



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:10 AM GMT

PDB ID : 1E7P
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-
GENES
Authors : Lancaster, C.R.D.; Kroeger, A.
Deposited on : 2000-09-01
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

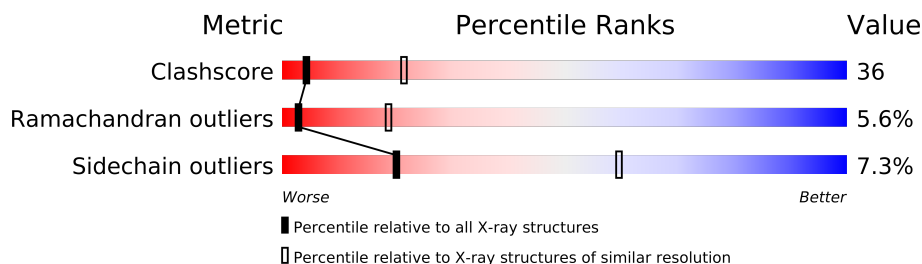
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	656	
1	D	656	
1	G	656	
1	J	656	
2	B	239	
2	E	239	
2	H	239	
2	K	239	
3	C	256	
3	F	256	
3	I	256	
3	L	256	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37080 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	33	0	0
			5094	3190	910	962	32			
1	D	655	Total	C	N	O	S	33	0	0
			5094	3190	910	962	32			
1	G	655	Total	C	N	O	S	33	0	0
			5094	3190	910	962	32			
1	J	655	Total	C	N	O	S	33	0	0
			5094	3190	910	962	32			

- Molecule 2 is a protein called FUMARATE REDUCTASE IRON-SULFUR PROTEIN.

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

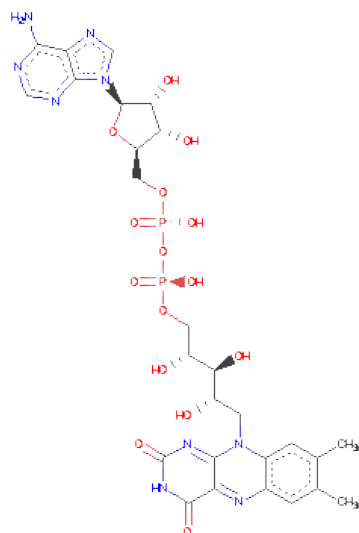
- Molecule 3 is a protein called FUMARATE REDUCTASE CYTOCHROME B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	254	Total	C	N	O	S	24	0	0
			2081	1388	334	345	14			
3	F	254	Total	C	N	O	S	24	0	0
			2081	1388	334	345	14			
3	I	254	Total	C	N	O	S	24	0	0
			2081	1388	334	345	14			
3	L	254	Total	C	N	O	S	24	0	0
			2081	1388	334	345	14			

There are 4 discrepancies between the modelled and reference sequences:

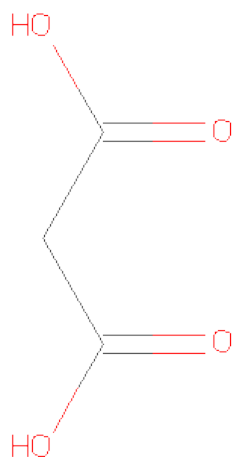
Chain	Residue	Modelled	Actual	Comment	Reference
C	66	GLN	GLU	ENGINEERED MUTATION	UNP P17413
F	66	GLN	GLU	ENGINEERED MUTATION	UNP P17413
I	66	GLN	GLU	ENGINEERED MUTATION	UNP P17413
L	66	GLN	GLU	ENGINEERED MUTATION	UNP P17413

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



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

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).

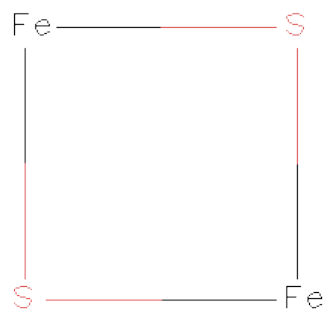


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		
5	G	1	Total	C	O	0	0
			7	3	4		
5	J	1	Total	C	O	0	0
			7	3	4		

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

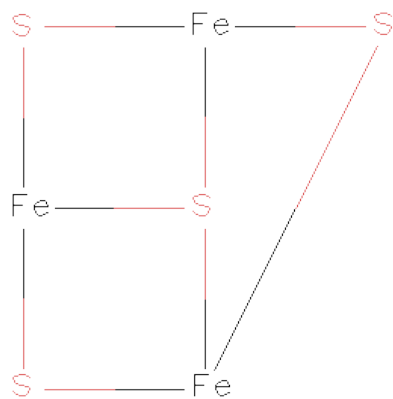
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Na	0	0
			1	1		
6	J	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

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



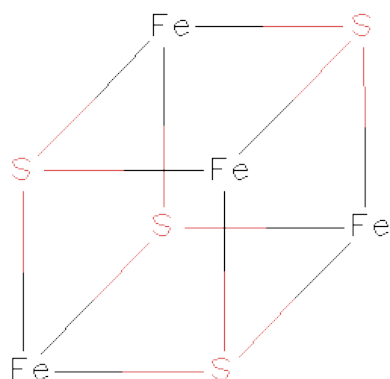
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		
7	H	1	Total	Fe	S	0	0
			4	2	2		
7	K	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



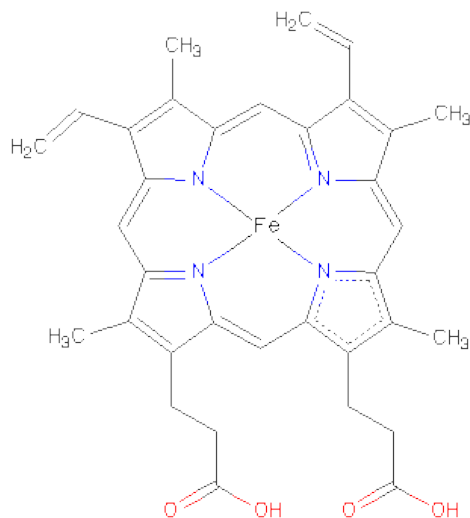
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		
8	H	1	Total	Fe	S	0	0
			7	3	4		
8	K	1	Total	Fe	S	0	0
			7	3	4		

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



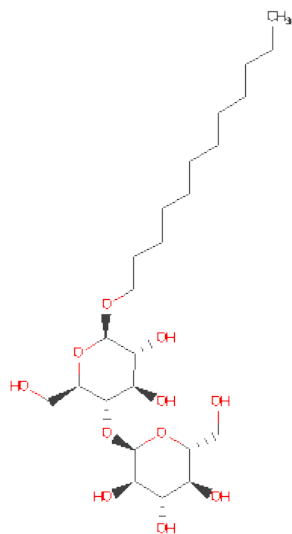
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	K	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- 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	17	0
			35	24	11		
11	F	1	Total	C	O	17	0
			35	24	11		
11	I	1	Total	C	O	17	0
			35	24	11		
11	L	1	Total	C	O	17	0
			35	24	11		

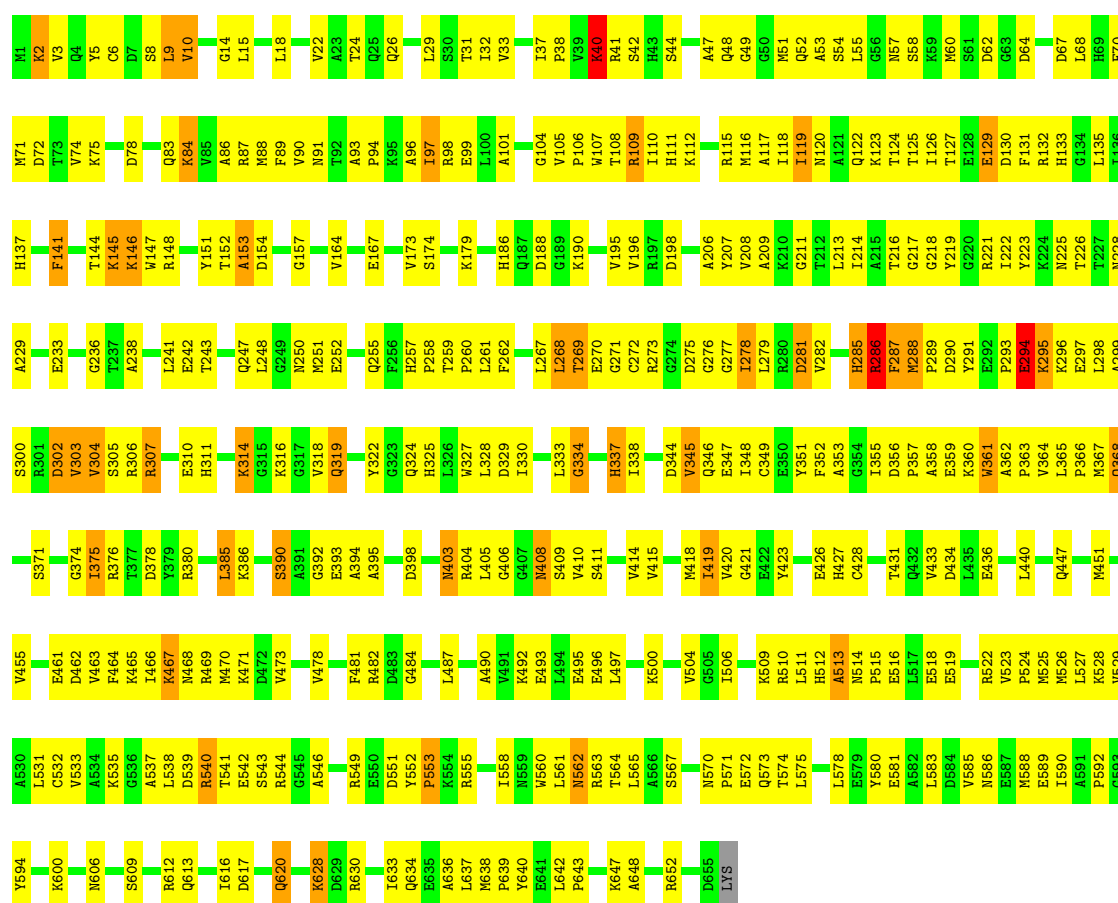
3 Residue-property plots

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.

Note EDS was not executed.

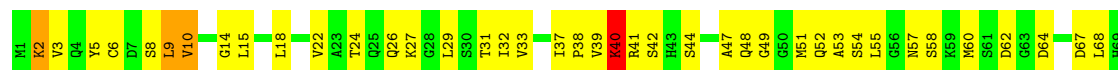
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT

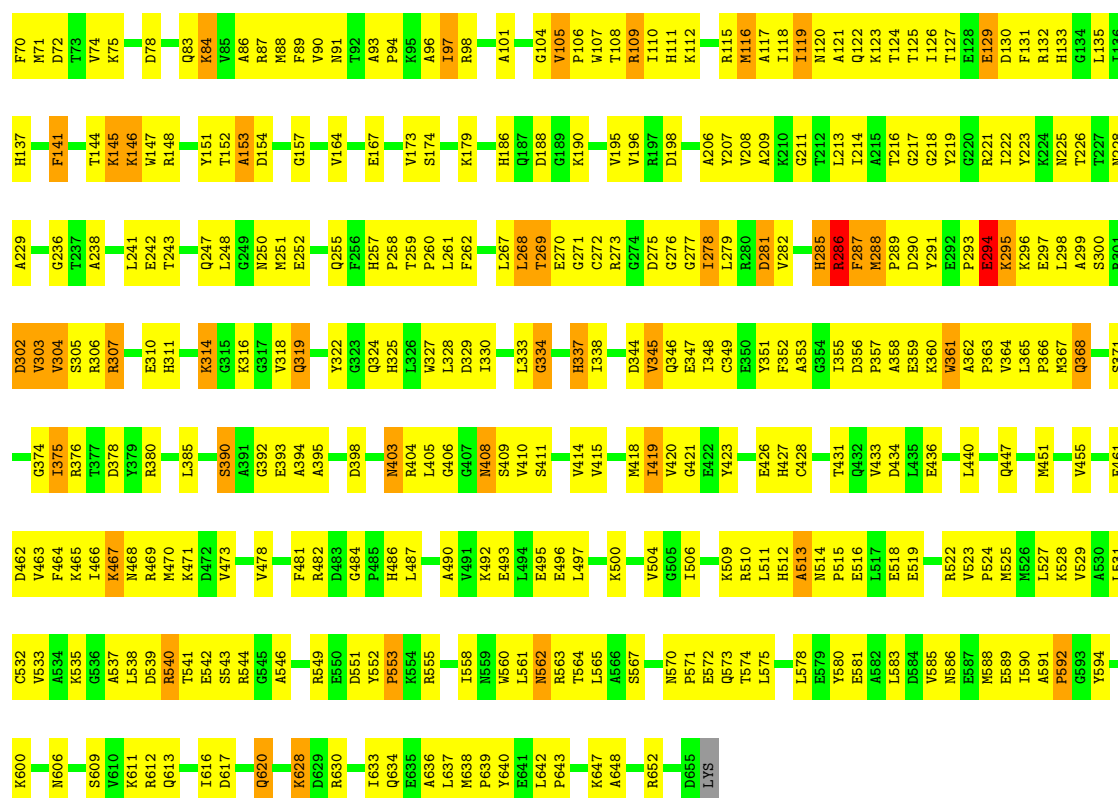
Chain A:

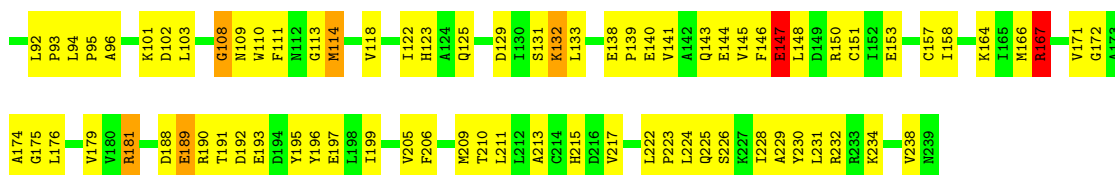


• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT

Chain D:

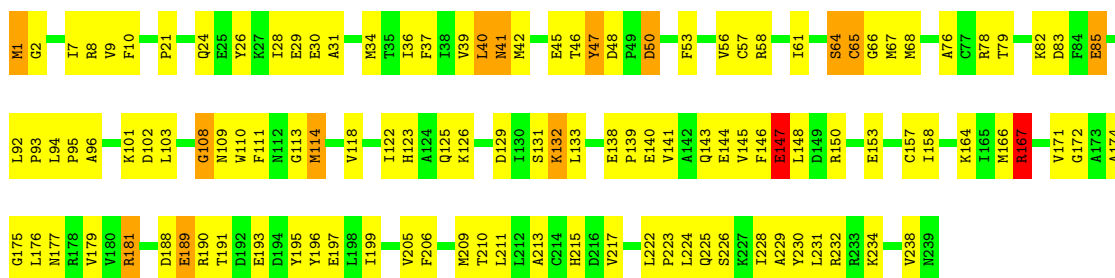






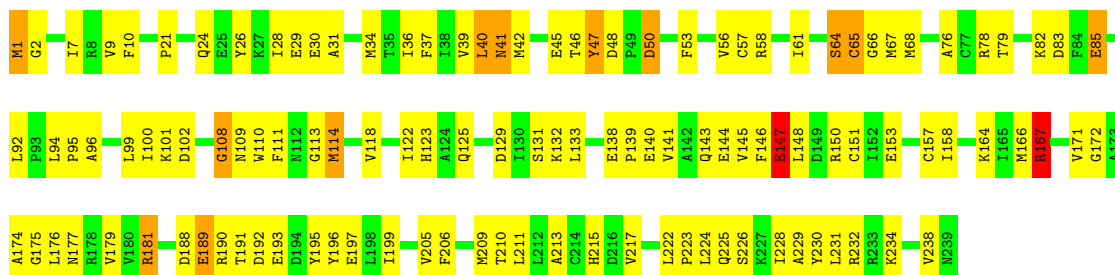
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain H:



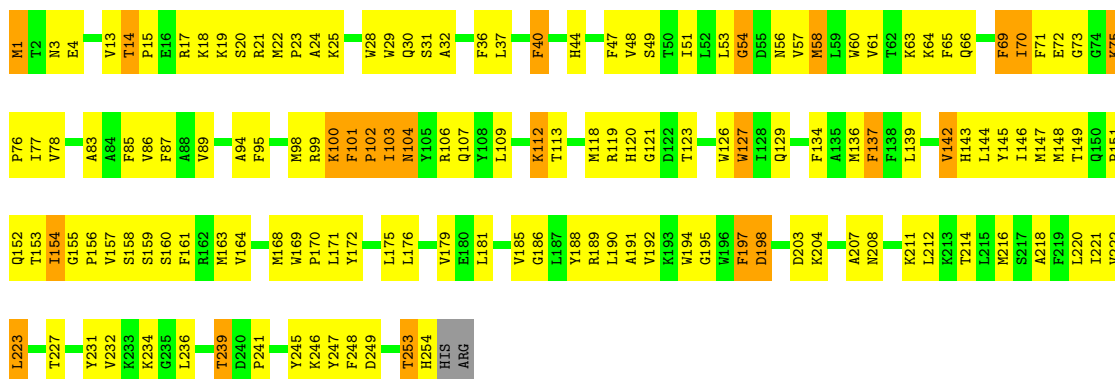
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain K:



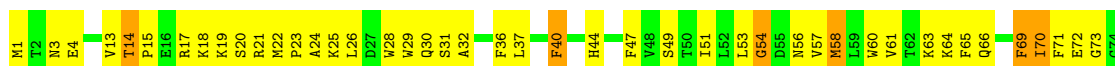
• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain C:



• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

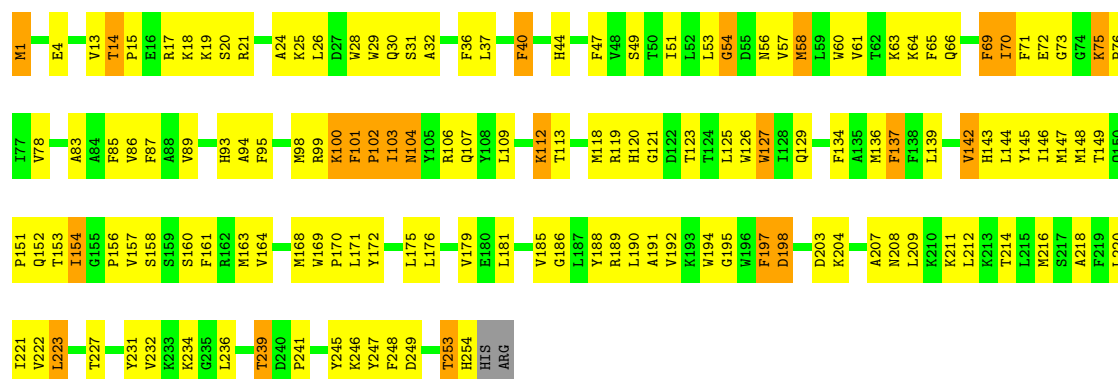
Chain F:





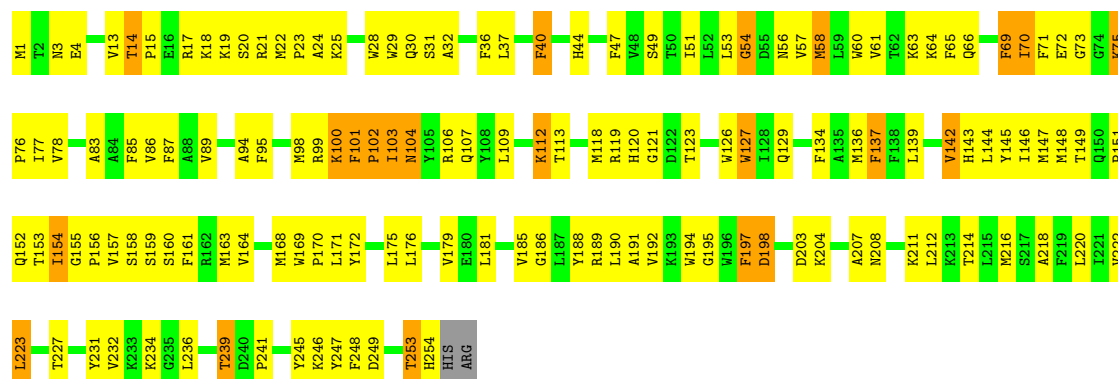
• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain I:



• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain L:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.07Å 290.24Å 153.61Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	80.8 (30.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	37080	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, NA, SF4, LMT, F3S, FES, 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	0.58	0/5190	0.73	0/6996
1	D	0.58	0/5190	0.73	0/6996
1	G	0.58	0/5190	0.73	0/6996
1	J	0.58	0/5190	0.73	0/6996
2	B	0.47	0/1931	0.70	1/2604 (0.0%)
2	E	0.47	0/1931	0.70	1/2604 (0.0%)
2	H	0.47	0/1931	0.70	1/2604 (0.0%)
2	K	0.47	0/1931	0.70	1/2604 (0.0%)
3	C	0.60	0/2147	0.67	1/2904 (0.0%)
3	F	0.60	0/2147	0.67	1/2904 (0.0%)
3	I	0.60	0/2147	0.67	1/2904 (0.0%)
3	L	0.60	0/2147	0.67	1/2904 (0.0%)
All	All	0.56	0/37072	0.71	8/50016 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	102	PRO	N-CA-C	-5.31	98.30	112.10
3	F	102	PRO	N-CA-C	-5.30	98.31	112.10
3	C	102	PRO	N-CA-C	-5.30	98.32	112.10
3	I	102	PRO	N-CA-C	-5.30	98.32	112.10
2	H	167	ARG	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5094	0	5069	407	11
1	D	5094	0	5069	408	16
1	G	5094	0	5069	416	13
1	J	5094	0	5069	413	14
2	B	1894	0	1861	105	0
2	E	1894	0	1861	106	0
2	H	1894	0	1861	107	0
2	K	1894	0	1861	103	0
3	C	2081	0	2103	163	0
3	F	2081	0	2103	163	0
3	I	2081	0	2103	166	0
3	L	2081	0	2103	162	0
4	A	53	0	29	4	0
4	D	53	0	29	4	0
4	G	53	0	29	4	0
4	J	53	0	29	4	0
5	A	7	0	2	5	0
5	D	7	0	2	5	0
5	G	7	0	2	6	0
5	J	7	0	2	5	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
7	H	4	0	0	0	0
7	K	4	0	0	0	0
8	B	7	0	0	2	0
8	E	7	0	0	2	0
8	H	7	0	0	2	0
8	K	7	0	0	2	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
9	H	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	8	0	0	0	0
10	C	86	0	60	11	0
10	F	86	0	60	12	0
10	I	86	0	60	11	0
10	L	86	0	60	11	0
11	C	35	0	46	3	0
11	F	35	0	46	3	0
11	I	35	0	46	3	0
11	L	35	0	46	3	0
All	All	37080	0	36680	2632	27

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

The worst 5 of 2632 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:216:THR:HG21	1:D:236:GLY:HA3	1.32	1.12
1:J:327:TRP:HB3	1:J:361:TRP:HB2	1.30	1.11
1:G:216:THR:HG21	1:G:236:GLY:HA3	1.32	1.09
3:L:152:GLN:HE21	3:L:153:THR:HG23	1.18	1.07
1:J:216:THR:HG21	1:J:236:GLY:HA3	1.32	1.06

The worst 5 of 27 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:580:TYR:C	1:G:122:GLN:NE2[1_455]	0.81	1.39
1:A:122:GLN:NE2	1:J:581:GLU:N[1_554]	0.84	1.36
1:D:581:GLU:N	1:G:122:GLN:NE2[1_455]	1.03	1.17
1:A:122:GLN:NE2	1:J:580:TYR:C[1_554]	1.10	1.10
1:A:122:GLN:OE1	1:J:581:GLU:CA[1_554]	1.30	0.90

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	2	16
1	D	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	2	15
1	G	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	2	16
1	J	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	2	15
2	B	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	4	27
2	E	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	4	27
2	H	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	4	27
2	K	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	4	27
3	C	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	4	23
3	F	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	4	23
3	I	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	4	23
3	L	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	4	23
All	All	4568/4604 (99%)	3556 (78%)	758 (17%)	254 (6%)	3	19

5 of 254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	THR
1	A	288	MET
1	A	294	GLU
1	A	319	GLN
1	A	333	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	532/533 (100%)	497 (93%)	35 (7%)	24	64
1	D	532/533 (100%)	497 (93%)	35 (7%)	24	64
1	G	532/533 (100%)	497 (93%)	35 (7%)	24	64
1	J	532/533 (100%)	497 (93%)	35 (7%)	24	64
2	B	211/211 (100%)	199 (94%)	12 (6%)	29	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	211/211 (100%)	199 (94%)	12 (6%)	29	70
2	H	211/211 (100%)	199 (94%)	12 (6%)	29	70
2	K	211/211 (100%)	199 (94%)	12 (6%)	29	70
3	C	221/223 (99%)	198 (90%)	23 (10%)	10	36
3	F	221/223 (99%)	198 (90%)	23 (10%)	10	36
3	I	221/223 (99%)	198 (90%)	23 (10%)	10	36
3	L	221/223 (99%)	198 (90%)	23 (10%)	10	36
All	All	3856/3868 (100%)	3576 (93%)	280 (7%)	20	59

5 of 280 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	78	VAL
1	G	302	ASP
3	L	14	THR
3	F	123	THR
1	G	40	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	225	GLN
1	G	158	HIS
1	J	562	ASN
3	F	3	ASN
1	G	26	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	701	1	58,58,58	2.17	14 (24%)	85,89,89	1.75	16 (18%)
5	MLA	A	702	-	6,6,6	1.92	2 (33%)	7,7,7	0.65	0
7	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	B	302	2	3,9,9	14.47	3 (100%)	0,15,15	0.00	-
9	SF4	B	303	2	12,12,12	13.32	11 (91%)	0,24,24	0.00	-
10	HEM	C	301	3	49,50,50	1.97	14 (28%)	46,82,82	1.79	6 (13%)
10	HEM	C	302	3	49,50,50	2.14	15 (30%)	46,82,82	1.53	5 (10%)
11	LMT	C	303	-	36,36,36	1.11	2 (5%)	47,47,47	1.23	4 (8%)
4	FAD	D	701	1	58,58,58	2.17	14 (24%)	85,89,89	1.75	16 (18%)
5	MLA	D	702	-	6,6,6	1.92	2 (33%)	7,7,7	0.66	0
7	FES	E	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	E	302	2	3,9,9	14.47	3 (100%)	0,15,15	0.00	-
9	SF4	E	303	2	12,12,12	13.32	11 (91%)	0,24,24	0.00	-
11	LMT	F	301	-	36,36,36	1.11	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	F	302	3	49,50,50	1.97	14 (28%)	46,82,82	1.79	6 (13%)
10	HEM	F	303	3	49,50,50	2.12	15 (30%)	46,82,82	1.52	5 (10%)
4	FAD	G	701	1	58,58,58	2.16	14 (24%)	85,89,89	1.75	16 (18%)
5	MLA	G	702	-	6,6,6	1.92	2 (33%)	7,7,7	0.65	0
7	FES	H	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	H	302	2	3,9,9	14.50	3 (100%)	0,15,15	0.00	-
9	SF4	H	303	2	12,12,12	13.32	11 (91%)	0,24,24	0.00	-
10	HEM	I	301	3	49,50,50	1.98	14 (28%)	46,82,82	1.78	6 (13%)
10	HEM	I	302	3	49,50,50	2.15	15 (30%)	46,82,82	1.53	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LMT	I	303	-	36,36,36	1.11	2 (5%)	47,47,47	1.23	4 (8%)
4	FAD	J	701	1	58,58,58	2.17	14 (24%)	85,89,89	1.75	16 (18%)
5	MLA	J	702	-	6,6,6	1.94	2 (33%)	7,7,7	0.65	0
7	FES	K	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	K	302	2	3,9,9	14.50	3 (100%)	0,15,15	0.00	-
9	SF4	K	303	2	12,12,12	13.34	11 (91%)	0,24,24	0.00	-
11	LMT	L	301	-	36,36,36	1.11	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	L	302	3	49,50,50	1.97	14 (28%)	46,82,82	1.78	5 (10%)
10	HEM	L	303	3	49,50,50	2.13	15 (30%)	46,82,82	1.53	5 (10%)

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	701	1	-	0/34/50/50	0/1/6/6
5	MLA	A	702	-	-	0/4/4/4	0/0/0/0
7	FES	B	301	2	-	0/0/4/4	0/0/1/1
8	F3S	B	302	2	-	0/0/24/24	0/0/3/3
9	SF4	B	303	2	-	0/0/48/48	0/0/5/5
10	HEM	C	301	3	-	0/14/114/114	0/0/8/8
10	HEM	C	302	3	-	0/14/114/114	0/0/8/8
11	LMT	C	303	-	-	0/21/61/61	0/2/2/2
4	FAD	D	701	1	-	0/34/50/50	0/1/6/6
5	MLA	D	702	-	-	0/4/4/4	0/0/0/0
7	FES	E	301	2	-	0/0/4/4	0/0/1/1
8	F3S	E	302	2	-	0/0/24/24	0/0/3/3
9	SF4	E	303	2	-	0/0/48/48	0/0/5/5
11	LMT	F	301	-	-	0/21/61/61	0/2/2/2
10	HEM	F	302	3	-	0/14/114/114	0/0/8/8
10	HEM	F	303	3	-	0/14/114/114	0/0/8/8
4	FAD	G	701	1	-	0/34/50/50	0/1/6/6
5	MLA	G	702	-	-	0/4/4/4	0/0/0/0
7	FES	H	301	2	-	0/0/4/4	0/0/1/1
8	F3S	H	302	2	-	0/0/24/24	0/0/3/3
9	SF4	H	303	2	-	0/0/48/48	0/0/5/5
10	HEM	I	301	3	-	0/14/114/114	0/0/8/8
10	HEM	I	302	3	-	0/14/114/114	0/0/8/8
11	LMT	I	303	-	-	0/21/61/61	0/2/2/2
4	FAD	J	701	1	-	0/34/50/50	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLA	J	702	-	-	0/4/4/4	0/0/0/0
7	FES	K	301	2	-	0/0/4/4	0/0/1/1
8	F3S	K	302	2	-	0/0/24/24	0/0/3/3
9	SF4	K	303	2	-	0/0/48/48	0/0/5/5
11	LMT	L	301	-	-	0/21/61/61	0/2/2/2
10	HEM	L	302	3	-	0/14/114/114	0/0/8/8
10	HEM	L	303	3	-	0/14/114/114	0/0/8/8

The worst 5 of 244 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	303	SF4	S4-FE3	-24.81	2.16	2.33
9	B	303	SF4	S4-FE3	-24.76	2.16	2.33
9	K	303	SF4	S4-FE3	-24.73	2.16	2.33
9	H	303	SF4	S4-FE3	-24.69	2.16	2.33
8	K	302	F3S	S3-FE3	-24.24	2.16	2.33

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302	HEM	C3B-C4B-NB	-6.89	109.07	114.00
10	C	301	HEM	C3B-C4B-NB	-6.87	109.08	114.00
10	I	301	HEM	C3B-C4B-NB	-6.87	109.08	114.00
10	F	302	HEM	C3B-C4B-NB	-6.86	109.09	114.00
10	I	301	HEM	CBA-CAA-C2A	6.11	123.46	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.