



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:56 AM GMT

PDB ID : 1FPM  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATESYNTHETASE FROM MOORELLA THERMOACETICA  
Authors : Radfar, R.; Leaphart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.  
Deposited on : 2000-08-31  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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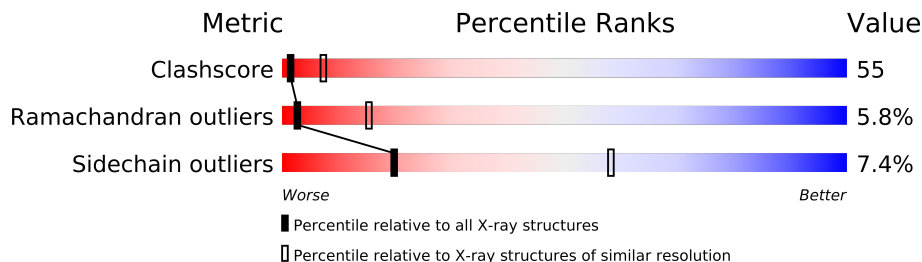
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8585 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

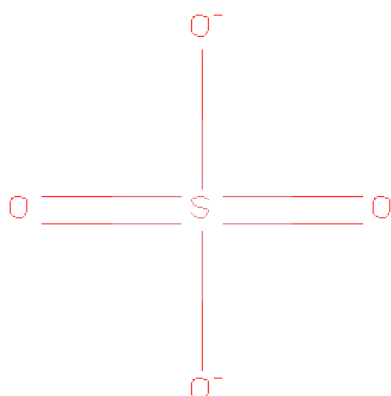
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATELIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4133	2617	715	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4125	2613	714	777	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P21164
A	?	-	VAL	DELETION	UNP P21164
B	?	-	GLU	DELETION	UNP P21164
B	?	-	VAL	DELETION	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cs 1 1	0	0
3	A	1	Total Cs 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

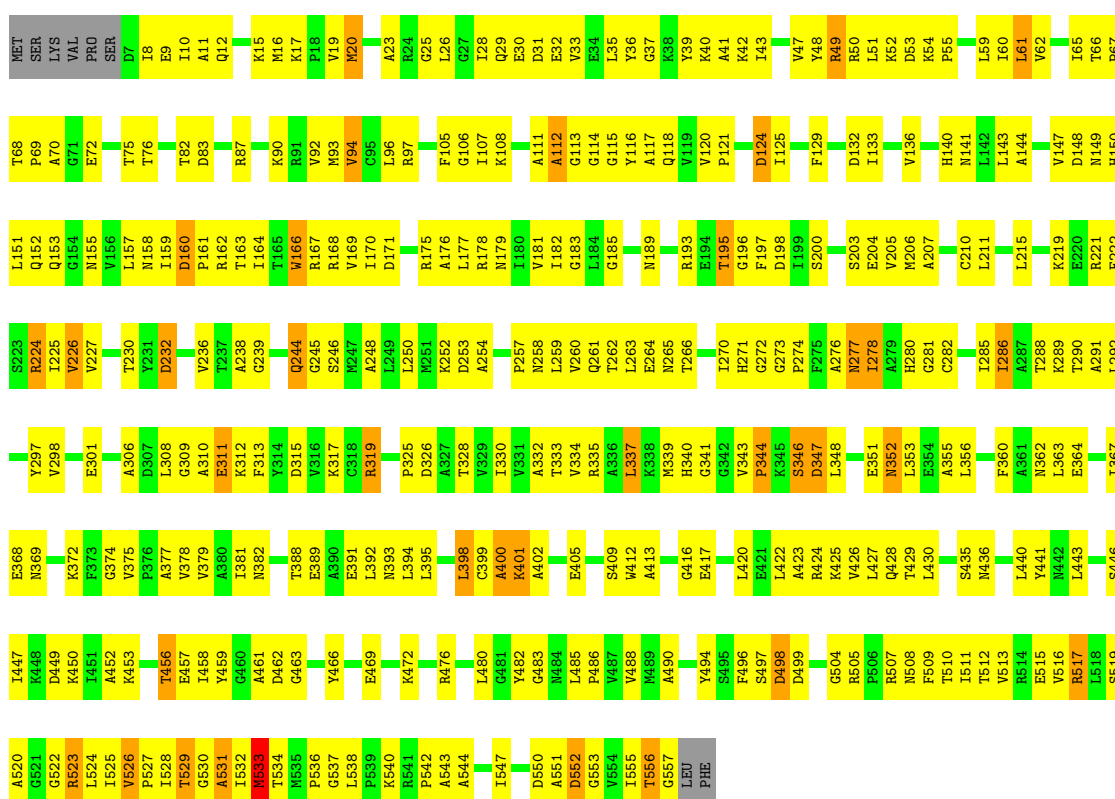
### 3 Residue-property plots

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.

Note EDS was not executed.

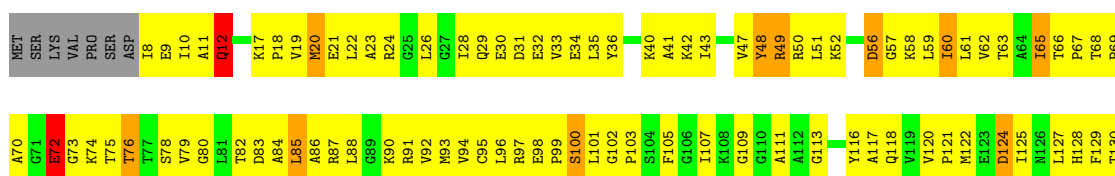
#### • Molecule 1: FORMATE--TETRAHYDROFOLATELIGASE

Chain A:



#### • Molecule 1: FORMATE--TETRAHYDROFOLATELIGASE

Chain B:



A520	G521	G522	R523	L524	I525	V526	P527	T528	T529	I532	M535	L538	P539	K540	R541	P542	A543	I547	D548	I549	D550	A551	D552	G553	V554	I555	T556	G557	LEU	PHE																													
I454	A455	T456	E457	I458	I459	G460	A461	D462	G463	Y466	A470	D471	K472	A473	I474	G475	R476	Y477	E478	L480	G481	Y482	G483	N484	L485	P486	V487	V488	M489	A490	K491	T492	Q493	Y494	S495	F496	S497	D498	L503	G504	R505	P506	N507	R508	F509	T510	T511	V512	V513	R514	E515	V516	R517	L518	S519				
D387	T388	E389	L392	N393	L394	L395	L396	E397	L398	G399	A400	K401	A402	G403	A404	E405	L408	S409	N412	K414	G415	G416	E417	L418	G419	L420	P421	L422	A423	R424	K425	V426	T429	L430	R433	P434	S435	N436	F437	L440	Y441	N442	L443	D444	L445	S446	T447	R448	D449	K450	I451	A452	K453						
P325	D326	A327	T328	L329	I330	V331	A332	T333	V334	R335	A336	L337	K338	M339	G340	G341	G342	V343	P344	D347	L348	A349	T350	E351	N352	L353	E354	A355	L356	R357	E358	G359	F360	A361	N362	L363	E364	K365	H366	T367	E368	N369	I370	F373	G374	V375	P376	A377	V378	V379	K317	A380	C318	R319	V320	A321	G322	F323	T386
K265	T266	P267	A268	F269	L270	H271	G272	G273	P274	F275	A276	N277	I278	A279	H280	G281	C282	N283	S284	I285	L286	A287	T288	K289	T290	A291	L292	K293	L294	A295	D296	I297	V298	V299	T300	E301	A302	G303	F304	G305	A306	D307	L308	G309	A310	E311	K312	F313	V314	D315	V316	K317	C318	R319	V320	A321	G322	F323	K324
E197	D198	I199	S200	V201	A202	S203	E204	V205	M206	L142	A207	C208	L209	C210	L211	A212	L215	K219	E220	R221	G154	F222	S223	R224	I225	Y229	T230	Y231	D232	V236	G239	L241	D240	E242	A243	Q244	G245	S246	M247	A248	L249	L250	M251	K252	D253	A254	I255	K256	P257	N258	G190	L259	P192	Q261	L262	L263	E264		
G131	D132	I133	H134	A135	V136	H140	N141	L142	L143	A207	L144	A145	H146	V147	D148	N149	H150	L151	Q152	Q153	G154	N155	V156	L157	H158	I159	D160	P161	R162	T163	I164	T165	W166	R167	R168	V169	L172	N173	D174	R175	A176	L177	R178	I182	G185	G186	K187	A188	N189	G190	V191	P192	R193	E194	T195	G196			

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	84.0 (40.00-3.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.266 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: CS, SO4

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	0.52	0/4201	0.72	0/5690
1	B	0.43	0/4193	0.67	0/5679
All	All	0.48	0/8394	0.70	0/11369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4133	0	4219	382	0
1	B	4125	0	4215	545	1
2	A	35	0	0	10	0
2	B	20	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	200	0	0	27	0
4	B	70	0	0	14	1
All	All	8585	0	8434	927	1



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 55.

The worst 5 of 927 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:TRP:CZ3	1:B:225:ILE:HD11	1.30	1.59
1:A:166:TRP:CZ3	1:A:225:ILE:HD11	1.42	1.53
1:B:166:TRP:CH2	1:B:225:ILE:HD11	1.58	1.38
1:B:166:TRP:CH2	1:B:225:ILE:CD1	2.11	1.34
1:B:166:TRP:CZ3	1:B:225:ILE:CD1	2.10	1.33

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	6	32
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	1	6
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	3	15

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LYS
1	A	352	ASN
1	A	556	THR
1	B	65	ILE

### 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	432/440 (98%)	399 (92%)	33 (8%)	19	57
1	B	431/440 (98%)	400 (93%)	31 (7%)	21	59
All	All	863/880 (98%)	799 (93%)	64 (7%)	20	58

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	ARG
1	B	72	GLU
1	B	526	VAL
1	A	526	VAL
1	A	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	546	ASN
1	B	118	GLN
1	B	362	ASN
1	B	12	GLN
1	A	189	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	SO4	A	560	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	561	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	562	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	563	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	564	-	4,4,4	1.65	1 (25%)	6,6,6	0.47	0
2	SO4	A	565	-	4,4,4	1.66	1 (25%)	6,6,6	0.47	0
2	SO4	A	566	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	560	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	561	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	562	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	563	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0

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	SO4	A	560	-	-	0/0/0/0	0/0/0/0
2	SO4	A	561	-	-	0/0/0/0	0/0/0/0
2	SO4	A	562	-	-	0/0/0/0	0/0/0/0
2	SO4	A	563	-	-	0/0/0/0	0/0/0/0
2	SO4	A	564	-	-	0/0/0/0	0/0/0/0
2	SO4	A	565	-	-	0/0/0/0	0/0/0/0
2	SO4	A	566	-	-	0/0/0/0	0/0/0/0
2	SO4	B	560	-	-	0/0/0/0	0/0/0/0
2	SO4	B	561	1	-	0/0/0/0	0/0/0/0
2	SO4	B	562	-	-	0/0/0/0	0/0/0/0
2	SO4	B	563	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	566	SO4	O1-S	-2.28	1.39	1.47
2	B	563	SO4	O1-S	-2.28	1.39	1.47
2	A	565	SO4	O1-S	-2.28	1.39	1.47
2	B	561	SO4	O1-S	-2.27	1.39	1.47
2	A	563	SO4	O1-S	-2.27	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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