



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:47 PM GMT

PDB ID : 1QLB
Title : respiratory complex II-like fumarate reductase from Wolinella succinogenes
Authors : Lancaster, C.R.D.; Kroeger, A.; Auer, M.; Michel, H.
Deposited on : 1999-08-25
Resolution : 2.33 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

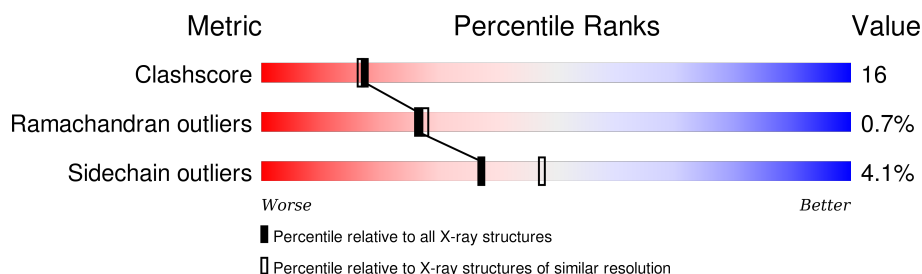
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	656	 75% 23% •
1	D	656	 74% 24% •
2	B	239	 74% 24% •
2	E	239	 74% 24% •
3	C	256	 65% 31% • •
3	F	256	 63% 34% • •

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19056 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 FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	88	0	0
			5101	3194	913	962	32			
1	D	655	Total	C	N	O	S	88	0	0
			5101	3194	913	962	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ASP	ARG	CONFLICT (SEE REMARK	UNP P17412
A	282	VAL	CYS	CONFLICT (SEE REMARK	UNP P17412
A	283	ASP	GLY	CONFLICT (SEE REMARK	UNP P17412
A	284	GLY	TRP	CONFLICT (SEE REMARK	UNP P17412
A	285	HIS	THR	CONFLICT (SEE REMARK	UNP P17412
A	286	ARG	PRO	CONFLICT (SEE REMARK	UNP P17412
A	287	PHE	ILE	CONFLICT (SEE REMARK	UNP P17412
A	288	MET	HIS	CONFLICT (SEE REMARK	UNP P17412
A	289	PRO	ALA	CONFLICT (SEE REMARK	UNP P17412
D	281	ASP	ARG	CONFLICT (SEE REMARK	UNP P17412
D	282	VAL	CYS	CONFLICT (SEE REMARK	UNP P17412
D	283	ASP	GLY	CONFLICT (SEE REMARK	UNP P17412
D	284	GLY	TRP	CONFLICT (SEE REMARK	UNP P17412
D	285	HIS	THR	CONFLICT (SEE REMARK	UNP P17412
D	286	ARG	PRO	CONFLICT (SEE REMARK	UNP P17412
D	287	PHE	ILE	CONFLICT (SEE REMARK	UNP P17412
D	288	MET	HIS	CONFLICT (SEE REMARK	UNP P17412
D	289	PRO	ALA	CONFLICT (SEE REMARK	UNP P17412

- 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
			1893	1194	322	354	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	239	Total	C	N	O	S	0	0	0
			1893	1194	322	354	23			

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 3 | C | 254 | Total
2080 | C
1388 | N
333 | O
345 | S
14 | 111 | 0 | 0 |
| 3 | F | 254 | Total
2080 | C
1388 | N
333 | O
345 | S
14 | 111 | 0 | 0 |

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- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

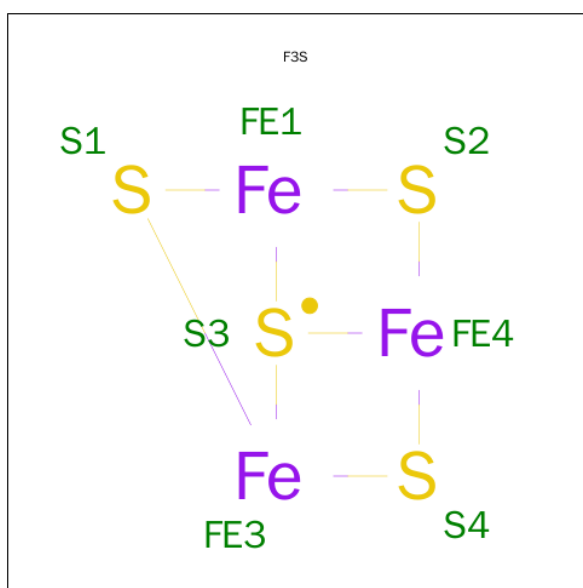
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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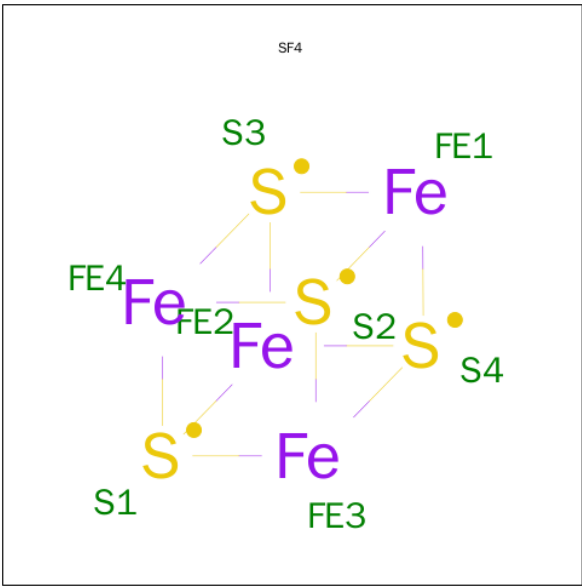
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			4	2	2		
5	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



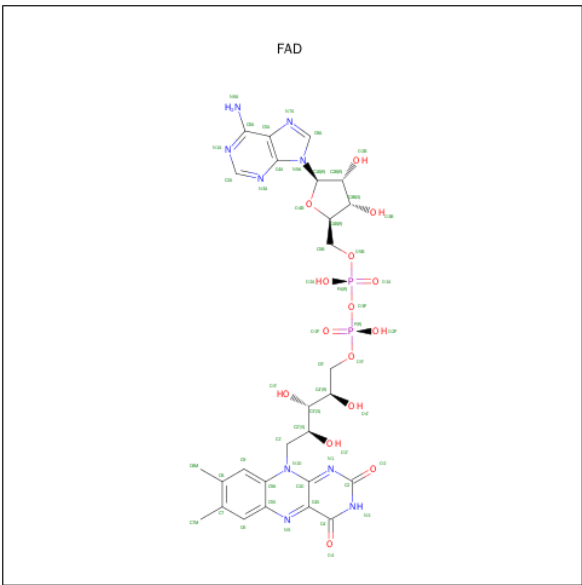
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



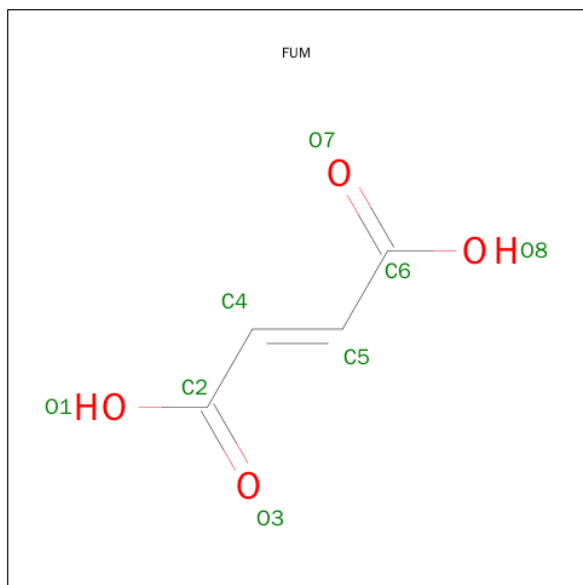
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



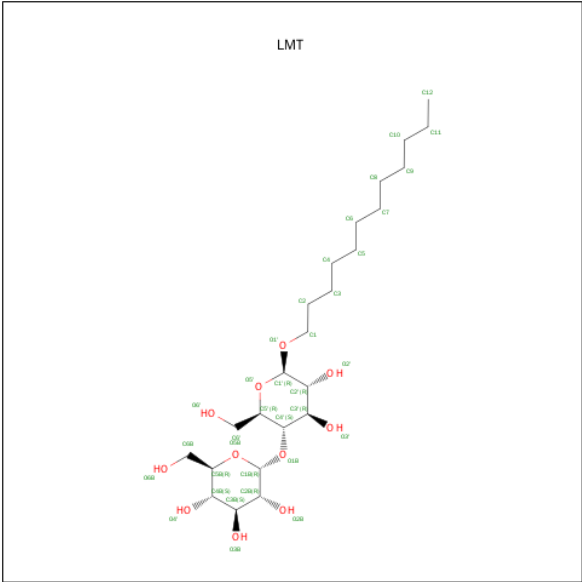
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 9 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



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

- Molecule 10 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		
11	D	1	Total	Ca	0	0
			1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	149	Total	O	0	0
			149	149		
12	B	79	Total	O	0	0
			79	79		
12	C	23	Total	O	0	0
			23	23		
12	D	148	Total	O	0	0
			148	148		
12	E	83	Total	O	0	0
			83	83		

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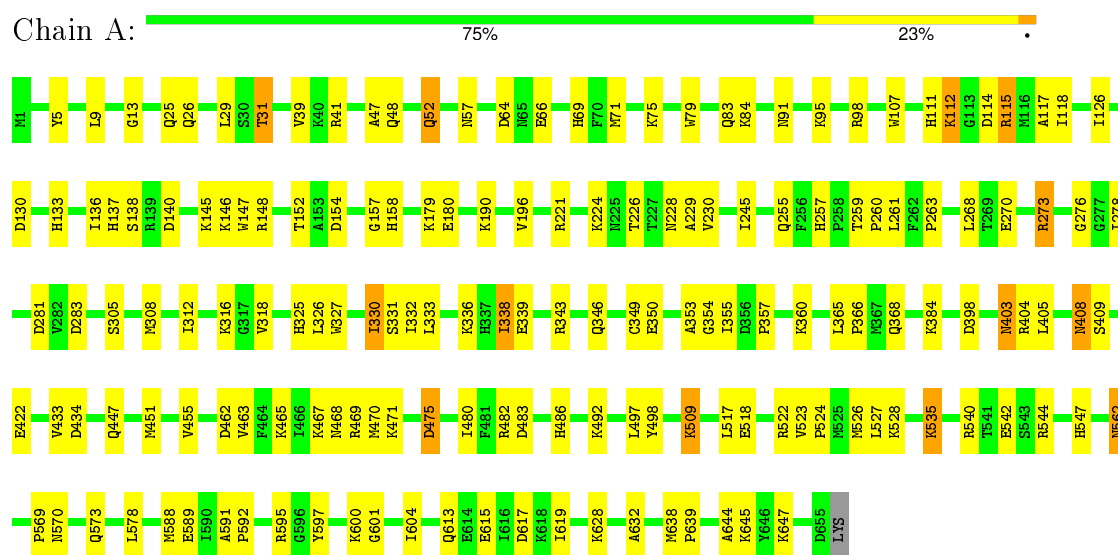
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	F	22	Total	O	0	0
			22	22		

3 Residue-property plots

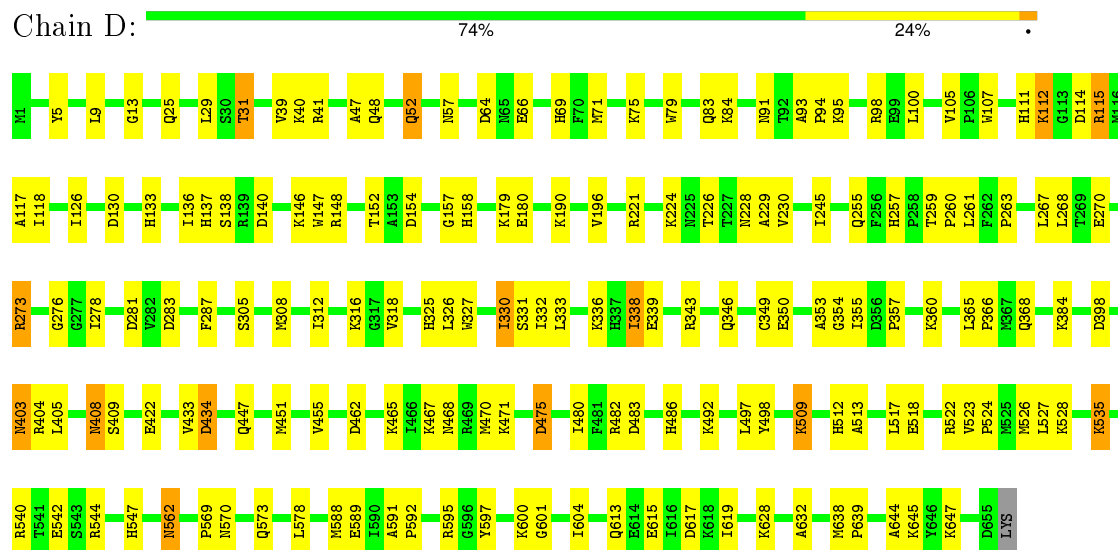
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

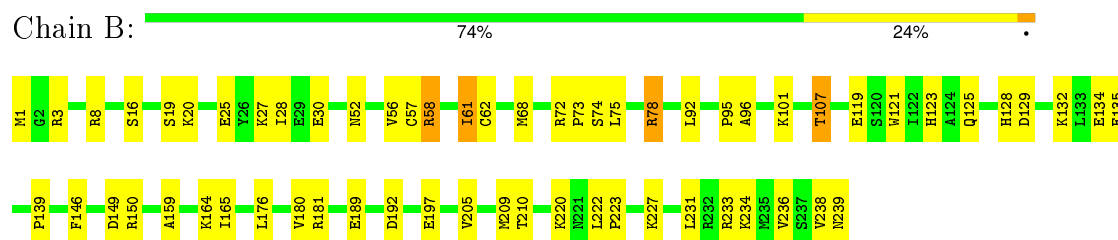
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT



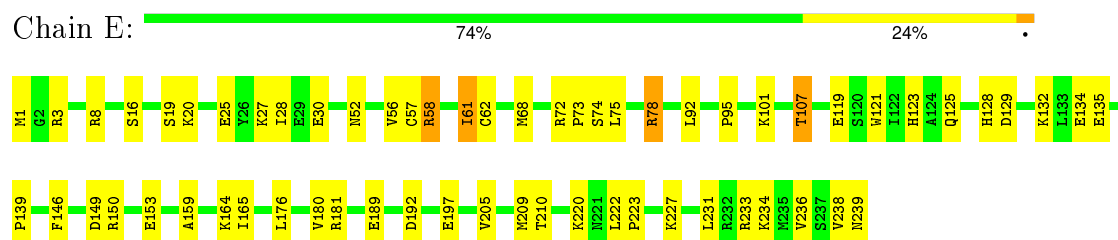
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT



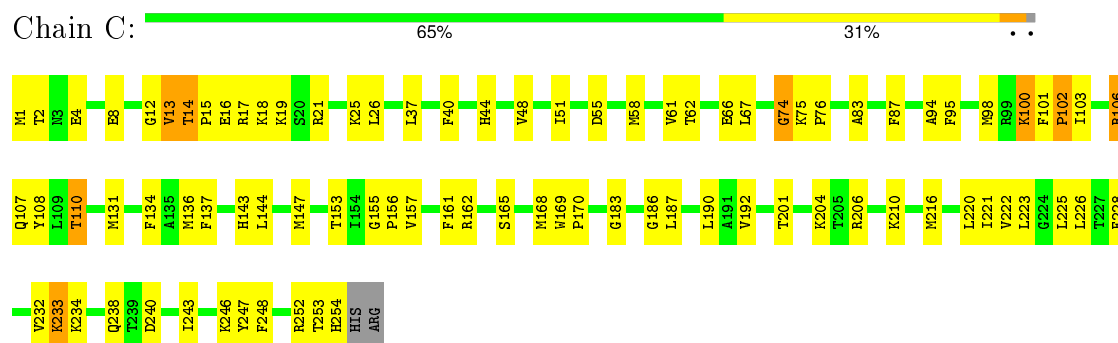
- Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN



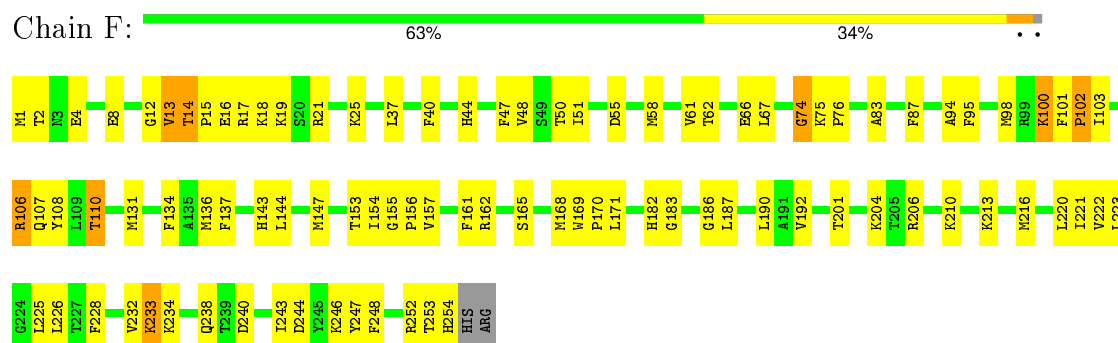
- Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN



- Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT



- Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT



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	118.40Å 85.05Å 188.85Å 90.00° 96.46° 90.00°	Depositor
Resolution (Å)	38.87 – 2.33	Depositor
% Data completeness (in resolution range)	95.8 (38.87-2.33)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.213 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19056	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: SF4, LMT, F3S, FES, HEM, FUM, CA, 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	0.32	0/5197	0.60	0/7006
1	D	0.32	0/5197	0.60	0/7006
2	B	0.35	0/1930	0.59	0/2604
2	E	0.34	0/1930	0.59	0/2604
3	C	0.32	0/2146	0.50	1/2904 (0.0%)
3	F	0.33	0/2146	0.50	1/2904 (0.0%)
All	All	0.33	0/18546	0.58	2/25028 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	PRO	N-CA-C	-5.88	96.82	112.10
3	F	102	PRO	N-CA-C	-5.86	96.85	112.10

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	5101	0	5079	148	0
1	D	5101	0	5079	149	0
2	B	1893	0	1861	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1893	0	1861	63	0
3	C	2080	0	2101	98	0
3	F	2080	0	2101	103	0
4	C	86	0	60	7	0
4	F	86	0	60	8	0
5	B	4	0	0	0	0
5	E	4	0	0	0	0
6	B	7	0	0	0	0
6	E	7	0	0	0	0
7	B	8	0	0	0	0
7	E	8	0	0	0	0
8	A	53	0	29	1	0
8	D	53	0	29	1	0
9	A	8	0	2	2	0
9	D	8	0	2	1	0
10	C	35	0	46	7	0
10	F	35	0	46	8	0
11	A	1	0	0	0	0
11	D	1	0	0	0	0
12	A	149	0	0	8	0
12	B	79	0	0	2	0
12	C	23	0	0	0	0
12	D	148	0	0	6	0
12	E	83	0	0	3	0
12	F	22	0	0	0	0
All	All	19056	0	18356	576	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 16.

The worst 5 of 576 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:253:THR:HG22	3:F:254:HIS:H	1.25	0.99
3:C:253:THR:HG22	3:C:254:HIS:H	1.25	0.98
2:B:239:ASN:ND2	3:C:21:ARG:HH21	1.64	0.96
2:E:239:ASN:ND2	3:F:21:ARG:HH21	1.64	0.95
2:E:239:ASN:HD22	3:F:21:ARG:HH21	1.15	0.91

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	653/656 (100%)	615 (94%)	33 (5%)	5 (1%)	24	25
1	D	653/656 (100%)	615 (94%)	33 (5%)	5 (1%)	24	25
2	B	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
2	E	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
3	C	252/256 (98%)	234 (93%)	15 (6%)	3 (1%)	16	14
3	F	252/256 (98%)	235 (93%)	14 (6%)	3 (1%)	16	14
All	All	2284/2302 (99%)	2157 (94%)	111 (5%)	16 (1%)	26	28

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ALA
1	A	338	ILE
3	C	67	LEU
1	D	117	ALA
1	D	338	ILE

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	534/535 (100%)	511 (96%)	23 (4%)	35	45
1	D	534/535 (100%)	510 (96%)	24 (4%)	34	42
2	B	211/211 (100%)	205 (97%)	6 (3%)	51	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	211/211 (100%)	205 (97%)	6 (3%)	51	64
3	C	221/223 (99%)	211 (96%)	10 (4%)	34	42
3	F	221/223 (99%)	211 (96%)	10 (4%)	34	42
All	All	1932/1938 (100%)	1853 (96%)	79 (4%)	37	47

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	100	LYS
1	D	115	ARG
3	F	58	MET
3	C	106	ARG
1	D	31	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	208	ASN
1	D	133	HIS
3	F	3	ASN
3	C	238	GLN
1	D	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 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$
8	FAD	A	1656	1	48,58,58	1.90	11 (22%)	54,89,89	2.03	12 (22%)
9	FUM	A	1657	-	1,7,7	1.74	0	0,8,8	0.00	-
5	FES	B	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
6	F3S	B	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	B	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
4	HEM	C	1255	3	30,50,50	3.00	11 (36%)	24,82,82	2.28	9 (37%)
4	HEM	C	1256	3	30,50,50	2.99	11 (36%)	24,82,82	2.16	7 (29%)
10	LMT	C	1257	-	36,36,36	1.09	2 (5%)	47,47,47	1.26	4 (8%)
8	FAD	D	1656	1	48,58,58	1.88	12 (25%)	54,89,89	2.03	12 (22%)
9	FUM	D	1657	-	1,7,7	1.75	0	0,8,8	0.00	-
5	FES	E	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
6	F3S	E	1241	2	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	E	1242	2	0,12,12	0.00	-	0,24,24	0.00	-
4	HEM	F	1255	3	30,50,50	3.01	11 (36%)	24,82,82	2.26	8 (33%)
4	HEM	F	1256	3	30,50,50	3.00	11 (36%)	24,82,82	2.19	8 (33%)
10	LMT	F	1257	-	36,36,36	1.09	2 (5%)	47,47,47	1.26	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
8	FAD	A	1656	1	-	0/30/50/50	0/6/6/6
9	FUM	A	1657	-	-	0/0/5/5	0/0/0/0
5	FES	B	1240	2	-	0/0/4/4	0/1/1/1
6	F3S	B	1241	2	-	0/0/24/24	0/0/3/3
7	SF4	B	1242	2	-	0/0/48/48	0/6/5/5
4	HEM	C	1255	3	-	0/10/54/54	0/0/8/8
4	HEM	C	1256	3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	C	1257	-	-	0/21/61/61	0/2/2/2
8	FAD	D	1656	1	-	0/30/50/50	0/6/6/6
9	FUM	D	1657	-	-	0/0/5/5	0/0/0/0
5	FES	E	1240	2	-	0/0/4/4	0/1/1/1
6	F3S	E	1241	2	-	0/0/24/24	0/0/3/3
7	SF4	E	1242	2	-	0/0/48/48	0/6/5/5
4	HEM	F	1255	3	-	0/10/54/54	0/0/8/8
4	HEM	F	1256	3	-	0/10/54/54	0/0/8/8
10	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)
4	F	1255	HEM	C3B-C4B	-8.09	1.44	1.51
4	C	1255	HEM	C3B-C4B	-7.91	1.44	1.51
4	F	1256	HEM	C3B-C4B	-7.78	1.44	1.51
4	C	1256	HEM	C3B-C4B	-7.78	1.44	1.51
4	F	1256	HEM	C3B-CAB	-6.75	1.38	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1656	FAD	C1'-N10-C9A	-5.98	112.15	118.86
8	D	1656	FAD	C1'-N10-C9A	-5.92	112.22	118.86
8	D	1656	FAD	C4X-C4-N3	-4.63	117.26	123.59
8	A	1656	FAD	C4X-C4-N3	-4.58	117.33	123.59
8	A	1656	FAD	C4X-C10-N10	-4.34	117.96	120.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1656	FAD	1	0
9	A	1657	FUM	2	0
4	C	1255	HEM	3	0
4	C	1256	HEM	4	0
10	C	1257	LMT	7	0
8	D	1656	FAD	1	0
9	D	1657	FUM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1255	HEM	4	0
4	F	1256	HEM	4	0
10	F	1257	LMT	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](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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