



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FP7  
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 : 2000-08-30  
Resolution : 3.20 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](mailto: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.

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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 : 1.7 (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

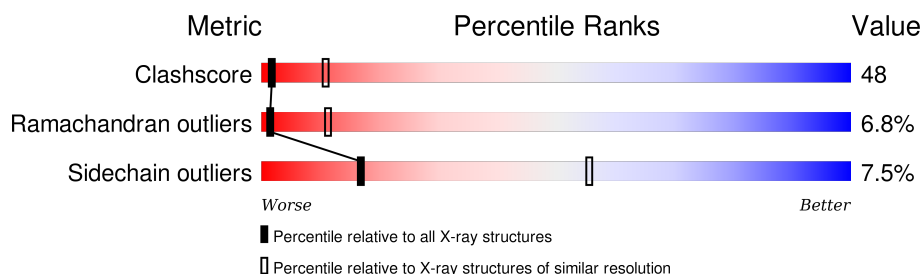
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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. 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	273	-	-	X	-
2	SO4	A	274	-	-	X	-
2	SO4	A	275	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	277	-	-	X	-
2	SO4	A	278	-	-	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: 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.

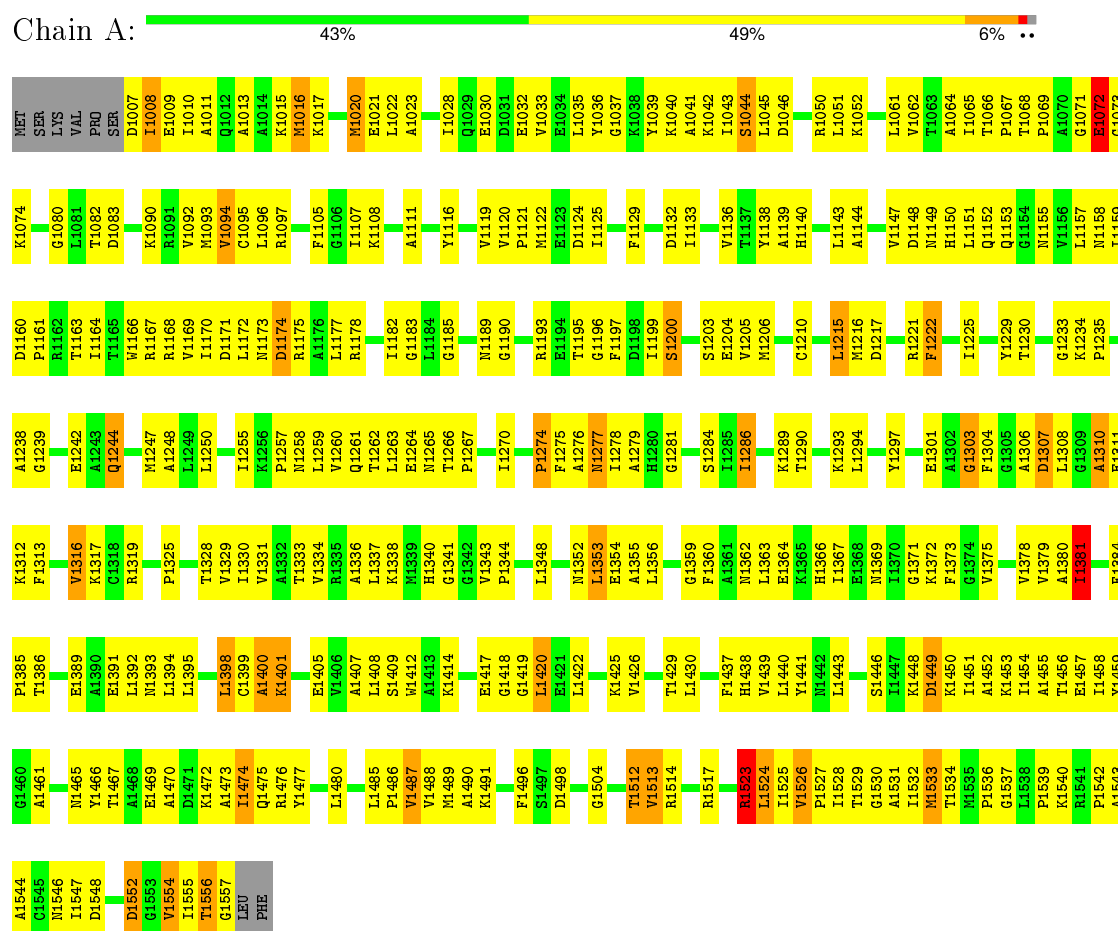
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

### 3 Residue-property plots

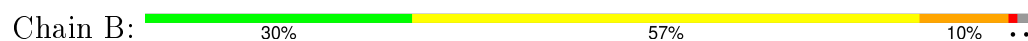
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



#### • Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



A1551	G1483	L1408	H1340	M1277	C1210	A1135	P1067
D1552	M1484	L1409	G1341	I1278	L1211	V1136	T1068
G1553	L1485	M1412	G1342	A1279	L1215	H1140	P1069
V1554	L1486	A1413	P1344	H1280	G1281	L1143	A1070
T1555	P1486	K1414	D1347	G1282	E1220	A1144	G1071
T1556	V1487	E1417	L1346	I1285	R1221	L1152	B1072
G1557	V1488	L1420	E1351	I1286	F1222	A1154	G1073
LEU	M1489	L1421	E1352	A1287	R1223	V1147	R1074
PHE	K1491	L1422	L1353	T1288	R1224	D1148	T1075
	Q1493	E1423	L1356	K1289	I1225	N1149	T1076
	Y1494	K1425	L1357	G1290	V1226	H1150	T1077
	S1495	V1426	R1357	T1291	G1226	L1151	S1078
	F1496	L1427	E1358	A1291	O1229	Q1152	V1079
	D1498	Q1428	G1359	L1292	I1229	G1153	G1080
	D1499	T1429	F1360	K1293	T1230	G1154	L1081
	M1500	L1430	A1361	L1294	Y1231	N1155	T1082
	T1501	E1431	M1362	A1295	D1232	V1156	D1083
	K1502	S1432	L1363	D1296	G1233	L1157	A1084
		P1433	E1364	Y1297	R1234	N1158	L1085
		R1434	K1365	V1298	P1235	I1159	A1086
		P1435	K1366	V1299	V1236	D1160	R1087
		S1435	H1367	T1300	T1237	P1161	L1088
		M1436	L1367	G1303	A1238		G1089
		F1437	E1368	F1304	G1239	W1166	K1090
		H1438	M1369	G1305	D1240	R1167	R1091
		V1439	I1370	A1306		R1168	V1092
		T1510	G1371	D1307	Q1244	R1169	M1093
		V1512	L1440	L1308	G1245	V1169	V1094
		V1513	Y1441	G1309	I1170	G1171	C1095
		R1514	N1442	F1373	S1246	D1171	L1096
		E1515	L1443	A1310	M1247	L1172	R1097
		V1516	D1444	E1311	A1248	N1173	
		R1517	L1445	E1312	L1249	D1174	P1103
		S1519	I1447	F1313	L1250	R1175	S1104
		A1520	K1448	Y1314	M1251	A1176	F1105
			T1449	V1378	K1252	L1177	G1106
			D1449	V1379	D1263	R1178	I1107
			K1450	A1380	A1254		K1108
			I1451	I1381	I1255	I1182	G1109
			A1452	M1382	K1256	G1183	G1110
			K1453	A1383	P1257		A1111
			I1454	F1384	N1258	G1186	A1112
			A1455	P1385	L1259	K1187	G1113
			T1456	T1386	V1260	A1188	G1114
			E1457	D1387	Q1261		G1115
			I1458		T1262	R1193	G1116
			Y1459	A1390	L1263	E1194	Y1116
			G1460	E1391	E1264	T1195	A1117
			A1461	L1392	N1265	G1196	Q1118
			D1462	N1393	T1266	F1197	V1119
				L1394	P1267	D1198	V1120
				L1395	A1268	I1199	P1121
				Y1396	F1269	S1200	
				E1397	I1270		D1124
				L1398	H1271	I1125	I1125
				C1399	G1272	S1203	F1129
				A1400	G1273	E1204	
				K1401	P1274	V1205	D1132
				A1402	F1275	M1206	I1133
				E1476		L1209	H1134
				Y1477			
				E1478			

## 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 [i](#)

### 5.1 Standard geometry [i](#)

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 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	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
4	B	71	0	0	16	0
All	All	8585	0	8430	806	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 48.

The worst 5 of 806 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: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 [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%)	437 (80%)	90 (16%)	20 (4%)	4	29
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	1	4
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1	11

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%)	18	57
1	B	431/440 (98%)	397 (92%)	34 (8%)	15	53
All	All	863/880 (98%)	798 (92%)	65 (8%)	17	55

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 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	271	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	274	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	A	278	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	272	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	279	1	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	281	-	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.22	1.39	1.47
2	B	281	SO4	O1-S	-2.21	1.39	1.47
2	A	277	SO4	O1-S	-2.21	1.39	1.47
2	B	279	SO4	O1-S	-2.21	1.39	1.47
2	A	275	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.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	273	SO4	4	0
2	A	274	SO4	2	0
2	A	275	SO4	4	0
2	A	277	SO4	2	0
2	A	278	SO4	2	0
2	B	272	SO4	1	0
2	B	280	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 ⓘ

### 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.