



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:58 AM GMT

PDB ID : 1FP7  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATESYNTHEASE FROM MOORELLA THERMOACETICA  
Authors : Radfar, R.; Leapheart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.  
Deposited on : 2000-08-30  
Resolution : 3.20 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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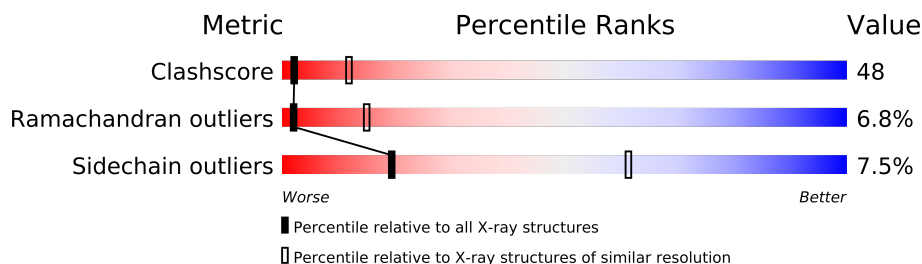
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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.

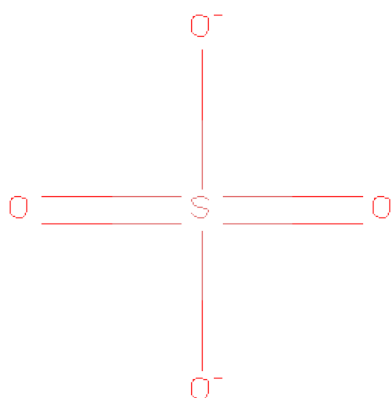
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATELIGASE.

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 POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 2 2	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

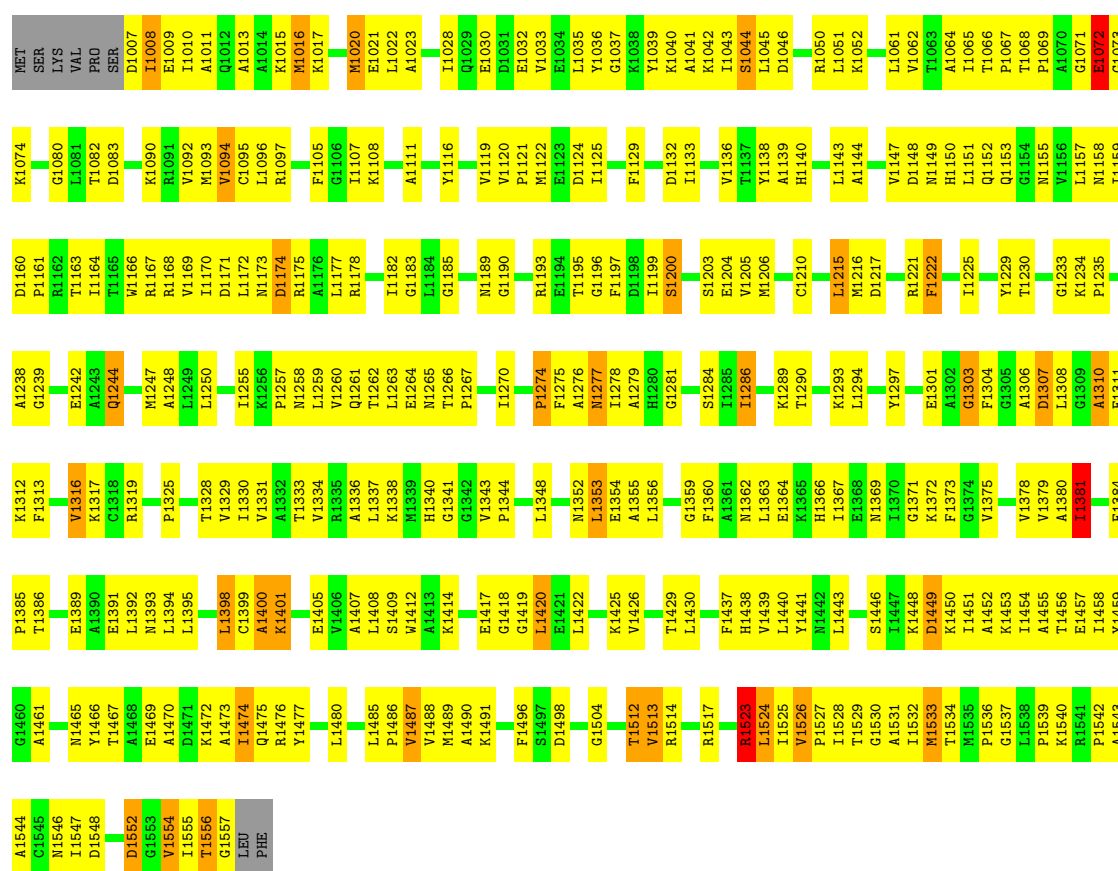
### 3 Residue-property plots

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:



A1551	G1483	L1408	H1340	M1277	G1210	A1135	P1067
D1552	N1484	S1409	G1341	I1278	L1211	V1136	T1068
G1553	L1485	S1412	G1342	A1279			P1069
V1554	L1486	A1413	V1343	H1280	L1215	H1140	A1070
T1555	P1486	A1413	P1344	G1281			G1071
T1556	V1487	K1414		G1282	E1220	L1143	S1072
G1557	V1488		D1347		R1221	A1144	G1073
LEU	M1489	E1417	L1346	I1285	F1222		R1074
PHE	A1490			I1286	S1223	V1147	T1075
	K1491	L1420	E1351	A1287	D1224	D1148	T1076
	T1492	E1421	N1352	T1288	I1225	N1149	T1077
	Q1493	L1422	L1353	K1289	V1226	H1150	S1078
	Y1494			T1290	V1227	L1151	V1079
	S1495	K1425	L1356	A1291	G1228	Q1152	G1080
	S1496	V1426	R1357	L1292	Y1229	L1153	L1081
	F1497	L1427	E1358	K1293	T1230	G1154	T1082
	D1498	Q1428	G1359	L1294	Y1231	N1155	D1083
	D1499	T1429	F1360	A1295	D1232	V1156	A1084
	M1500	L1430	A1361	D1296	G1233	L1157	L1085
	T1501	E1431	N1362	Y1297	K1234	N1158	A1086
	K1502	S1432	L1363	V1298	P1235	I1159	R1087
		P1433	E1364	T1299	V1236	D1160	L1088
		P1434	K1365	T1300	T1237	P1161	G1089
		S1435	H1366		A1238		K1090
	P1506		I1367	G1303	G1239	W1166	R1091
	R1507	N1436		F1304	D1240	R1167	V1092
	N1508	F1437	E1368	G1305		R1168	M1093
	F1509	H1438	N1369	A1306	G1244	V1169	V1094
	T1510	V1439	I1370	D1307	G1245	I1170	C1095
	I1511	L1440	G1371	L1308	S1246	D1171	L1096
	T1512	Y1441	K1372	G1309	M1247	L1172	R1097
	V1513	N1442	F1373	A1310	A1248	N1173	
	R1514	L1443	G1374	E1311	L1249	D1174	P1103
	E1515	D1444	V1375	K1312	L1250	R1175	S1104
	V1516	L1445	A1376	F1313	M1251	A1176	F1105
	R1517	S1446	A1377	Y1314	K1252	L1177	G1106
	L1518	I1447	V1378	D1315	D1253	R1178	I1107
	S1519	K1448	V1379	V1316	A1254		K1108
	A1520	D1449	A1380	K1317	I1255	I1182	G1109
		K1450	I1381	C1318	K1256	G1183	G1110
	R1523	I1451	N1382	F1319	P1257		A1111
	L1524	A1452	A1383	Y1320	N1258	G1186	A1112
	I1525	K1453	F1384		L1259	K1187	G1113
	V1526	I1454	P1385		V1260	A1188	G1114
	P1527	A1455	T1386	F1323	Q1261		G1115
	I1528	A1455	D1387	K1324	T1262	R1193	G1116
	T1529	T1456		P1325	L1263	E1194	A1117
		E1457		D1326	E1264	T1195	Q1118
	I1532	I1458	A1390	A1327	N1265	G1196	V1119
	M1533	Y1459	E1391	T1328	T1266	F1197	V1120
	T1534	G1460	L1392	V1329	P1267	D1198	P1121
	M1535	A1461	N1393	I1330	A1269	I1199	
	P1536	D1462	L1394	V1331	F1270	S1200	D1124
			L1395	T1332	I1271	I1125	
		N1465	Y1396	A1332	G1272		F1129
	A1543	Y1466	E1397	T1333	H1271	S1203	
	A1544		L1398	V1334	R1335	E1204	D1132
	C1545	K1472	O1399	R1335	A1336	V1205	I1133
	N1546		A1400	A1336	L1337	M1206	
	I1547		K1401	A1402	F1275		
	D1548	R1476	A1402	K1338	A1276		
	I1549	Y1477	A1402	K1338			
	D1550	E1478	G1403	M1339			

## 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)	19.99 – 3.20	Depositor
% Data completeness (in resolution range)	87.2 (19.99-3.20)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.285 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: K, 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	0.44	0/4201	0.72	1/5690 (0.0%)
1	B	0.40	0/4193	0.68	0/5679
All	All	0.42	0/8394	0.70	1/11369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1524	LEU	N-CA-C	5.35	125.44	111.00

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	357	0
1	B	4125	0	4211	448	0
2	A	35	0	0	14	0
2	B	20	0	0	2	0
3	A	2	0	0	1	0
4	A	199	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	71	0	0	16	0
All	All	8585	0	8430	806	0

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 48.

The worst 5 of 806 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1175:ARG:HD3	2:A:275:SO4:O3	1.40	1.22
1:B:1222:PHE:O	1:B:1225:ILE:HG22	1.40	1.19
1:A:1007:ASP:OD2	4:A:32:HOH:O	1.68	1.11
1:B:1079:VAL:HB	1:B:1117:ALA:HB1	1.34	1.08
1:B:1335:ARG:HD3	1:B:1348:LEU:HB3	1.33	1.07

There are no symmetry-related clashes.

## 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%)	437 (80%)	90 (16%)	20 (4%)	5	34
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	1	7
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	2	15

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1304	PHE
1	A	1533	MET
1	A	1556	THR
1	B	1056	ASP

### 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%)	401 (93%)	31 (7%)	21	63
1	B	431/440 (98%)	397 (92%)	34 (8%)	18	58
All	All	863/880 (98%)	798 (92%)	65 (8%)	19	61

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1546	ASN
1	B	1094	VAL
1	B	1518	LEU
1	A	1552	ASP
1	B	1059	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1362	ASN
1	B	1118	GLN
1	B	1382	ASN
1	A	1465	ASN
1	B	1029	GLN

### 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	271	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	273	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	274	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	275	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	276	-	4,4,4	1.65	1 (25%)	6,6,6	0.47	0
2	SO4	A	277	-	4,4,4	1.66	1 (25%)	6,6,6	0.47	0
2	SO4	A	278	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	272	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	279	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	280	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	281	-	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	271	-	-	0/0/0/0	0/0/0/0
2	SO4	A	273	-	-	0/0/0/0	0/0/0/0
2	SO4	A	274	1	-	0/0/0/0	0/0/0/0
2	SO4	A	275	-	-	0/0/0/0	0/0/0/0
2	SO4	A	276	-	-	0/0/0/0	0/0/0/0
2	SO4	A	277	-	-	0/0/0/0	0/0/0/0
2	SO4	A	278	1	-	0/0/0/0	0/0/0/0
2	SO4	B	272	1	-	0/0/0/0	0/0/0/0
2	SO4	B	279	1	-	0/0/0/0	0/0/0/0
2	SO4	B	280	-	-	0/0/0/0	0/0/0/0
2	SO4	B	281	-	-	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	278	SO4	O1-S	-2.28	1.39	1.47
2	B	281	SO4	O1-S	-2.28	1.39	1.47
2	A	277	SO4	O1-S	-2.28	1.39	1.47
2	B	279	SO4	O1-S	-2.27	1.39	1.47
2	A	275	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.