



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KFY  
Title : QUINOL-FUMARATE REDUCTASE WITH QUINOL INHIBITOR 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL  
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.  
Deposited on : 2001-11-24  
Resolution : 3.60 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) : **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

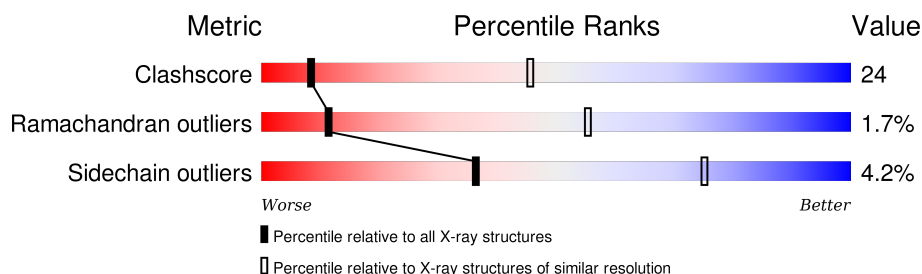
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)


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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	602	 67% 26% . .
1	M	602	 53% 39% . .
2	B	243	 69% 28% . .
2	N	243	 49% 47% .
3	C	130	 59% 34% 6% .
3	O	130	 55% 37% 7% .
4	D	119	 52% 43% . .

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Mol	Chain	Length	Quality of chain
4	P	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BRS	B	700	-	-	X	-
7	F3S	N	245	-	-	X	-
8	SF4	N	246	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16957 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

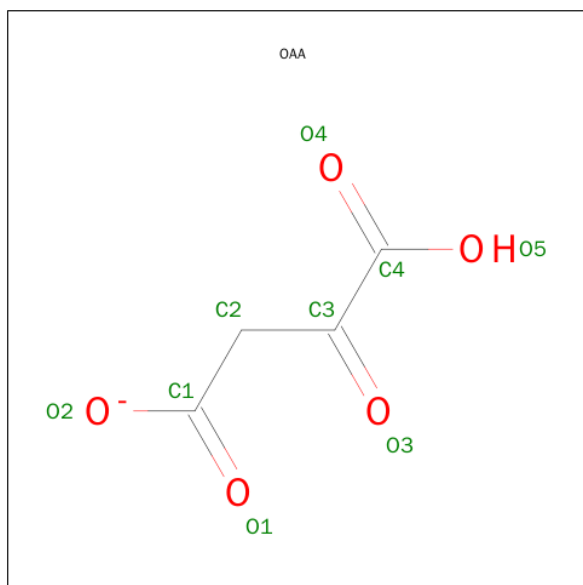
- Molecule 3 is a protein called FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

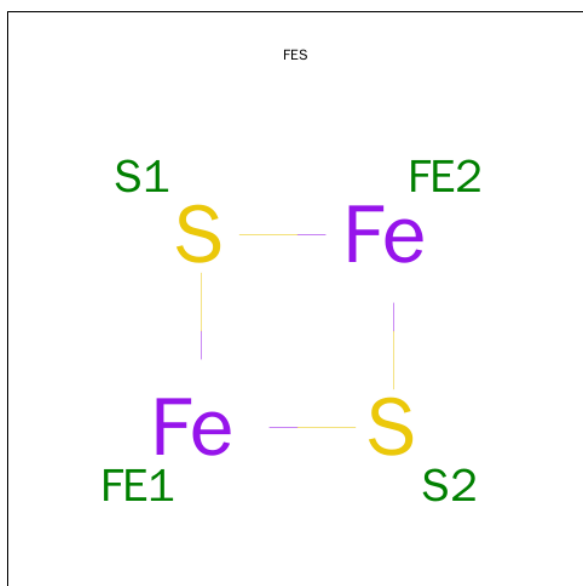
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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



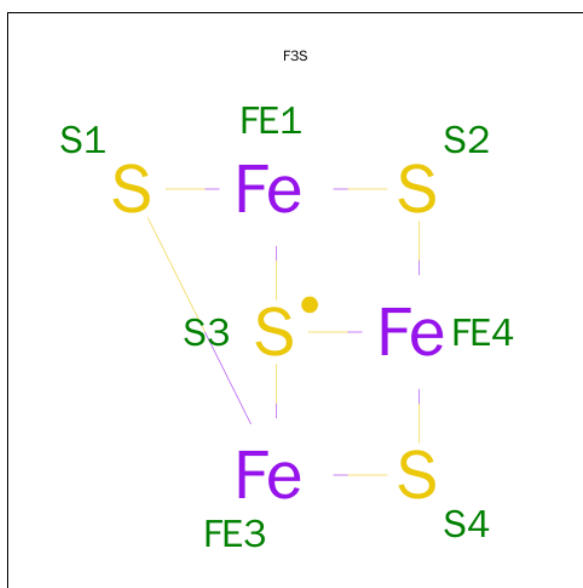
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		
5	M	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



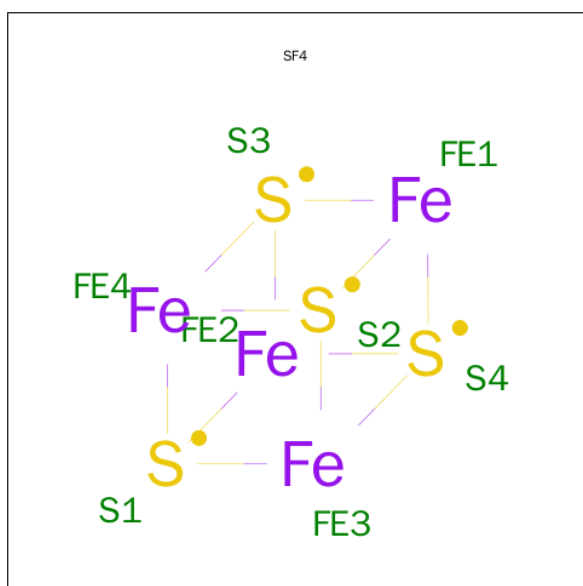
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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

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



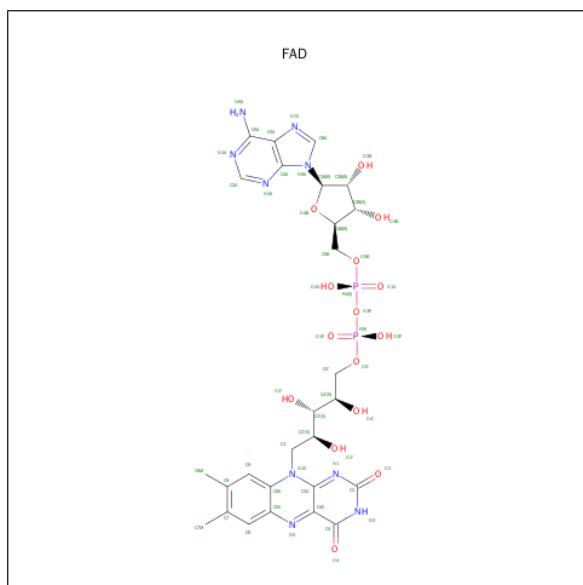
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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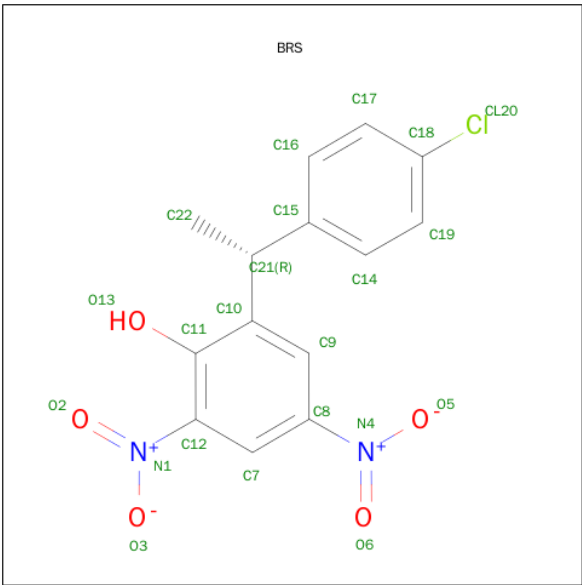
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



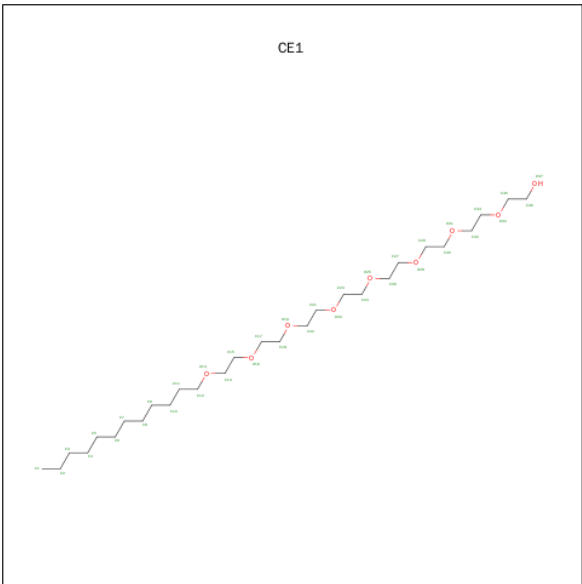
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
9	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 10 is 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL (three-letter code: BRS) (formula:  $C_{14}H_{11}ClN_2O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			22	14	1	2	5		
10	N	1	Total	C	Cl	N	O	0	0
			22	14	1	2	5		

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: C<sub>28</sub>H<sub>58</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	P	1	Total	C	O	0	0
			37	28	9		

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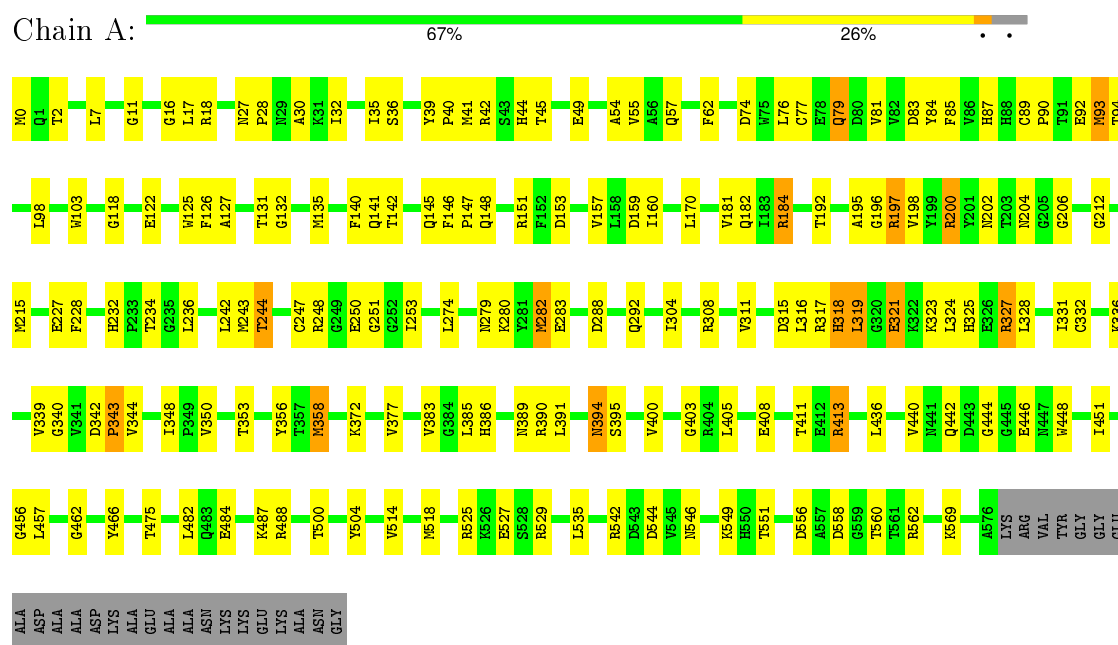
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			37	28	9		
11	O	1	Total	C	O	0	0
			37	28	9		

### 3 Residue-property plots

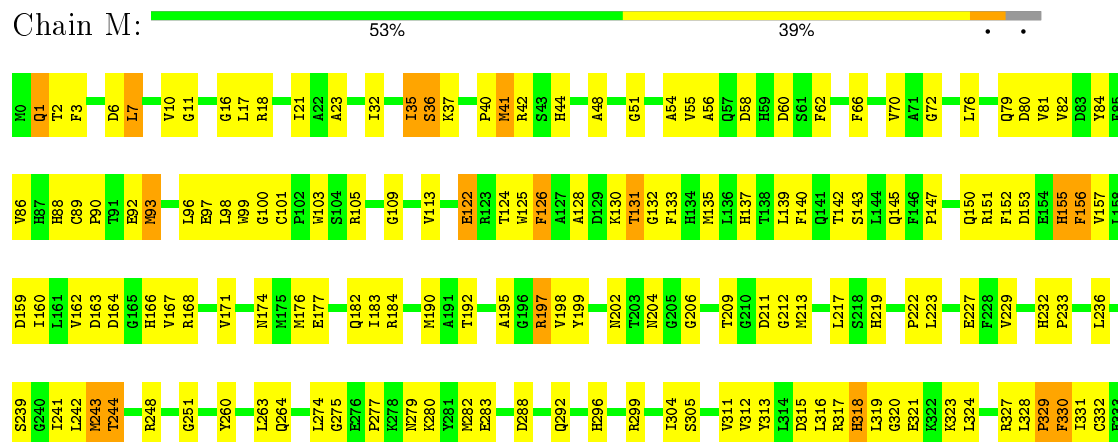
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

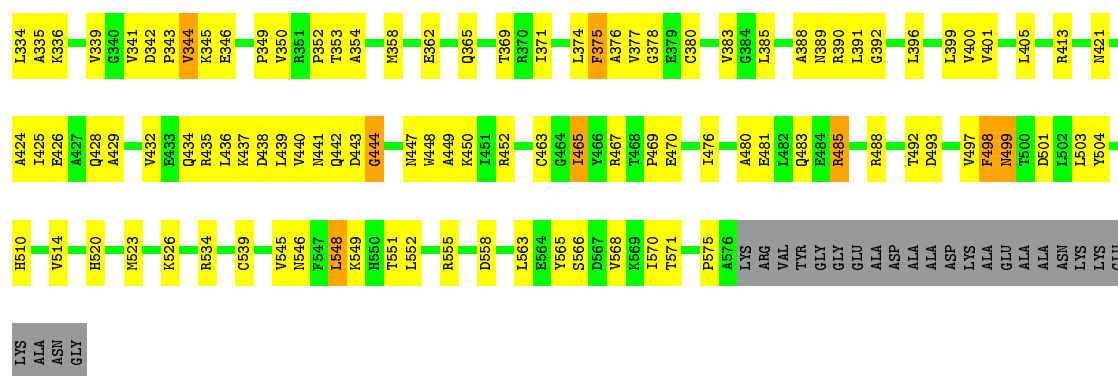
Note EDS was not executed.

#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

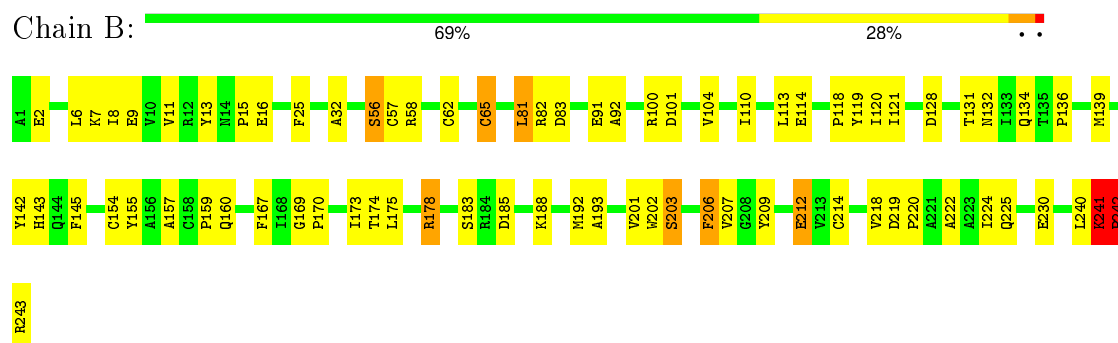


#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

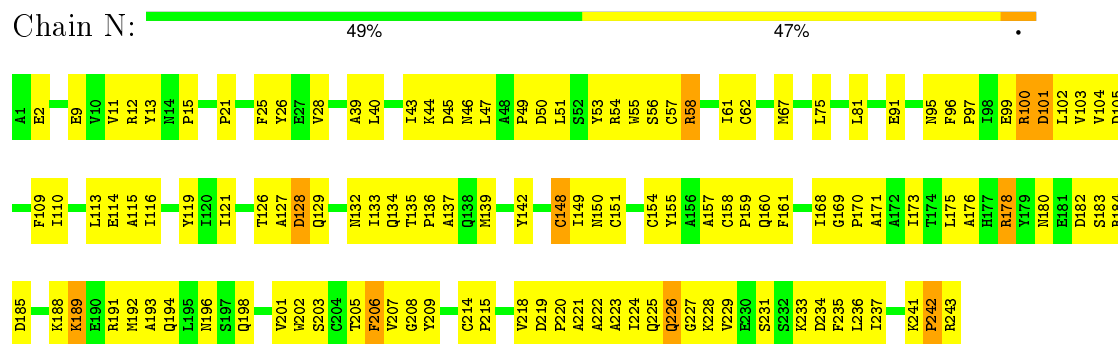




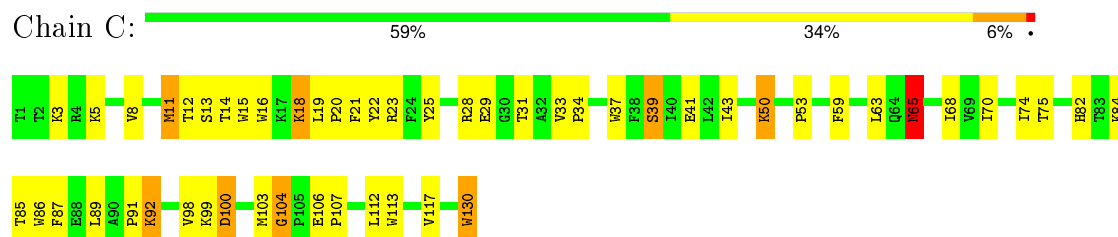
• Molecule 2: Fumarate reductase iron-sulfur protein



• Molecule 2: Fumarate reductase iron-sulfur protein

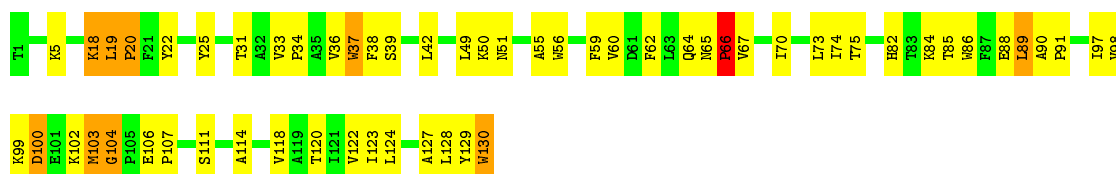


• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN



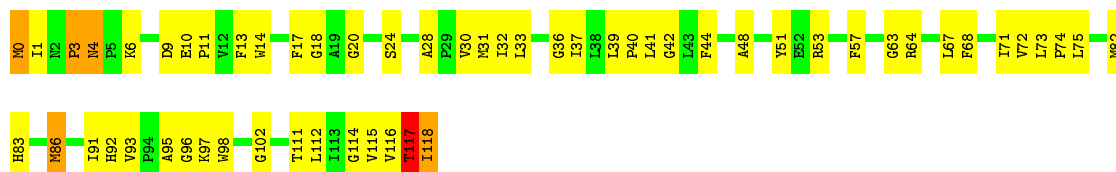
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN





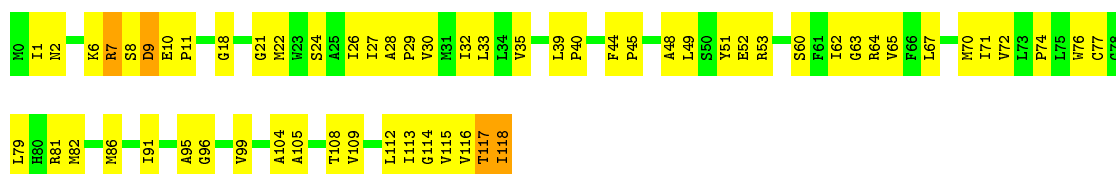
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D: 52% 43% . .



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P: 50% 47% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.15Å 137.81Å 270.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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: OAA, SF4, BRS, F3S, FES, CE1, 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	0.67	1/4540 (0.0%)	0.81	1/6139 (0.0%)
1	M	0.57	0/4540	0.76	0/6139
2	B	0.62	1/1931 (0.1%)	0.82	1/2617 (0.0%)
2	N	0.58	1/1931 (0.1%)	0.79	2/2617 (0.1%)
3	C	0.78	3/1094 (0.3%)	0.86	3/1496 (0.2%)
3	O	0.72	2/1094 (0.2%)	0.83	2/1496 (0.1%)
4	D	0.69	2/956 (0.2%)	0.91	3/1303 (0.2%)
4	P	0.66	1/956 (0.1%)	0.84	1/1303 (0.1%)
All	All	0.64	11/17042 (0.1%)	0.81	13/23110 (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	O	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	130	TRP	CB-CG	-8.82	1.34	1.50
4	D	117	THR	CA-C	-6.44	1.36	1.52
3	C	104	GLY	C-O	-6.43	1.13	1.23
3	O	104	GLY	C-O	-6.29	1.13	1.23
1	A	77	CYS	CB-SG	-6.04	1.72	1.82

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	117	THR	N-CA-C	8.57	134.14	111.00
3	C	65	ASN	N-CA-C	7.78	132.01	111.00
4	D	117	THR	CB-CA-C	-6.08	95.18	111.60
2	B	241	LYS	C-N-CD	-5.95	107.52	120.60
3	O	130	TRP	CA-CB-CG	5.85	124.82	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	129	TYR	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	4448	0	4335	150	0
1	M	4448	0	4335	263	0
2	B	1888	0	1837	72	0
2	N	1888	0	1837	121	0
3	C	1058	0	1108	63	0
3	O	1058	0	1108	64	0
4	D	926	0	971	78	0
4	P	926	0	971	74	0
5	A	9	0	2	1	0
5	M	9	0	2	2	0
6	B	4	0	0	0	0
6	N	4	0	0	0	0
7	B	7	0	0	0	0
7	N	7	0	0	2	0
8	B	8	0	0	0	0
8	N	8	0	0	7	0
9	A	53	0	31	7	0
9	M	53	0	31	10	0
10	B	22	0	11	11	0
10	N	22	0	11	5	0
11	D	37	0	58	5	0
11	O	37	0	58	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	37	0	58	2	0
All	All	16957	0	16764	810	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 24.

The worst 5 of 810 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:135:MET:SD	1:A:135:MET:CE	2.01	1.48
1:A:44:HIS:NE2	9:A:703:FAD:HM82	1.06	1.37
1:M:44:HIS:NE2	9:M:803:FAD:HM82	1.04	1.35
4:D:6:LYS:HG3	4:P:6:LYS:HB3	1.27	1.16
1:A:44:HIS:CE1	9:A:703:FAD:HM82	1.83	1.14

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	575/602 (96%)	525 (91%)	43 (8%)	7 (1%)	16	62
1	M	575/602 (96%)	506 (88%)	59 (10%)	10 (2%)	11	55
2	B	241/243 (99%)	218 (90%)	19 (8%)	4 (2%)	11	55
2	N	241/243 (99%)	212 (88%)	23 (10%)	6 (2%)	7	48
3	C	128/130 (98%)	116 (91%)	9 (7%)	3 (2%)	8	50
3	O	128/130 (98%)	114 (89%)	10 (8%)	4 (3%)	5	43
4	D	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	21	67
4	P	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	21	67
All	All	2122/2188 (97%)	1900 (90%)	186 (9%)	36 (2%)	11	55



5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	PRO
1	M	1	GLN
1	M	244	THR
3	O	18	LYS
1	A	79	GLN

### 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	460/475 (97%)	448 (97%)	12 (3%)	54	83
1	M	460/475 (97%)	435 (95%)	25 (5%)	27	68
2	B	205/205 (100%)	197 (96%)	8 (4%)	39	77
2	N	205/205 (100%)	196 (96%)	9 (4%)	35	74
3	C	111/111 (100%)	106 (96%)	5 (4%)	34	74
3	O	111/111 (100%)	105 (95%)	6 (5%)	27	68
4	D	97/97 (100%)	91 (94%)	6 (6%)	23	65
4	P	97/97 (100%)	94 (97%)	3 (3%)	47	81
All	All	1746/1776 (98%)	1672 (96%)	74 (4%)	36	75

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	36	SER
1	M	163	ASP
3	O	37	TRP
1	M	41	MET
1	M	126	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	182	GLN
1	M	366	ASN
3	O	65	ASN
1	M	204	ASN
1	M	230	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 ⓘ

15 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	OAA	A	702	-	2,8,8	3.75	2 (100%)	2,10,10	2.23	1 (50%)
9	FAD	A	703	1	48,58,58	1.60	7 (14%)	54,89,89	2.35	8 (14%)
6	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	B	245	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	B	246	2	0,12,12	0.00	-	0,24,24	0.00	-
10	BRS	B	700	-	18,23,23	2.11	7 (38%)	25,33,33	1.66	7 (28%)
11	CE1	D	710	-	36,36,36	1.11	2 (5%)	35,35,35	1.61	8 (22%)
5	OAA	M	802	-	2,8,8	0.96	0	2,10,10	0.71	0
9	FAD	M	803	1	48,58,58	1.71	7 (14%)	54,89,89	2.21	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	N	245	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	N	246	2	0,12,12	0.00	-	0,24,24	0.00	-
10	BRS	N	800	-	18,23,23	1.56	3 (16%)	25,33,33	1.48	5 (20%)
11	CE1	O	811	-	36,36,36	1.06	0	35,35,35	1.65	12 (34%)
11	CE1	P	810	-	36,36,36	1.05	2 (5%)	35,35,35	1.73	10 (28%)

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	OAA	A	702	-	-	0/2/8/8	0/0/0/0
9	FAD	A	703	1	-	0/30/50/50	0/6/6/6
6	FES	B	244	2	-	0/0/4/4	0/1/1/1
7	F3S	B	245	2	-	0/0/24/24	0/0/3/3
8	SF4	B	246	2	-	0/0/48/48	0/6/5/5
10	BRS	B	700	-	-	0/15/16/16	0/2/2/2
11	CE1	D	710	-	-	0/34/34/34	0/0/0/0
5	OAA	M	802	-	-	0/2/8/8	0/0/0/0
9	FAD	M	803	1	-	0/30/50/50	0/6/6/6
6	FES	N	244	2	-	0/0/4/4	0/1/1/1
7	F3S	N	245	2	-	0/0/24/24	0/0/3/3
8	SF4	N	246	2	-	0/0/48/48	0/6/5/5
10	BRS	N	800	-	-	0/15/16/16	0/2/2/2
11	CE1	O	811	-	-	0/34/34/34	0/0/0/0
11	CE1	P	810	-	-	0/34/34/34	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	703	FAD	P-O5'	-2.77	1.46	1.59
9	M	803	FAD	P-O5'	-2.19	1.49	1.59
10	B	700	BRS	C14-C15	2.05	1.42	1.39
9	A	703	FAD	C4A-N3A	2.17	1.38	1.35
11	P	810	CE1	O28-C29	2.21	1.51	1.42

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
9	A	703	FAD	N3A-C2A-N1A	-11.01	120.47	128.89
9	M	803	FAD	N3A-C2A-N1A	-10.97	120.50	128.89
9	M	803	FAD	C4X-C10-N10	-5.06	117.54	120.52
9	A	703	FAD	C4X-C10-N10	-5.03	117.56	120.52
10	N	800	BRS	C9-C10-C21	-3.41	117.89	122.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	OAA	1	0
9	A	703	FAD	7	0
10	B	700	BRS	11	0
11	D	710	CE1	5	0
5	M	802	OAA	2	0
9	M	803	FAD	10	0
7	N	245	F3S	2	0
8	N	246	SF4	7	0
10	N	800	BRS	5	0
11	O	811	CE1	1	0
11	P	810	CE1	2	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 ⓘ

### 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.