



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:00 PM GMT

PDB ID : 3VR8  
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum*  
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.  
Deposited on : 2012-04-07  
Resolution : 2.81 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](mailto: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.

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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

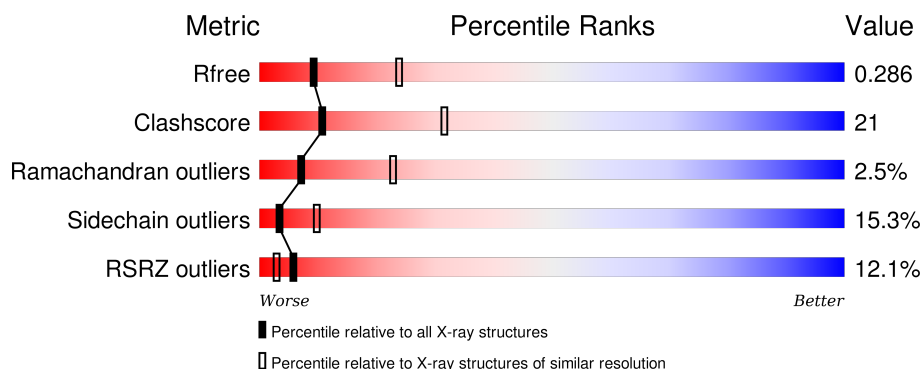
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	645	<div> <div>14%</div> <div>52% 37% 6% 5%</div> </div>
1	E	645	<div> <div>10%</div> <div>51% 38% 6% 5%</div> </div>
2	B	282	<div> <div>9%</div> <div>48% 30% 10% 12%</div> </div>
2	F	282	<div> <div>13%</div> <div>45% 35% 7% 12%</div> </div>
3	C	188	<div> <div>5%</div> <div>48% 27% 5% 19%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	RQX	C	202	-	-	-	X
11	RQX	G	202	-	-	-	X
5	MLI	A	701	-	-	X	-
6	FAD	A	702	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18232 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			
1	E	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			
2	F	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			

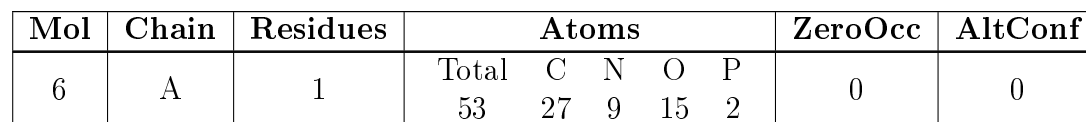
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	150	Total	C	N	O	S	0	0	0
			1195	798	201	190	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).

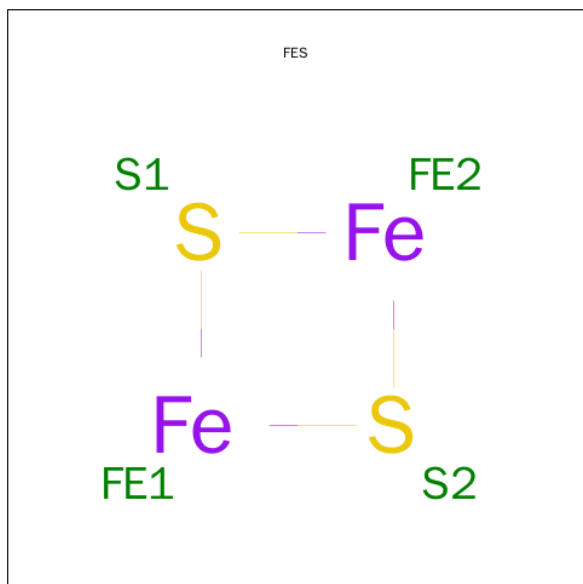


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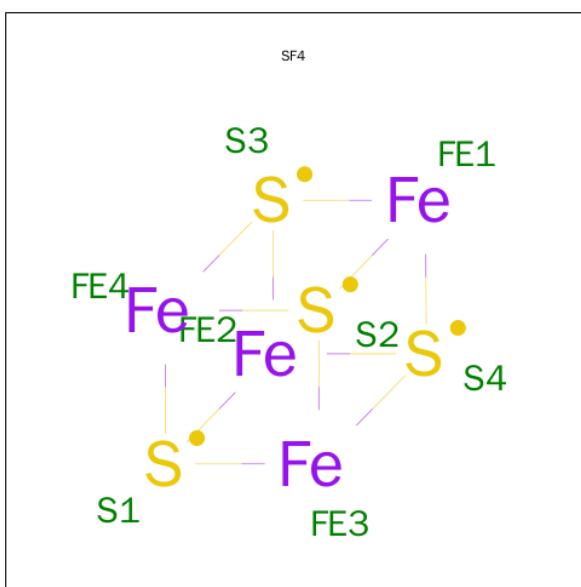
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



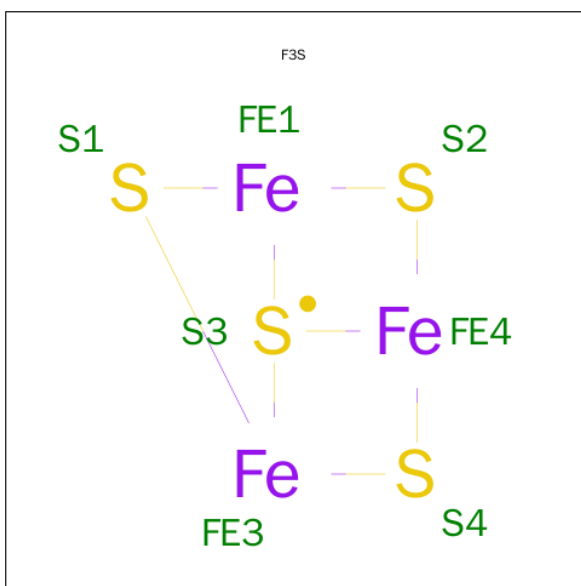
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



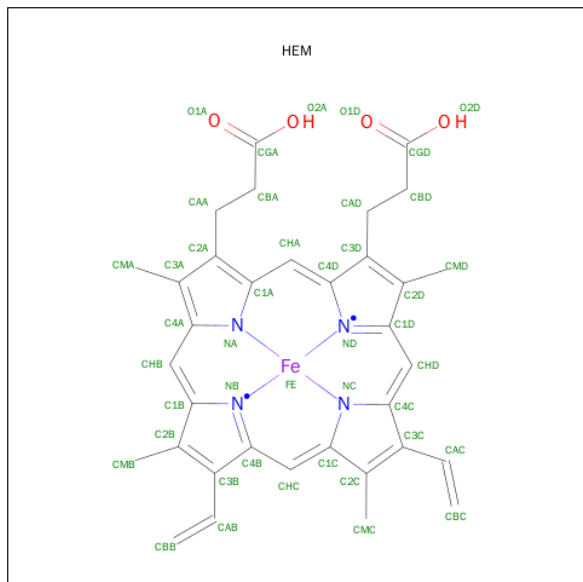
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



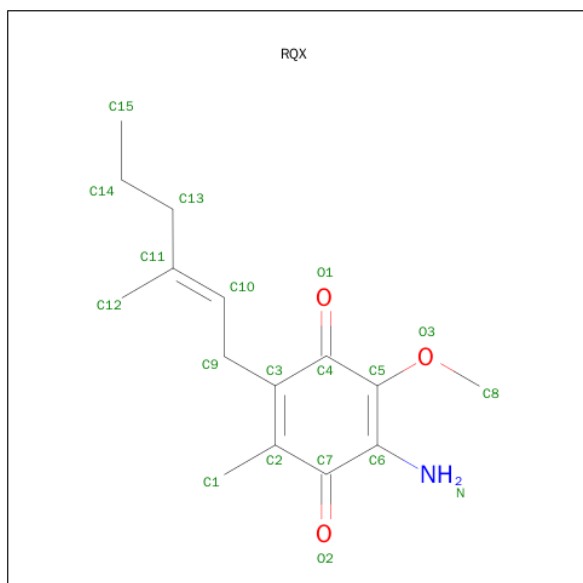
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- 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	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

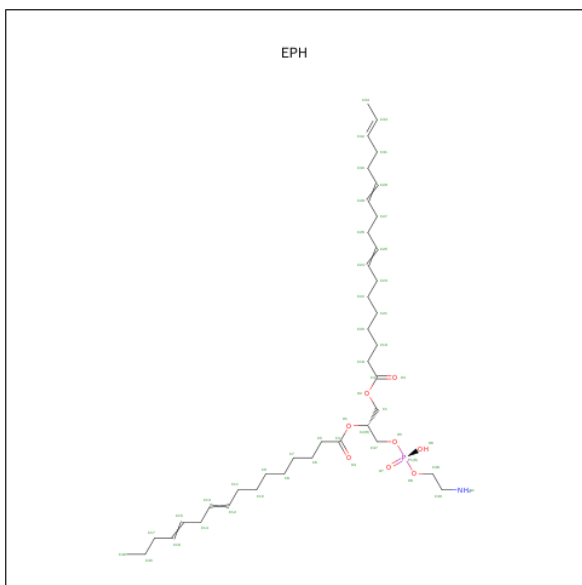
- Molecule 11 is 2-AMINO-3-METHOXY-6-METHYL-5-[(2E)-3-METHYLHEX-2-EN-1-YL] CYCLOHEXA-2,5-DIENE-1,4-DIONE (three-letter code: RQX) (formula:  $C_{15}H_{21}NO_3$ ).





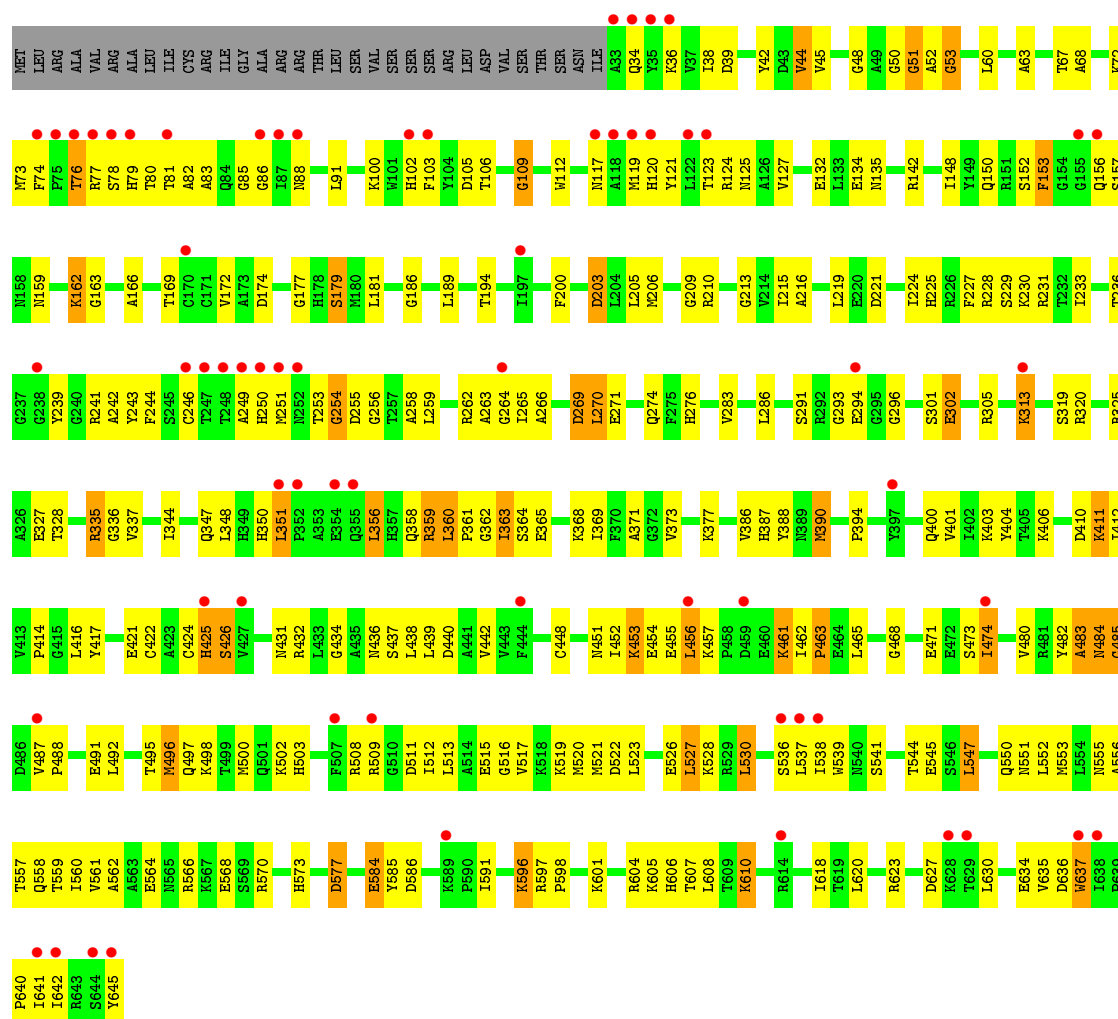
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			19	15	1	3		
11	G	1	Total	C	N	O	0	0
			19	15	1	3		

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

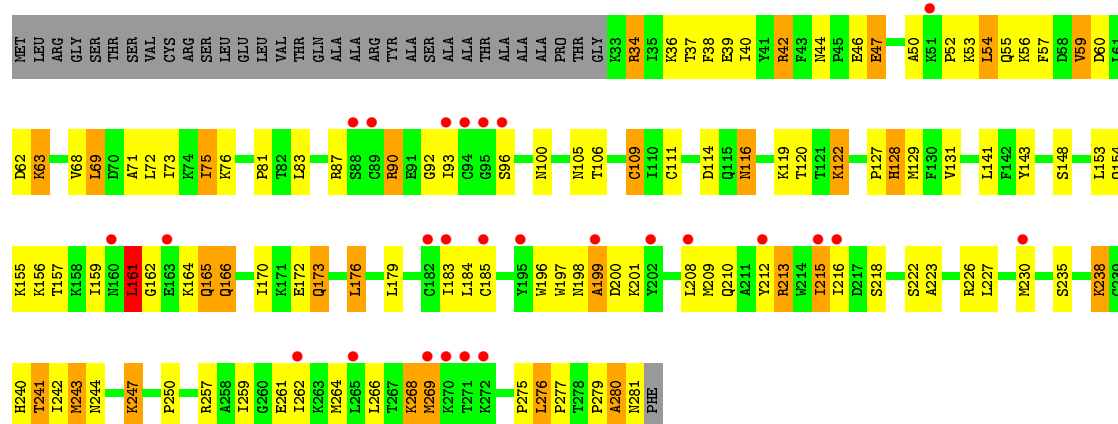


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		



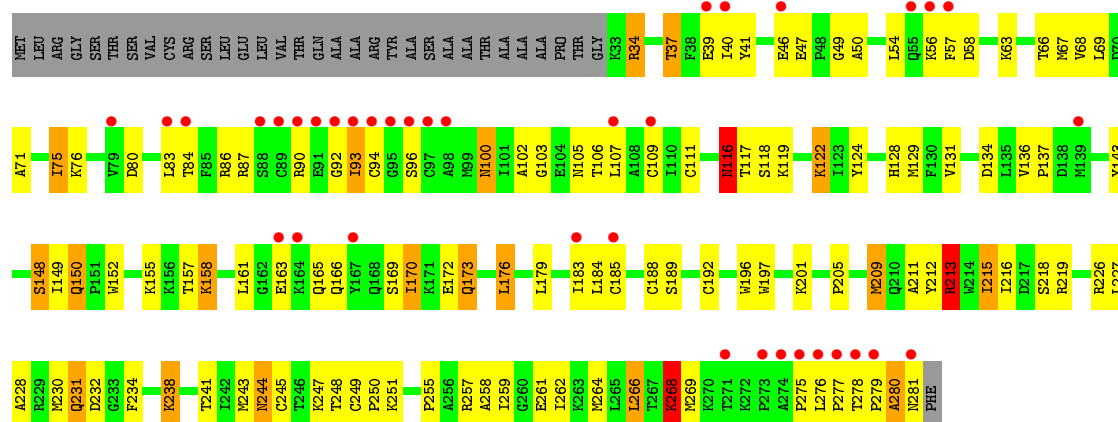


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

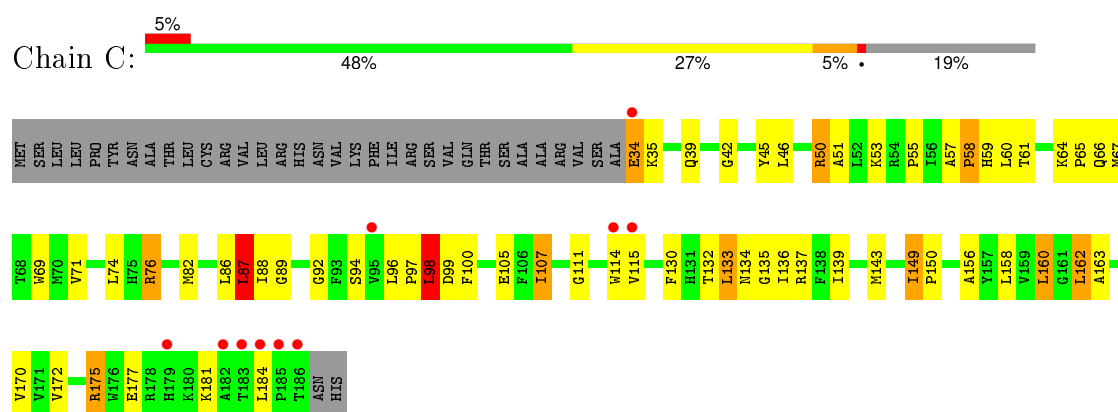


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

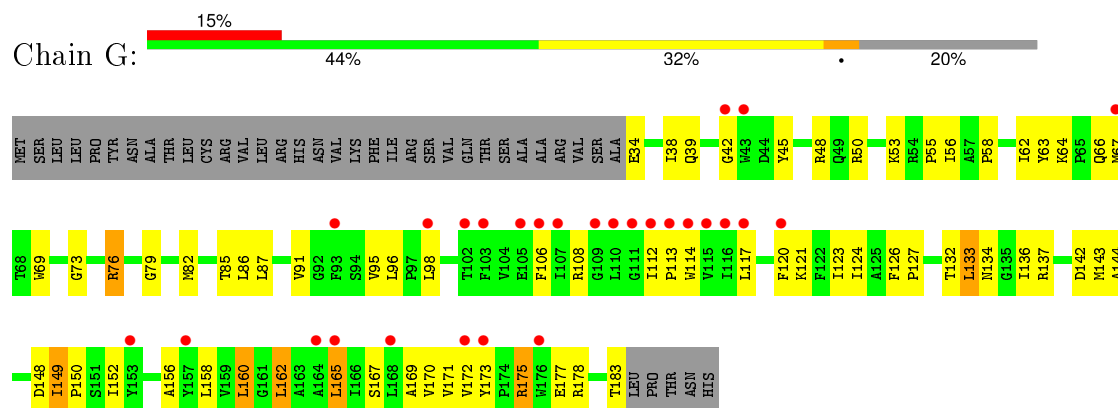




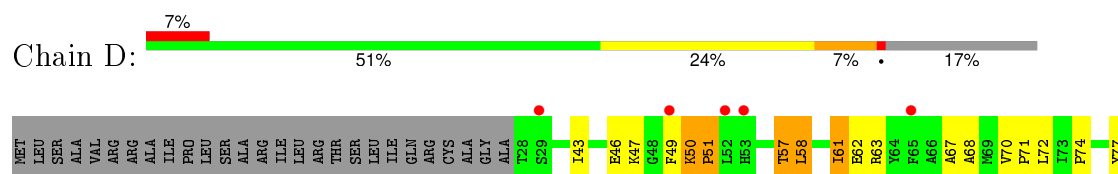
• Molecule 3: Cytochrome b-large subunit

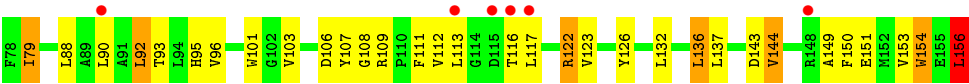


• Molecule 3: Cytochrome b-large subunit

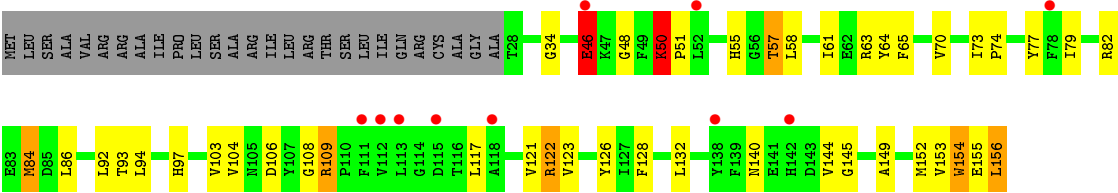


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.71Å 129.09Å 221.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.81 48.56 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.81) 92.0 (48.56-2.81)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.231 , 0.297 0.223 , 0.286	Depositor DCC
$R_{free}$ test set	4025 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 39.6	EDS
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 80036 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: SF4, MLI, RQX, F3S, FES, EPH, HEM, 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	0.62	0/4859	0.75	1/6564 (0.0%)
1	E	0.64	0/4859	0.77	1/6564 (0.0%)
2	B	0.68	0/2016	0.81	0/2723
2	F	0.74	0/2016	0.81	0/2723
3	C	0.65	0/1255	0.78	1/1709 (0.1%)
3	G	0.63	0/1232	0.68	0/1676
4	D	0.66	0/1026	0.74	1/1402 (0.1%)
4	H	0.63	0/1026	0.74	1/1402 (0.1%)
All	All	0.65	0/18289	0.77	5/24763 (0.0%)

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
1	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	98	LEU	CA-CB-CG	7.37	132.24	115.30
1	E	351	LEU	CA-CB-CG	6.39	130.00	115.30
4	D	156	LEU	CA-CB-CG	5.49	127.92	115.30
4	H	156	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	142	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	HIS	Peptide

## 5.2 Too-close contacts ⓘ

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	4758	0	4692	203	0
1	E	4758	0	4692	207	0
2	B	1973	0	1993	93	0
2	F	1973	0	1992	107	0
3	C	1217	0	1265	53	0
3	G	1195	0	1240	70	0
4	D	994	0	977	43	0
4	H	994	0	977	37	0
5	A	7	0	2	2	0
5	E	7	0	2	0	0
6	A	53	0	31	7	0
6	E	53	0	31	10	0
7	B	4	0	0	1	0
7	F	4	0	0	0	0
8	B	8	0	0	1	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	15	0
10	G	43	0	30	9	0
11	C	19	0	21	8	0
11	G	19	0	21	6	0
12	D	44	0	53	6	0
12	H	44	0	53	8	0
All	All	18232	0	18102	764	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 21.

The worst 5 of 764 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.00	1.31
1:E:79:HIS:NE2	6:E:702:FAD:HM82	0.88	1.20
1:A:446:ARG:HH11	1:A:446:ARG:HG3	1.07	1.18
2:F:34:ARG:HH21	2:F:34:ARG:HG2	1.14	1.12
1:E:79:HIS:CD2	6:E:702:FAD:HM82	1.85	1.10

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	611/645 (95%)	531 (87%)	68 (11%)	12 (2%)	9	29
1	E	611/645 (95%)	540 (88%)	56 (9%)	15 (2%)	7	23
2	B	247/282 (88%)	214 (87%)	26 (10%)	7 (3%)	6	20
2	F	247/282 (88%)	206 (83%)	33 (13%)	8 (3%)	5	16
3	C	151/188 (80%)	127 (84%)	18 (12%)	6 (4%)	4	11
3	G	148/188 (79%)	127 (86%)	18 (12%)	3 (2%)	9	29
4	D	127/156 (81%)	109 (86%)	16 (13%)	2 (2%)	12	36
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	5	17
All	All	2269/2542 (89%)	1959 (86%)	253 (11%)	57 (2%)	7	23

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	TYR
1	A	163	GLY
1	A	372	GLY
1	A	485	GLY
2	B	161	LEU

### 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	498/526 (95%)	425 (85%)	73 (15%)	4	11
1	E	498/526 (95%)	437 (88%)	61 (12%)	6	18
2	B	219/242 (90%)	173 (79%)	46 (21%)	1	4
2	F	219/242 (90%)	179 (82%)	40 (18%)	2	6
3	C	127/158 (80%)	107 (84%)	20 (16%)	3	9
3	G	124/158 (78%)	108 (87%)	16 (13%)	5	15
4	D	96/119 (81%)	79 (82%)	17 (18%)	2	6
4	H	96/119 (81%)	82 (85%)	14 (15%)	4	11
All	All	1877/2090 (90%)	1590 (85%)	287 (15%)	3	10

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	99	ASP
1	E	76	THR
3	G	133	LEU
3	C	149	ILE
4	D	90	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	240	HIS
1	E	120	HIS
2	F	165	GLN
2	B	244	ASN
1	E	88	ASN

### 5.3.3 RNA ⓘ

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](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	A	702	1	48,58,58	1.26	4 (8%)	54,89,89	2.40	13 (24%)
7	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	C	201	3,4	30,50,50	2.12	10 (33%)	24,82,82	2.49	11 (45%)
11	RQX	C	202	-	19,19,19	2.27	3 (15%)	21,26,26	2.24	5 (23%)
12	EPH	D	201	-	42,43,48	1.95	8 (19%)	43,48,53	2.68	9 (20%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	1	48,58,58	1.46	6 (12%)	54,89,89	2.59	12 (22%)
7	FES	F	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	G	201	3,4	30,50,50	2.09	6 (20%)	24,82,82	2.39	8 (33%)
11	RQX	G	202	-	19,19,19	2.47	2 (10%)	21,26,26	1.83	4 (19%)
12	EPH	H	201	-	42,43,48	1.95	9 (21%)	43,48,53	2.60	7 (16%)

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
5	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FAD	A	702	1	-	0/30/50/50	0/6/6/6
7	FES	B	301	2	-	0/0/4/4	0/1/1/1
8	SF4	B	302	2	-	0/0/48/48	0/6/5/5
9	F3S	B	303	2	-	0/0/24/24	0/0/3/3
10	HEM	C	201	3,4	-	0/10/54/54	0/0/8/8
11	RQX	C	202	-	-	0/10/34/34	0/1/1/1
12	EPH	D	201	-	-	0/47/47/52	0/0/0/0
5	MLI	E	701	-	-	0/0/4/4	0/0/0/0
6	FAD	E	702	1	-	0/30/50/50	0/6/6/6
7	FES	F	301	2	-	0/0/4/4	0/1/1/1
8	SF4	F	302	2	-	0/0/48/48	0/6/5/5
9	F3S	F	303	2	-	0/0/24/24	0/0/3/3
10	HEM	G	201	3,4	-	0/10/54/54	0/0/8/8
11	RQX	G	202	-	-	0/10/34/34	0/1/1/1
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	C3B-C4B	-7.97	1.44	1.51
10	C	201	HEM	C3B-C4B	-7.29	1.45	1.51
10	C	201	HEM	C3D-C4D	-3.93	1.46	1.51
12	D	201	EPH	C18-C4	-3.92	1.38	1.50
12	D	201	EPH	C27-C28	-3.82	1.33	1.50

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	N3A-C2A-N1A	-12.14	119.60	128.89
6	A	702	FAD	N3A-C2A-N1A	-11.79	119.87	128.89
6	E	702	FAD	P-O3P-PA	-5.24	118.02	132.73
10	G	201	HEM	C3C-CAC-CBC	-4.22	117.98	124.46
11	C	202	RQX	C1-C2-C3	-4.06	115.42	124.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	2	0
6	A	702	FAD	7	0
7	B	301	FES	1	0
8	B	302	SF4	1	0
10	C	201	HEM	15	0
11	C	202	RQX	8	0
12	D	201	EPH	6	0
6	E	702	FAD	10	0
10	G	201	HEM	9	0
11	G	202	RQX	6	0
12	H	201	EPH	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/645 (95%)	0.44	90 (14%) 3 2	71, 96, 118, 136	0
1	E	613/645 (95%)	0.23	64 (10%) 8 4	70, 90, 113, 126	0
2	B	249/282 (88%)	0.17	26 (10%) 8 4	72, 89, 117, 137	0
2	F	249/282 (88%)	0.46	37 (14%) 3 2	67, 86, 109, 120	0
3	C	153/188 (81%)	0.21	10 (6%) 22 13	78, 97, 142, 162	0
3	G	150/188 (79%)	0.62	28 (18%) 2 1	77, 100, 151, 156	0
4	D	129/156 (82%)	0.19	11 (8%) 13 6	89, 101, 129, 142	0
4	H	129/156 (82%)	0.17	10 (7%) 16 8	86, 103, 133, 146	0
All	All	2285/2542 (89%)	0.32	276 (12%) 6 3	67, 94, 124, 162	0

The worst 5 of 276 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	9.9
4	D	49	PHE	7.4
3	G	115	VAL	6.5
3	C	183	THR	6.3
3	G	112	ILE	6.3

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	RQX	G	202	19/19	0.80	0.35	2.94	120,125,127,127	0
11	RQX	C	202	19/19	0.79	0.29	2.16	113,116,119,119	0
12	EPH	H	201	44/49	0.80	0.34	1.53	97,113,134,135	0
12	EPH	D	201	44/49	0.88	0.24	1.12	94,102,121,122	0
5	MLI	A	701	7/7	0.90	0.32	1.06	102,103,106,106	0
6	FAD	A	702	53/53	0.92	0.40	0.75	77,83,87,89	0
10	HEM	C	201	43/43	0.97	0.20	0.22	89,93,96,98	0
10	HEM	G	201	43/43	0.98	0.19	0.22	92,97,103,106	0
9	F3S	F	303	7/7	0.99	0.18	0.20	82,83,84,87	0
8	SF4	F	302	8/8	0.99	0.22	-0.07	57,61,64,65	0
6	FAD	E	702	53/53	0.96	0.26	-0.12	63,79,88,89	0
8	SF4	B	302	8/8	0.99	0.20	-0.22	63,66,68,70	0
9	F3S	B	303	7/7	0.98	0.15	-0.39	83,85,86,87	0
5	MLI	E	701	7/7	0.95	0.21	-0.50	92,93,93,93	0
7	FES	B	301	4/4	1.00	0.27	-0.99	70,70,72,78	0
7	FES	F	301	4/4	0.99	0.29	-2.15	60,66,68,75	0

## 6.5 Other polymers

There are no such residues in this entry.