W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:26 AM GMT

PDB ID	:	3APY
Title	:	Properties and crystal structure of methylenetetrahydrofolate reductase from Thermus thermophilus HB8
Authors	:	Yamada, K.
Deposited on	:	2010-10-21
Resolution	:	2.80 Å(reported)

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

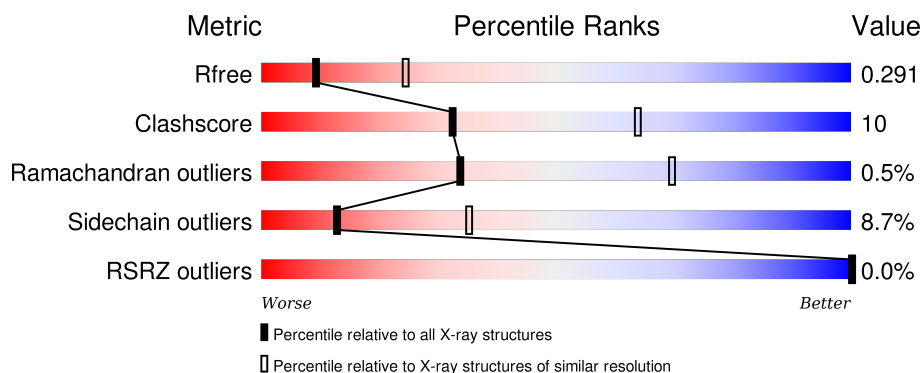|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.291
Clashscore		10
Ramachandran outliers		0.5%
Sidechain outliers		8.7%
RSRZ outliers		0.0%

Worse ... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 >=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 <=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	310	67% 23% • 6%
1	B	310	74% 17% • 6%
1	C	310	72% 20% • 6%
1	D	310	74% 16% • 6%
1	E	310	70% 21% • 6%

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Mol	Chain	Length	Quality of chain
1	F	310	71% 21% • 6%
1	G	310	69% 21% • 6%
1	H	310	73% 18% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19755 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 Methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	B	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	C	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	D	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	E	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	F	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	G	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	H	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
A	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
A	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
A	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
A	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
B	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
B	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
B	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
B	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
C	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
C	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
C	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
C	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
D	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
D	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
D	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
D	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
E	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
E	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
E	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
E	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
F	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
F	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
F	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
F	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
G	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
G	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
G	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
G	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
H	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
H	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
H	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
H	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
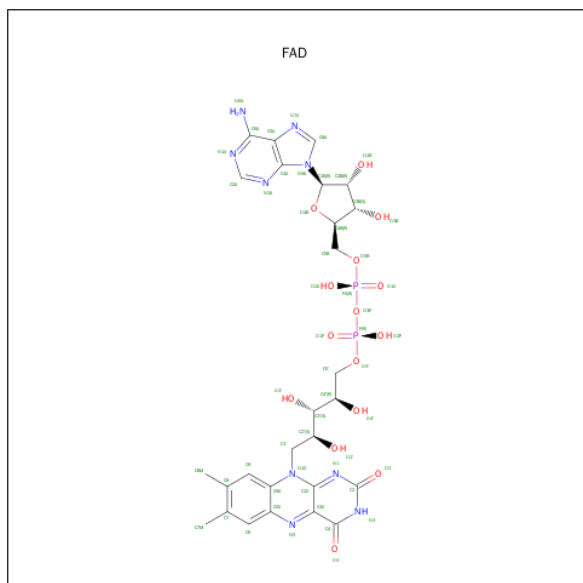
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	111	Total	O	0	0
			111	111		
4	C	117	Total	O	0	0
			117	117		
4	D	97	Total	O	0	0
			97	97		
4	E	127	Total	O	0	0
			127	127		
4	F	119	Total	O	0	0
			119	119		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	111	Total 111	O 111	0	0
4	H	115	Total 115	O 115	0	0

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.
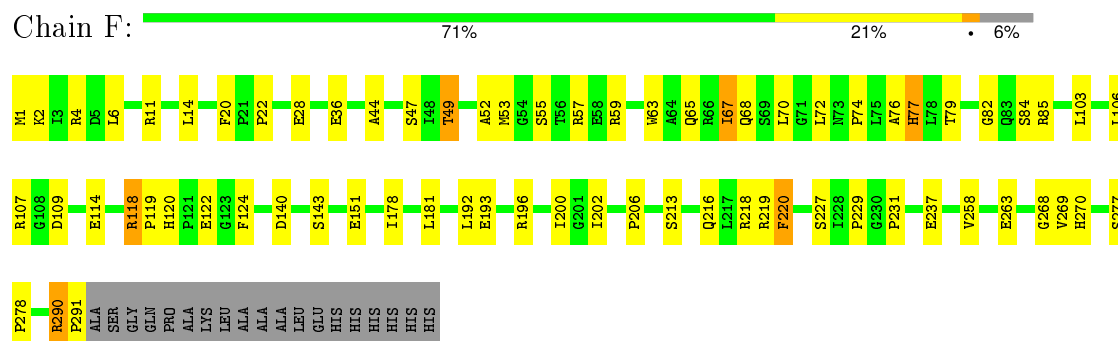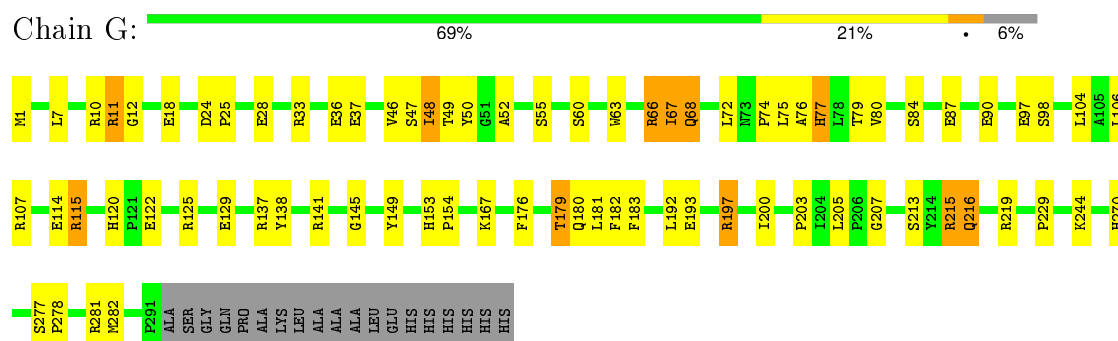
- Molecule 1: Methylenetetrahydrofolate reductase
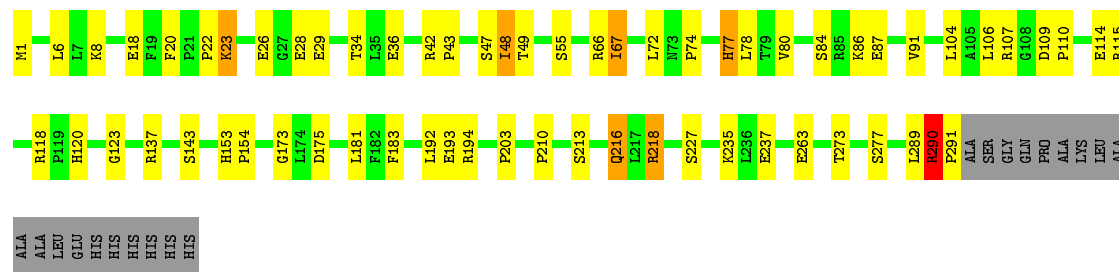

- Molecule 1: Methylenetetrahydrofolate reductase

- Molecule 1: Methylenetetrahydrofolate reductase

• Molecule 1: Methylenetetrahydrofolate reductase

Chain D:

74%   16%   ·   6%

M1 L6 F20 P21 P22 K23 D24 E28 F32 R42 V46 S47 I48 T49 M53 G54 S55 E58 V61 A62 W63 A64 Q65 R66 I67 Q68 S69 L70 P74 L75 A76 H77 V80 A81 G82 V91 L104 A105 L106 R107 R137 S143 P154 E155

L181 F182 F183 L192 E193 R194 A195 R196 I200 M209 P210 V211 Q216 L217 R218 G225 A226 S227 I228 P229 K235 L236 E237 R238 V258 E263 V269 S277 P278 R281 R290 P291 ALA SER GLY GLN PRO ALA LYS LEU ALA ALA LEU GLU HIS HIS

HIS HIS HIS HIS

• Molecule 1: Methylenetetrahydrofolate reductase

Chain E:

70%   21%   ·   6%

M1 K2 L7 K8 F17 E18 F19 F20 P21 P22 P25 E29 F32 R33 T34 L35 E36 E37 I38 K39 R42 P43 S47 I48 T49 M53 E58 W63 R66 I67 Q68 L72 N73 P74 L75 A76 H77 G82 R85 E90 V91 L92 F95

S98 R115 R118 P119 H120 P121 E122 R137 Y138 R141 V142 S143 V144 G145 F166 V170 G173 F176 Q180 L192 R197 P203 C224 G225 A226 S227 K235 L236 E237 R238 K244 E252 H253 A254 V258 L261 E267 G268 V269 S277

P278 R281 L289 R290 P291 ALA SER GLY GLN PRO ALA LYS LEU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Methylenetetrahydrofolate reductase

Chain F:

71%   21%   ·   6%

M1 K2 I3 R4 D5 L6 R11 L14 F20 P21 P22 E28 E36 A44 S47 I48 T49 A52 M53 G54 S55 T56 R57 E58 R59 W63 A64 Q65 R66 I67 Q68 S69 L70 G71 L72 N73 P74 L75 A76 H77 L78 T79 G82 Q83 S84 R85 L103 L106

R107 G108 D109 E114 R118 P119 H120 P121 E122 G123 F124 D140 S143 E151 I178 L181 L192 E193 R196 I200 G201 I202 P206 S213 Q216 L217 R218 R219 F220 S227 I228 P229 G230 P231 E237 V258 E263 G268 V269 H270 S277

P278 R290 P291 ALA SER GLY GLN PRO ALA LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Methylenetetrahydrofolate reductase

Chain G:

69%   21%   ·   6%

M1 L7 R10 R11 G12 E18 D24 P25 E28 R33 E36 E37 V46 S47 I48 T49 Y50 G51 A52 S55 S60 W63 R66 I67 Q68 L72 N73 P74 L75 A76 H77 L78 T79 V80 S84 E87 E90 E97 S98 L104 A105 L106

R107 E114 R115 H120 P121 E122 R125 E129 R137 Y138 R141 G145 Y149 H153 P154 K167 F176 T179 Q180 L181 F182 F183 L192 E193 R197 I200 P203 I204 L205 P206 G207 S213 Y214 R215 Q216 R219 P229 K244 H270

S277 P278 R281 M282 P291 ALA SER GLY GLN PRO ALA LYS LEU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Methylenetetrahydrofolate reductase

Chain H:

73%   18%   6%

M1 L6 L7 K8 E18 F19 F20 P21 P22 K23 E26 G27 E28 E29 T34 L35 E36 R42 P43 S47 I48 T49 S55 R66 I67 L72 N73 P74 H77 L78 T79 V80 S84 R85 K86 E87 V91 L104 A105 L106 R107 G108 D109 P110 E114 R115

R118 P119 H120 G123 R137 S143 H153 P154 G173 L174 D175 L181 F182 F183 L192 E193 R194 P203 P210 S213 Q216 I217 R218 S227 K235 L236 E237 E263 T273 S277 L289 R290 P291 ALA SER GLY GLN PRO ALA LYS LEU ALA

ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.59Å 90.93Å 125.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.96-2.80) 93.8 (19.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.64 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.306 0.203 , 0.291	Depositor DCC
R_{free} test set	3050 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 2.9	EDS
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	13 of 60581 reflections (0.021%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19755	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 55.73 % 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 3.0318e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: FAD, CL

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	0.70	0/2357	0.78	1/3185 (0.0%)
1	B	0.67	0/2357	0.73	0/3185
1	C	0.71	0/2357	0.77	1/3185 (0.0%)
1	D	0.68	0/2357	0.75	0/3185
1	E	0.70	0/2357	0.74	1/3185 (0.0%)
1	F	0.69	0/2357	0.73	0/3185
1	G	0.71	0/2357	0.75	0/3185
1	H	0.65	0/2357	0.72	0/3185
All	All	0.69	0/18856	0.75	3/25480 (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	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	GLY	N-CA-C	-7.63	94.02	113.10
1	C	52	ALA	N-CA-C	-6.78	92.70	111.00
1	E	33	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	290	ARG	Peptide

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	2302	0	2319	71	0
1	B	2302	0	2319	46	0
1	C	2302	0	2319	47	0
1	D	2302	0	2319	46	0
1	E	2302	0	2319	55	0
1	F	2302	0	2319	45	0
1	G	2302	0	2319	66	0
1	H	2302	0	2319	39	0
2	A	53	0	31	5	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	E	53	0	31	0	0
2	F	53	0	31	2	0
2	G	53	0	31	3	0
2	H	53	0	31	1	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
4	A	112	0	0	6	0
4	B	111	0	0	5	0
4	C	117	0	0	7	0
4	D	97	0	0	4	0
4	E	127	0	0	7	0
4	F	119	0	0	5	0
4	G	111	0	0	3	0
4	H	115	0	0	7	0
All	All	19755	0	18800	395	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 10.

The worst 5 of 395 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:67:ILE:HD11	1:D:74:PRO:HB3	1.36	1.04
1:A:290:ARG:HH11	1:A:290:ARG:HG2	1.24	0.99
1:H:290:ARG:O	1:H:290:ARG:HD3	1.61	0.99
1:A:52:ALA:HB2	1:A:56:THR:HG23	1.46	0.98
1:A:237:GLU:HG3	1:B:218:ARG:HH12	1.27	0.98

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	289/310 (93%)	280 (97%)	8 (3%)	1 (0%)	46	79
1	B	289/310 (93%)	278 (96%)	8 (3%)	3 (1%)	19	52
1	C	289/310 (93%)	275 (95%)	13 (4%)	1 (0%)	46	79
1	D	289/310 (93%)	274 (95%)	13 (4%)	2 (1%)	26	62
1	E	289/310 (93%)	277 (96%)	11 (4%)	1 (0%)	46	79
1	F	289/310 (93%)	275 (95%)	12 (4%)	2 (1%)	26	62
1	G	289/310 (93%)	272 (94%)	17 (6%)	0	100	100
1	H	289/310 (93%)	279 (96%)	8 (3%)	2 (1%)	26	62
All	All	2312/2480 (93%)	2210 (96%)	90 (4%)	12 (0%)	34	69

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	ARG
1	C	52	ALA

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Mol	Chain	Res	Type
1	D	290	ARG
1	H	290	ARG
1	B	114	GLU

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	236/249 (95%)	215 (91%)	21 (9%)	12	34
1	B	236/249 (95%)	219 (93%)	17 (7%)	18	45
1	C	236/249 (95%)	220 (93%)	16 (7%)	20	49
1	D	236/249 (95%)	211 (89%)	25 (11%)	8	24
1	E	236/249 (95%)	213 (90%)	23 (10%)	10	29
1	F	236/249 (95%)	216 (92%)	20 (8%)	13	36
1	G	236/249 (95%)	218 (92%)	18 (8%)	16	42
1	H	236/249 (95%)	211 (89%)	25 (11%)	8	24
All	All	1888/1992 (95%)	1723 (91%)	165 (9%)	13	35

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	228	ILE
1	E	118	ARG
1	H	114	GLU
1	D	237	GLU
1	E	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	GLN
1	E	68	GLN

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Mol	Chain	Res	Type
1	H	68	GLN
1	D	77	HIS
1	D	83	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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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
2	FAD	A	311	-	48,58,58	1.37	6 (12%)	54,89,89	2.05	13 (24%)
2	FAD	B	311	-	48,58,58	1.35	6 (12%)	54,89,89	2.44	11 (20%)
2	FAD	C	311	-	48,58,58	1.17	6 (12%)	54,89,89	2.31	12 (22%)
2	FAD	D	311	-	48,58,58	1.21	5 (10%)	54,89,89	2.03	8 (14%)
2	FAD	E	311	-	48,58,58	1.24	4 (8%)	54,89,89	2.12	9 (16%)
2	FAD	F	311	-	48,58,58	1.38	7 (14%)	54,89,89	2.23	9 (16%)
2	FAD	G	311	-	48,58,58	1.32	6 (12%)	54,89,89	2.32	13 (24%)
2	FAD	H	311	-	48,58,58	1.24	5 (10%)	54,89,89	2.22	7 (12%)

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
2	FAD	A	311	-	-	0/30/50/50	0/6/6/6
2	FAD	B	311	-	-	0/30/50/50	0/6/6/6
2	FAD	C	311	-	-	0/30/50/50	0/6/6/6
2	FAD	D	311	-	-	0/30/50/50	0/6/6/6
2	FAD	E	311	-	-	0/30/50/50	0/6/6/6
2	FAD	F	311	-	-	0/30/50/50	0/6/6/6
2	FAD	G	311	-	-	0/30/50/50	0/6/6/6
2	FAD	H	311	-	-	0/30/50/50	0/6/6/6

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	311	FAD	C6-C5X	-2.60	1.37	1.41
2	D	311	FAD	C6-C5X	-2.09	1.38	1.41
2	B	311	FAD	C6-C5X	-2.06	1.38	1.41
2	H	311	FAD	C5X-N5	2.00	1.38	1.35
2	F	311	FAD	C1'-N10	2.06	1.50	1.48

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	311	FAD	N3A-C2A-N1A	-13.90	118.25	128.89
2	H	311	FAD	N3A-C2A-N1A	-12.93	118.99	128.89
2	G	311	FAD	N3A-C2A-N1A	-12.26	119.50	128.89
2	C	311	FAD	N3A-C2A-N1A	-11.86	119.82	128.89
2	D	311	FAD	N3A-C2A-N1A	-11.11	120.39	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	311	FAD	5	0
2	B	311	FAD	2	0
2	C	311	FAD	1	0
2	D	311	FAD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	311	FAD	2	0
2	G	311	FAD	3	0
2	H	311	FAD	1	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, 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(Å²)	Q<0.9
1	A	291/310 (93%)	-0.76	0	100	100	6, 17, 33, 45	1 (0%)
1	B	291/310 (93%)	-0.69	1 (0%)	94	92	5, 18, 34, 46	1 (0%)
1	C	291/310 (93%)	-0.73	0	100	100	5, 18, 34, 56	1 (0%)
1	D	291/310 (93%)	-0.69	0	100	100	5, 18, 33, 46	1 (0%)
1	E	291/310 (93%)	-0.74	0	100	100	7, 18, 36, 52	1 (0%)
1	F	291/310 (93%)	-0.72	0	100	100	7, 18, 35, 47	1 (0%)
1	G	291/310 (93%)	-0.72	0	100	100	6, 17, 33, 50	1 (0%)
1	H	291/310 (93%)	-0.69	0	100	100	5, 18, 35, 47	1 (0%)
All	All	2328/2480 (93%)	-0.72	1 (0%)	100	100	5, 18, 34, 56	8 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	3.5

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($Å^2$)	Q<0.9
2	FAD	A	311	53/53	0.97	0.12	0.04	9,11,14,14	0
2	FAD	C	311	53/53	0.98	0.12	-0.18	5,10,15,15	0
2	FAD	F	311	53/53	0.97	0.12	-0.20	2,16,19,22	0
2	FAD	B	311	53/53	0.97	0.12	-0.24	6,14,18,19	0
2	FAD	H	311	53/53	0.98	0.12	-0.36	11,15,18,19	0
2	FAD	E	311	53/53	0.97	0.11	-0.40	6,9,13,14	0
2	FAD	D	311	53/53	0.97	0.13	-0.49	7,12,18,19	0
2	FAD	G	311	53/53	0.98	0.11	-0.65	4,9,13,13	0
3	CL	F	312	1/1	0.90	0.10	-	41,41,41,41	0
3	CL	E	312	1/1	0.97	0.15	-	37,37,37,37	0
3	CL	D	312	1/1	0.92	0.15	-	40,40,40,40	0
3	CL	A	312	1/1	0.97	0.09	-	31,31,31,31	0
3	CL	H	312	1/1	0.96	0.21	-	31,31,31,31	0
3	CL	G	312	1/1	0.91	0.08	-	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.