



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:35 PM GMT

PDB ID : 1U6I
Title : The Structure of native coenzyme F420-dependent methylenetetrahydromethanopterin dehydrogenase at 2.2Å resolution
Authors : Warkentin, E.; Hagemeier, C.H.; Shima, S.; Thauer, R.K.; Ermler, U.
Deposited on : 2004-07-30
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

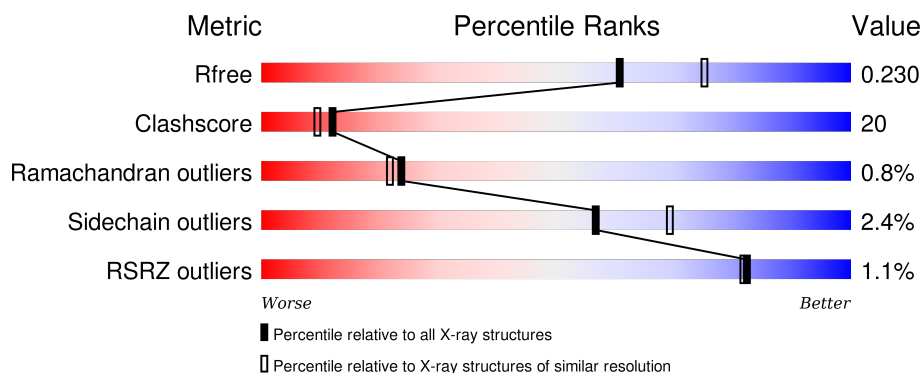
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.









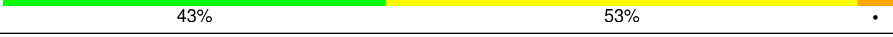
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	<div> <div>73%</div> <div>26%</div> </div>
1	B	283	<div> <div>70%</div> <div>29%</div> <div>•</div> </div>
1	C	283	<div> <div>2%</div> <div>62%</div> <div>36%</div> <div>•</div> </div>
1	D	283	<div> <div>61%</div> <div>38%</div> <div>•</div> </div>
1	E	283	<div> <div>59%</div> <div>40%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	283	
1	G	283	
1	H	283	
1	I	283	
1	J	283	
1	K	283	
1	L	283	

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
2	MG	H	6012	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26858 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 F420-dependent methylenetetrahydromethanopterin dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	B	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	C	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	D	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	E	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	F	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	G	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	H	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	I	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	J	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	K	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	L	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P94951
B	1	MET	-	INITIATING METHIONINE	UNP P94951
C	1	MET	-	INITIATING METHIONINE	UNP P94951
D	1	MET	-	INITIATING METHIONINE	UNP P94951

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	INITIATING METHIONINE	UNP P94951
F	1	MET	-	INITIATING METHIONINE	UNP P94951
G	1	MET	-	INITIATING METHIONINE	UNP P94951
H	1	MET	-	INITIATING METHIONINE	UNP P94951
I	1	MET	-	INITIATING METHIONINE	UNP P94951
J	1	MET	-	INITIATING METHIONINE	UNP P94951
K	1	MET	-	INITIATING METHIONINE	UNP P94951
L	1	MET	-	INITIATING METHIONINE	UNP P94951

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0
3	B	112	Total O 112 112	0	0
3	C	27	Total O 27 27	0	0
3	D	35	Total O 35 35	0	0
3	E	38	Total O 38 38	0	0
3	F	42	Total O 42 42	0	0
3	G	88	Total O 88 88	0	0
3	H	100	Total O 100 100	0	0
3	I	32	Total O 32 32	0	0

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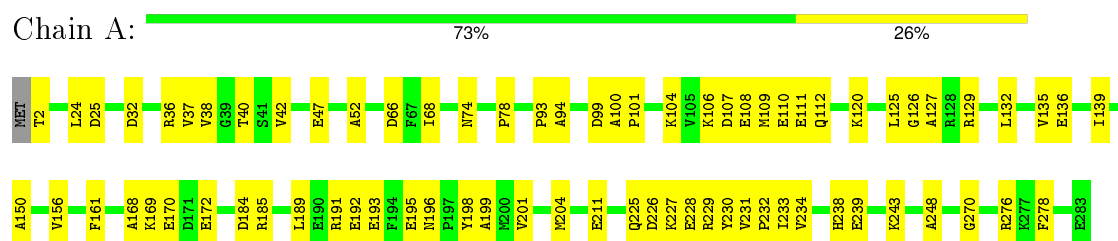
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	35	Total	O	0	0
			35	35		
3	K	39	Total	O	0	0
			39	39		
3	L	37	Total	O	0	0
			37	37		

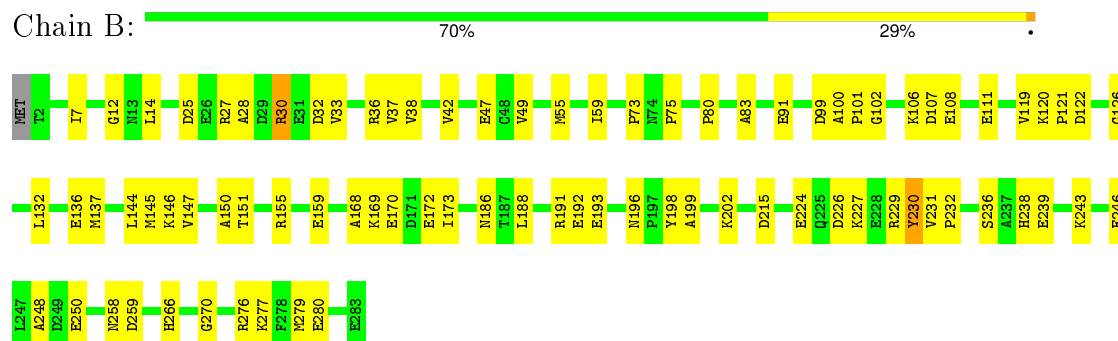
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

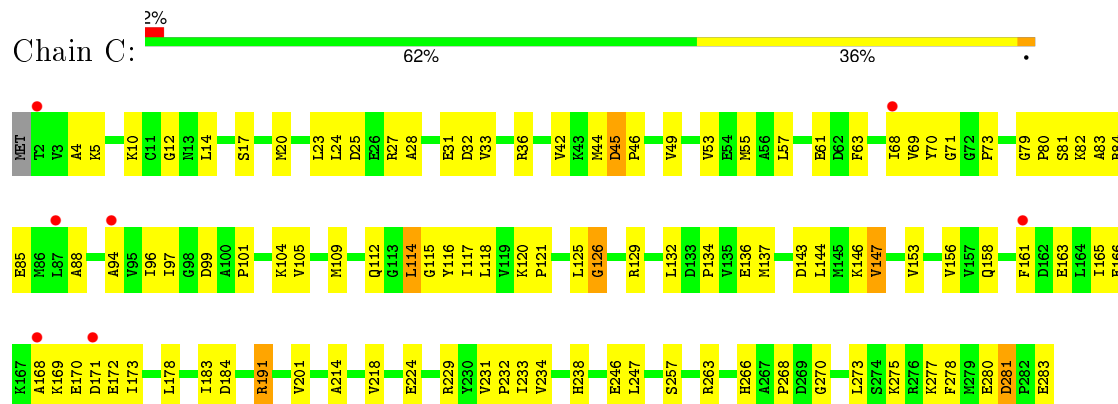
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

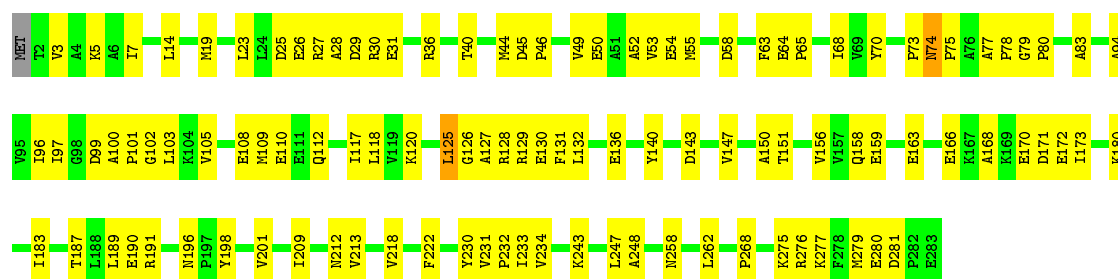


- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



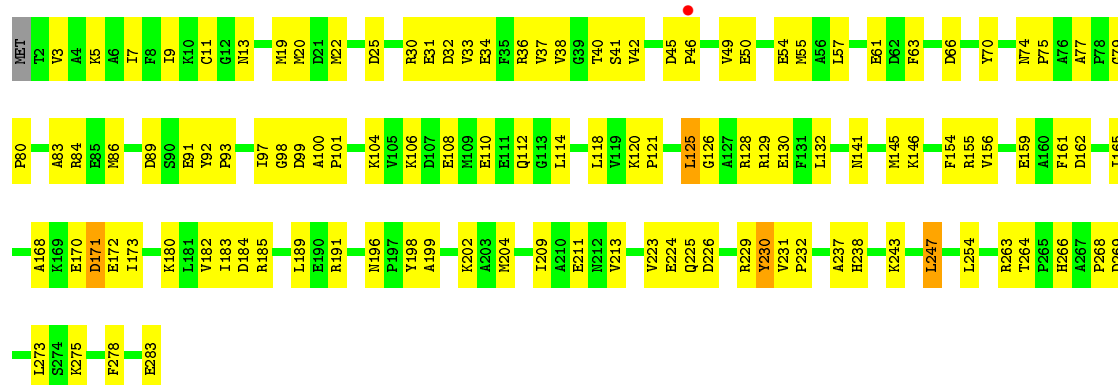
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

Chain D:  61% 38%



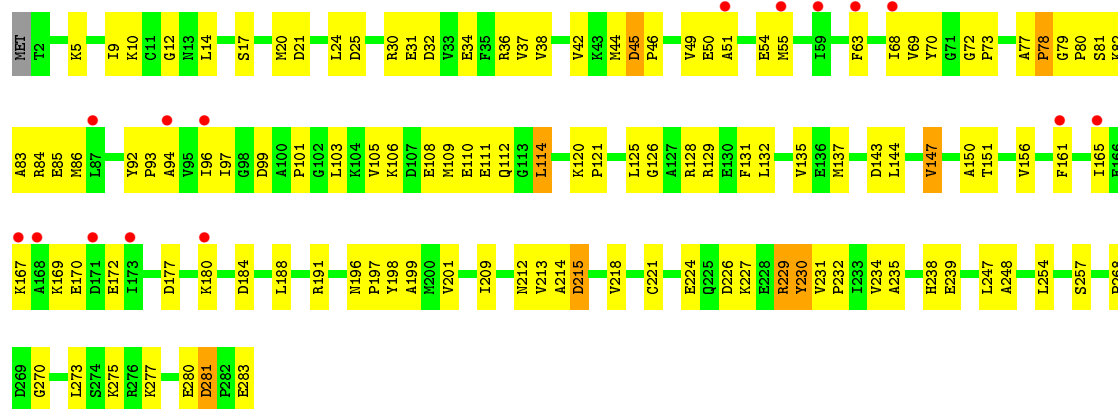
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

Chain E:  59% 40%



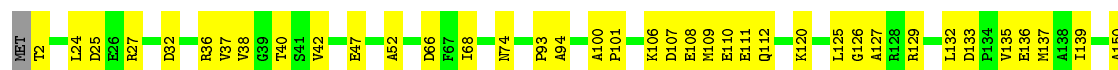
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

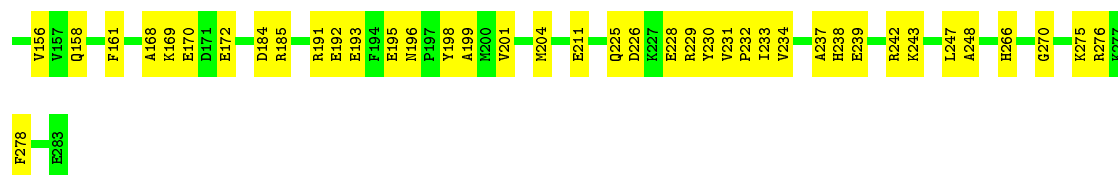
Chain F:  5% 57% 40%



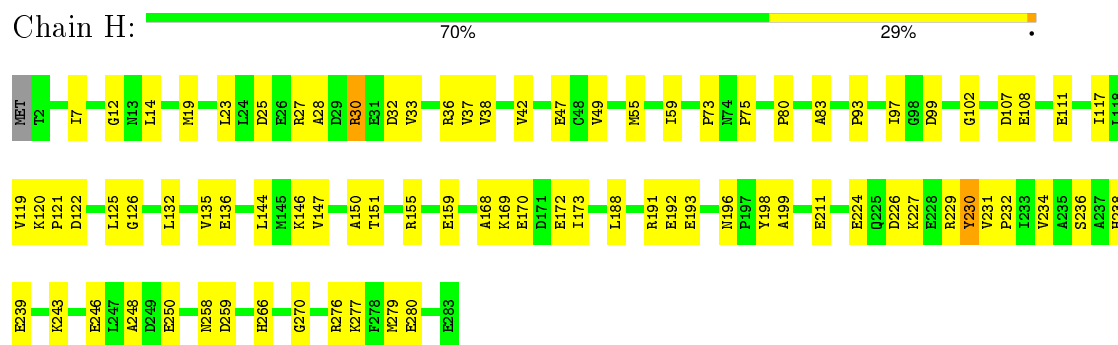
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

Chain G:  72% 28%

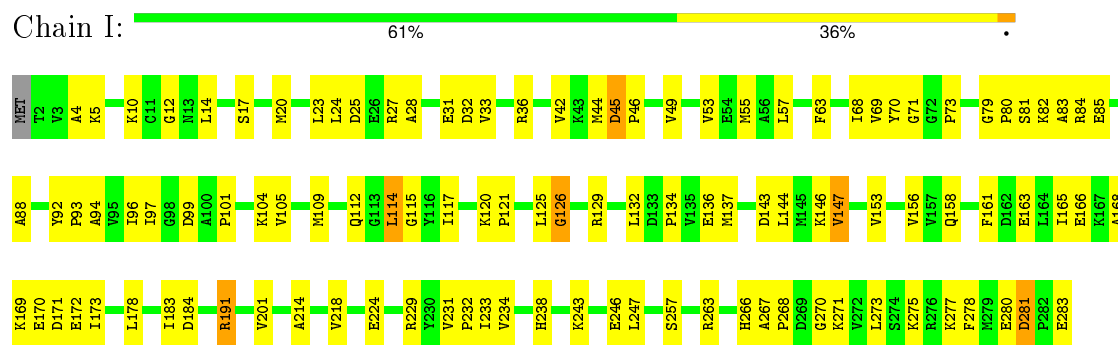




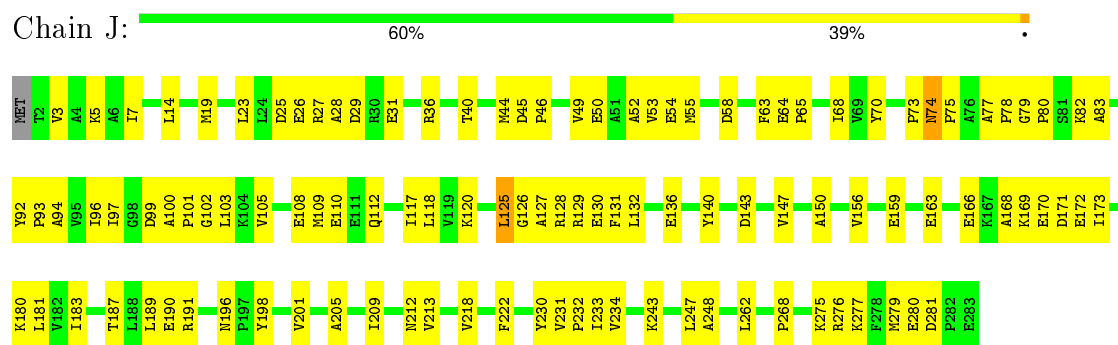
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



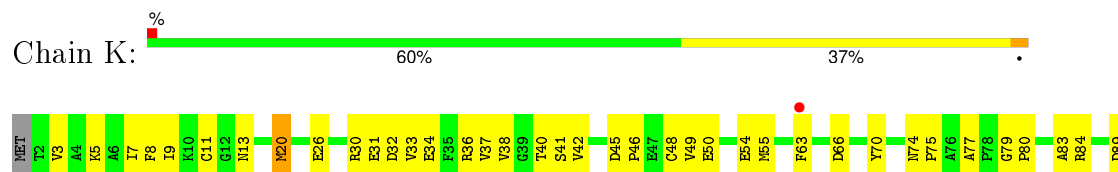
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

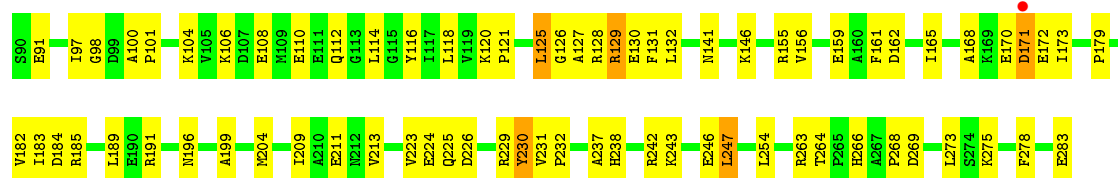


- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

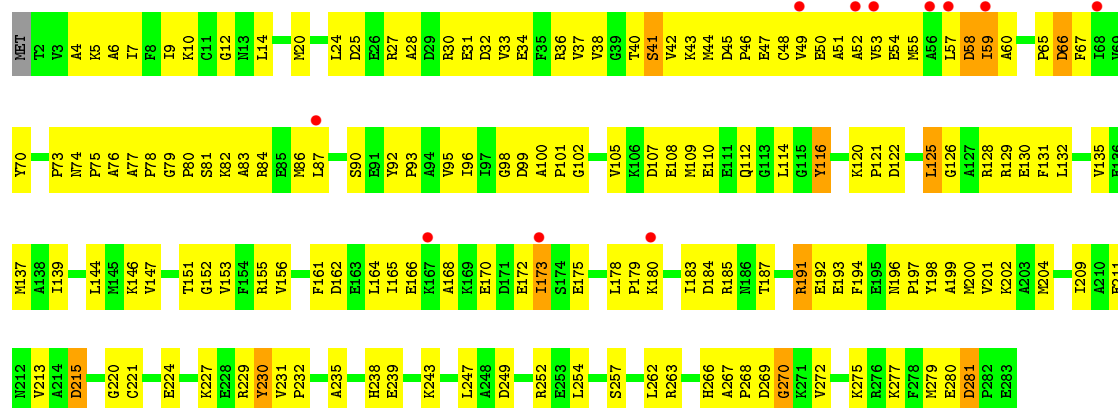


- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase





- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.90Å 118.90Å 219.20Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	19.35 – 2.20 19.35 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.35-2.20) 94.2 (19.35-1.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.235 0.188 , 0.230	Depositor DCC
R_{free} test set	9126 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	7 of 247785 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26858	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 92.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0800e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.37	0/2215	0.61	0/2989
1	B	0.37	0/2215	0.61	0/2989
1	C	0.36	0/2215	0.58	0/2989
1	D	0.35	0/2215	0.58	0/2989
1	E	0.34	0/2215	0.56	0/2989
1	F	0.36	0/2215	0.63	0/2989
1	G	0.37	0/2215	0.61	0/2989
1	H	0.36	0/2215	0.61	0/2989
1	I	0.34	0/2215	0.58	0/2989
1	J	0.34	0/2215	0.58	0/2989
1	K	0.33	0/2215	0.56	0/2989
1	L	0.34	0/2215	0.61	0/2989
All	All	0.35	0/26580	0.59	0/35868

There are no bond length outliers.

There are no bond angle outliers.

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	2182	0	2157	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2182	0	2157	69	0
1	C	2182	0	2157	100	0
1	D	2182	0	2157	99	0
1	E	2182	0	2157	103	0
1	F	2182	0	2157	113	0
1	G	2182	0	2157	70	0
1	H	2182	0	2157	68	0
1	I	2182	0	2157	101	0
1	J	2182	0	2157	99	0
1	K	2182	0	2157	103	0
1	L	2182	0	2157	157	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	81	0	0	6	0
3	B	112	0	0	9	0
3	C	27	0	0	1	0
3	D	35	0	0	1	0
3	E	38	0	0	5	0
3	F	42	0	0	2	0
3	G	88	0	0	7	0
3	H	100	0	0	8	0
3	I	32	0	0	1	0
3	J	35	0	0	2	0
3	K	39	0	0	3	0
3	L	37	0	0	4	0
All	All	26858	0	25884	1038	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 20.

The worst 5 of 1038 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:D:156:VAL:HG22	1:D:191:ARG:HH11	1.13	1.14
1:J:156:VAL:HG22	1:J:191:ARG:HH11	1.14	1.08
1:G:132:LEU:HG	3:G:8432:HOH:O	1.61	0.98
1:L:5:LYS:HG2	1:L:34:GLU:HB3	1.49	0.92
1:F:126:GLY:H	1:F:238:HIS:HE1	1.21	0.87

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	280/283 (99%)	263 (94%)	15 (5%)	2 (1%)	26	25
1	B	280/283 (99%)	265 (95%)	15 (5%)	0	100	100
1	C	280/283 (99%)	255 (91%)	23 (8%)	2 (1%)	26	25
1	D	280/283 (99%)	263 (94%)	16 (6%)	1 (0%)	39	42
1	E	280/283 (99%)	258 (92%)	18 (6%)	4 (1%)	14	10
1	F	280/283 (99%)	258 (92%)	20 (7%)	2 (1%)	26	25
1	G	280/283 (99%)	263 (94%)	15 (5%)	2 (1%)	26	25
1	H	280/283 (99%)	266 (95%)	14 (5%)	0	100	100
1	I	280/283 (99%)	255 (91%)	23 (8%)	2 (1%)	26	25
1	J	280/283 (99%)	263 (94%)	16 (6%)	1 (0%)	39	42
1	K	280/283 (99%)	258 (92%)	18 (6%)	4 (1%)	14	10
1	L	280/283 (99%)	232 (83%)	42 (15%)	6 (2%)	9	5
All	All	3360/3396 (99%)	3099 (92%)	235 (7%)	26 (1%)	24	22

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	129	ARG
1	K	129	ARG
1	E	171	ASP
1	K	171	ASP
1	L	41	SER

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	233/234 (100%)	228 (98%)	5 (2%)	61	74
1	B	233/234 (100%)	231 (99%)	2 (1%)	84	92
1	C	233/234 (100%)	224 (96%)	9 (4%)	39	48
1	D	233/234 (100%)	231 (99%)	2 (1%)	84	92
1	E	233/234 (100%)	226 (97%)	7 (3%)	48	60
1	F	233/234 (100%)	226 (97%)	7 (3%)	48	60
1	G	233/234 (100%)	228 (98%)	5 (2%)	61	74
1	H	233/234 (100%)	230 (99%)	3 (1%)	76	87
1	I	233/234 (100%)	225 (97%)	8 (3%)	44	54
1	J	233/234 (100%)	231 (99%)	2 (1%)	84	92
1	K	233/234 (100%)	226 (97%)	7 (3%)	48	60
1	L	233/234 (100%)	224 (96%)	9 (4%)	39	48
All	All	2796/2808 (100%)	2730 (98%)	66 (2%)	57	69

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	215	ASP
1	G	230	TYR
1	L	125	LEU
1	F	229	ARG
1	G	47	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	196	ASN
1	G	238	HIS
1	K	238	HIS
1	F	238	HIS

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Mol	Chain	Res	Type
1	G	158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	282/283 (99%)	-0.56	0 100 100	11, 26, 45, 55	0
1	B	282/283 (99%)	-0.55	0 100 100	13, 24, 39, 61	0
1	C	282/283 (99%)	-0.08	7 (2%) 61 60	18, 45, 75, 88	0
1	D	282/283 (99%)	-0.38	0 100 100	18, 41, 61, 74	0
1	E	282/283 (99%)	-0.27	1 (0%) 93 93	20, 45, 69, 85	0
1	F	282/283 (99%)	0.09	15 (5%) 30 29	16, 49, 79, 91	0
1	G	282/283 (99%)	-0.57	0 100 100	13, 27, 43, 52	0
1	H	282/283 (99%)	-0.58	0 100 100	13, 24, 40, 59	0
1	I	282/283 (99%)	-0.16	0 100 100	15, 46, 70, 81	0
1	J	282/283 (99%)	-0.31	0 100 100	18, 42, 64, 76	0
1	K	282/283 (99%)	-0.25	2 (0%) 89 88	21, 46, 67, 79	0
1	L	282/283 (99%)	0.05	11 (3%) 43 42	18, 48, 78, 91	0
All	All	3384/3396 (99%)	-0.30	36 (1%) 82 82	11, 36, 69, 91	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	57	LEU	4.3
1	F	94	ALA	4.0
1	L	53	VAL	3.9
1	F	168	ALA	3.6
1	L	167	LYS	3.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	H	6012	1/1	0.98	0.13	3.09	27,27,27,27	0
2	MG	G	6008	1/1	0.97	0.10	-0.87	29,29,29,29	0
2	MG	G	6009	1/1	0.86	0.09	-1.58	47,47,47,47	0
2	MG	A	6002	1/1	0.96	0.08	-1.89	32,32,32,32	0
2	MG	B	6005	1/1	0.96	0.09	-2.07	17,17,17,17	0
2	MG	A	6001	1/1	0.93	0.08	-3.31	19,19,19,19	0
2	MG	H	6011	1/1	0.97	0.05	-	26,26,26,26	0
2	MG	B	6006	1/1	0.96	0.08	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.