



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:28 PM GMT

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

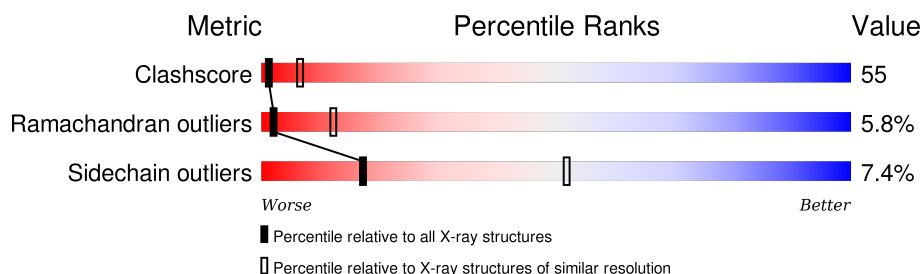
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 ≥ 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	557	
1	B	557	

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	SO4	A	561	-	-	X	-
2	SO4	A	565	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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.

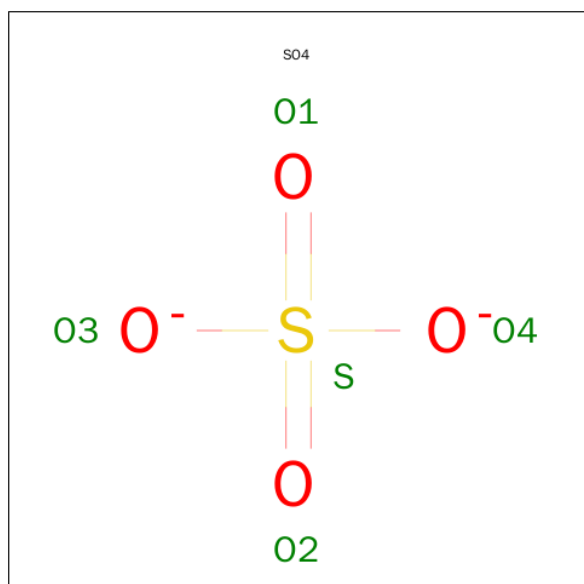
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

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: SO₄) (formula: O₄S).



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.

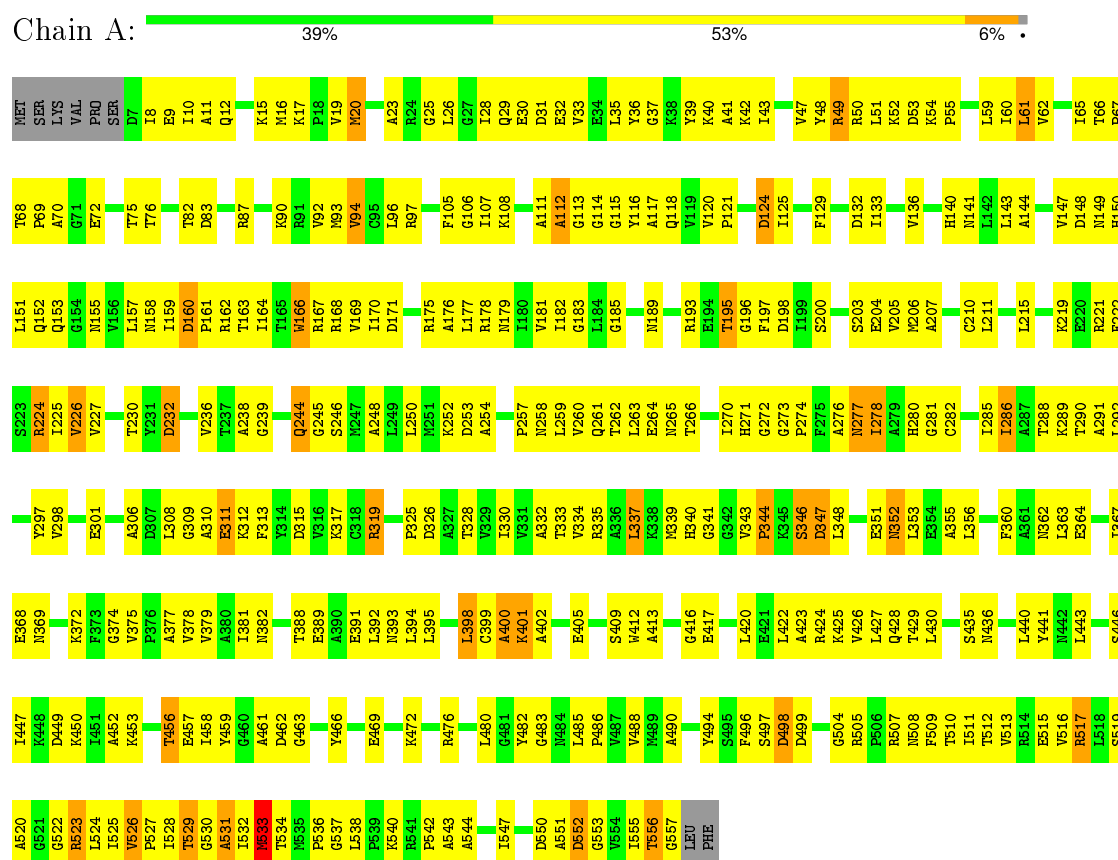
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

3 Residue-property plots

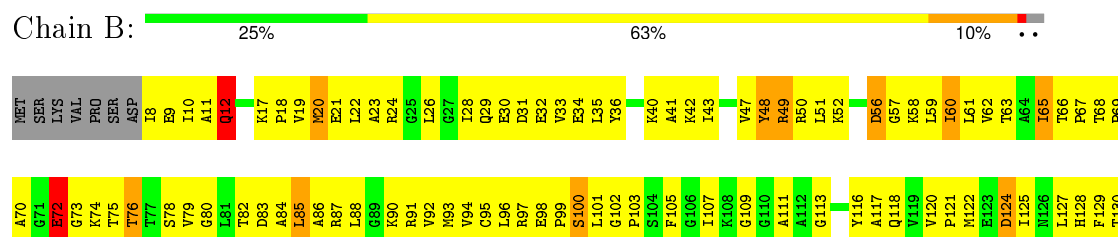
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



A520	I454	D887	P325	I265	F197	G131
G521	A455	T388	D326	T266	D198	D132
R522	T456	E389	A327	P267	I199	I133
R523	E457	T328	T328	A268	S200	H134
I524	I458	I392	I329	F269	V201	A135
I525	Y459	N393	I330	I270	A202	V136
V526	G460	L394	V331	H271	S203	
P527	A461	L395	A332	G272	E204	H140
T528	D462	I396	T333	G273	V205	N141
T529	G463	I397	V334	F274	M206	L142
		L398	R335	F275	A207	L143
	Y466	C399	A336	A276	C208	A144
		A400	I337	N277	L209	A145
M535	A470	K401	K338	I278	C210	H146
	D471	A402	M339	I279	A212	V147
L538	K472	G403	H340	H280	L211	D148
P539	A473	A404	G341	G281		N149
K540	I474	E405	G342	C282	L215	H150
R541			V343	N283		L151
P542	Q475		P344	S284	K219	Q152
A543	R476	L408		I285	E220	Q153
	Y477	S409	D347	T286	R221	G154
	Y478	N412	L348	A287	F222	N155
I547	S479	A413	A349	T288	S223	V156
D548	L480	K414	T350	T289	R224	L157
I549	G481	G415	E351	T290		H158
D550	Y482	G416	N352	A291	Y229	I159
A551	G483	E417	L353	L292	T230	D160
D552	N484	G418	E354	K293	Y231	P161
G553	L485	G419	A355	L294	D332	R162
V554	P486	L420	L356	A295		T163
I555	V487	E421	R357	D296	V236	I164
T556	V488	L422	E358	I297		T165
	M489	A423	G359	V298	G239	W166
G557	A490	R424	F360	V299	D240	R167
LEU	K491	K425	A361	T300	L241	R168
PHE	Q492	V426	N362	E301		V169
	Y493		L363	A302		
	Y494	T429	E364	G303	A242	L172
	S495	L430	R365	F304	G243	N173
	F496				Q244	D174
	S497	R433	H366	G305	S246	R175
	D498	P434	I367	A306	M247	A176
		S435	E368	D307	A248	L177
		N436	N369	L303	L249	R178
		F437	I370	G309		
	L503			A310	L250	
	R505	L440	F373	E311	M251	I182
	P506	Y441	G374	K312		
	R507	N442	V375	F313	D253	G185
	N508	L443	P376	X314	A254	G186
	F509	D444	A377	X315	I255	K187
T510	T511	L445	V378	V316	K256	A188
T512	S446	S446	V379	K317	P257	N189
V513	V513	I447	A380	C318	N258	G190
R514	R514	K448	I381	R319	L259	V191
E515	E515	D449	N382	X320	V260	P192
V516	V516	K450	A383	A321	Q261	R193
R517	R517	I451	F384	G322	T262	E194
L518	L518	A452	P385	F323	L263	T195
S519	S519	K453	T386	K324	E264	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, α , β , γ	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 ²)	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 Too-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 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	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

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 55.

The worst 5 of 927 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: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	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

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	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	5	26
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	1	5
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	2	12

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%)	16	51
1	B	431/440 (98%)	400 (93%)	31 (7%)	18	53
All	All	863/880 (98%)	799 (93%)	64 (7%)	17	52

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 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 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	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	561	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	562	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	563	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	564	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	565	-	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	A	566	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	560	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	561	1	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	B	562	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	563	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.22	1.39	1.47
2	B	563	SO4	O1-S	-2.21	1.39	1.47
2	A	565	SO4	O1-S	-2.21	1.39	1.47
2	B	561	SO4	O1-S	-2.21	1.39	1.47
2	A	563	SO4	O1-S	-2.21	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 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	SO4	4	0
2	A	563	SO4	1	0
2	A	565	SO4	4	0
2	A	566	SO4	1	0
2	B	560	SO4	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](#)

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.