



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 10:41 AM EST

PDB ID : 1FP7
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

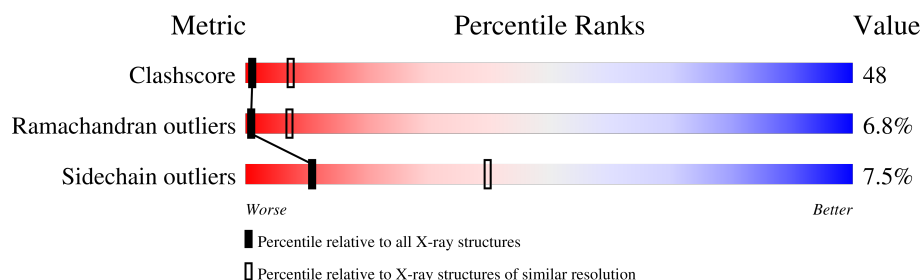
1 Overall quality at a glance

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	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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	-
2	SO4	A	277	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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.

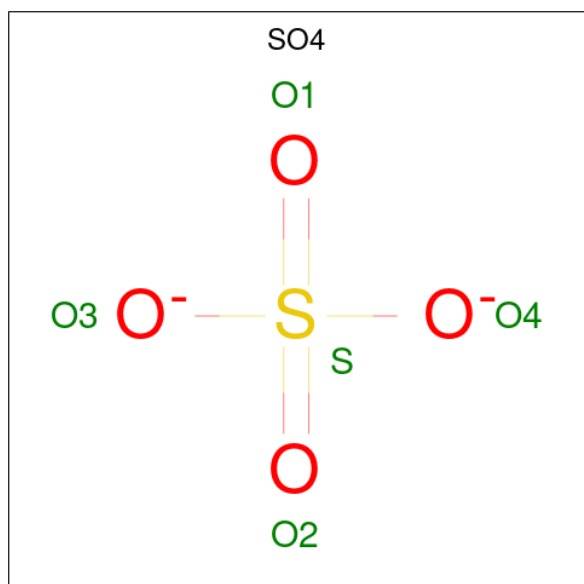
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

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: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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
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.

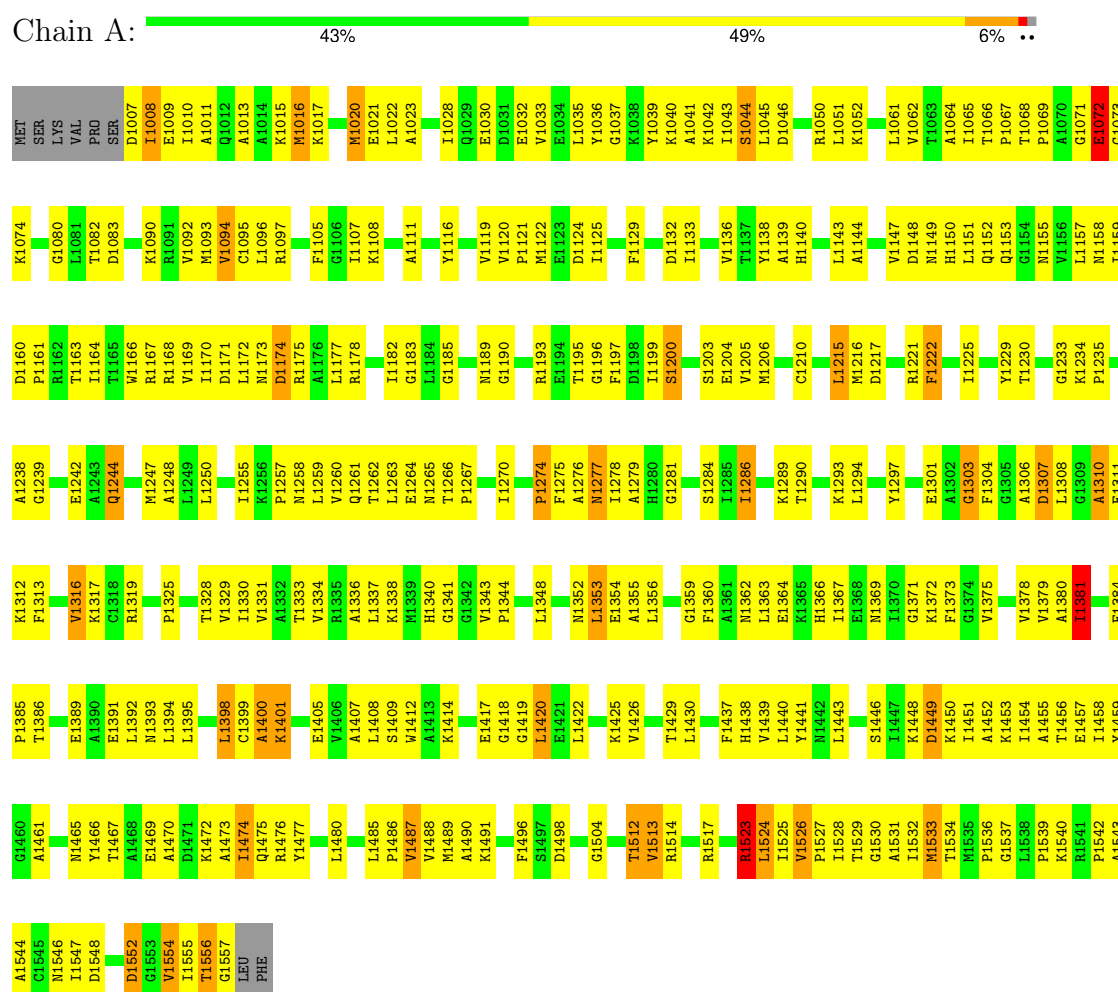
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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	N1484	L1409	G1341	I1278	L1211	V1136	T1068
G1553	L1485	S1409	G1342	A1279	L1215	H1140	P1069
V1554	P1486	W1412	V1343	H1280	L1215	L1143	A1070
T1555	P1486	A1413	P1344	G1281	L1215	A1144	G1071
T1556	V1487	K1414	D1347	G1282	E1220	L1152	E1072
G1557	V1488	E1417	L1348	L1285	R1221	Q1152	G1073
LEU	M1489	L1420	E1351	L1286	F1222	G1154	R1074
PHE	A1490	E1421	N1352	A1287	S1223	V1147	T1075
	T1491	N1352	L1353	T1288	R1224	D1148	T1076
	Q1493	L1422	L1356	K1289	V1226	N1149	T1077
	Y1494	K1425	R1357	T1290	V1227	H1150	S1078
S1495	F1496	V1426	L1358	A1291	G1228	L1151	V1079
S1497	S1497	L1427	R1358	L1292	Y1229	Q1152	G1080
Q1428	D1498	Q1428	G1359	K1293	T1230	G1154	L1081
D1499	M1500	T1429	F1360	L1294	Y1231	G1155	T1082
M1500	T1501	L1430	A1361	A1295	D1232	N1156	D1083
T1501	K1501	E1431	N1362	D1296	G1233	L1157	A1084
	S1432	S1432	L1363	V1298	K1234	L1085	L1085
	R1433	P1434	E1364	V1299	P1235	N1158	A1086
	S1435	P1434	K1365	T1237	V1236	L1159	R1087
	N1436	S1435	H1366	T1300	T1237	D1160	G1088
	F1437	N1436	L1367	G1303	A1238	P1161	L1089
	H1438	F1437	E1368	F1304	G1239	W1166	K1090
	V1439	N1369	L1370	G1305	D1240	R1167	R1091
	T1511	I1370	I1371	A1306	Q1244	R1168	V1092
	T1512	L1440	G1371	D1307	G1245	R1169	M1093
	V1513	Y1441	K1372	L1308	S1246	V1094	C1095
	R1514	N1442	F1373	G1309	M1247	D1171	L1096
	E1515	L1443	G1374	A1310	A1248	L1172	R1097
	V1516	D1444	V1375	E1311	L1249	N1173	P1103
	R1517	S1445	P1376	K1312	L1250	D1174	S1104
	S1519	I1447	A1377	F1313	M1251	R1175	S1104
	A1520	K1448	V1378	Y1314	K1252	A1176	F1105
		D1449	V1379	R1315	D1253	L1177	G1106
		K1450	A1380	V1316	A1254	R1178	I1107
		I1451	I1381	K1317	I1255	I1182	K1108
		A1452	N1382	C1318	K1256	G1183	G1109
		K1453	A1383	R1319	P1257	G1186	G1110
		I1454	F1384	Y1320	N1258	A1111	A1111
		A1455	P1385		L1259	G1187	A1112
		T1456	T1386	F1323	V1260	K1187	G1113
		E1457	D1387	K1324	Q1261	G1114	G1114
		I1458		P1325	T1262	G1115	G1115
		Y1459	A1390	D1326	L1263	Y1116	Y1116
		G1460	E1391	A1327	E1264	E1194	A1117
		A1461	N1392	T1328	N1265	T1195	Q1118
		D1462	L1393	V1329	T1266	G1196	V1119
			L1394	I1330	P1267	F1197	V1120
			Y1395	V1331	A1268	D1198	P1121
			E1396	T1332	F1269	I1199	
			L1397	T1333	I1270	S1200	D1124
			L1398	V1334	H1271	I1125	I1125
			C1399	R1335	G1273	S1203	F1129
			A1400	A1336	G1273	V1205	
			K1401	L1337	P1274	M1206	
			L1402	K1338	F1275	I1132	D1132
			G1403	M1339	A1276	I1133	I1133
							H1134

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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)	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	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 ²)	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	358	1
1	B	4125	0	4211	449	0
2	A	35	0	0	15	1
2	B	20	0	0	3	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	808	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 48.

The worst 5 of 808 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:1175:ARG:NH1	2:B:279:SO4:O3	1.58	1.33
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

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:A:1007:ASP:OD1	2:A:278:SO4:O3[3_665]	1.60	0.60

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%)	2	19
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	0	2
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1	7

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

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Mol	Chain	Res	Type
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%)	12	41
1	B	431/440 (98%)	397 (92%)	34 (8%)	10	38
All	All	863/880 (98%)	798 (92%)	65 (8%)	11	40

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

Mol	Chain	Res	Type
1	B	1382	ASN
1	B	1499	ASP
1	A	1487	VAL
1	A	1449	ASP
1	B	1518	LEU

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

Mol	Chain	Res	Type
1	B	1140	HIS
1	B	1189	ASN
1	B	1153	GLN
1	B	1244	GLN
1	A	1261	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 oligosaccharides 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	B	281	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	278	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	274	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	279	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	272	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	271	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	0.68	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	278	SO4	2	1
2	A	274	SO4	3	0
2	B	279	SO4	1	0
2	A	275	SO4	4	0
2	A	277	SO4	2	0
2	B	272	SO4	1	0
2	B	280	SO4	1	0
2	A	273	SO4	4	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.