22	42,46,48,50	0
10	HEM	C	1256	43/43	0.96	0.13	0.37	38,40,43,45	0
10	HEM	F	1256	43/43	0.96	0.13	-0.00	36,40,43,45	0
10	HEM	C	1255	43/43	0.96	0.10	-0.21	26,31,34,38	0
10	HEM	F	1255	43/43	0.97	0.10	-0.24	26,32,35,38	0
6	NA	D	1658	1/1	0.96	0.08	-0.47	26,26,26,26	0
4	FAD	D	1656	53/53	0.97	0.09	-0.50	18,22,25,25	0
4	FAD	A	1656	53/53	0.98	0.08	-0.88	16,22,25,27	0
8	F3S	E	1241	7/7	0.99	0.09	-1.05	23,24,25,25	0
9	SF4	E	1242	8/8	0.99	0.06	-1.19	21,23,23,24	0
8	F3S	B	1241	7/7	0.99	0.07	-1.31	24,25,26,27	0
9	SF4	B	1242	8/8	0.99	0.05	-1.34	22,24,25,25	0
7	FES	E	1240	4/4	0.99	0.06	-1.48	21,21,21,23	0
7	FES	B	1240	4/4	0.99	0.06	-1.54	22,22,23,24	0
6	NA	A	1658	1/1	0.99	0.03	-3.90	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.