



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 1EG7 / pdb_00001eg7
Title : THE CRYSTAL STRUCTURE OF FORMYLTETRAHYDROFOLATE
SYNTHETASE FROM MOORELLA THERMOACETICA
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Deposited on : 2000-02-14
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

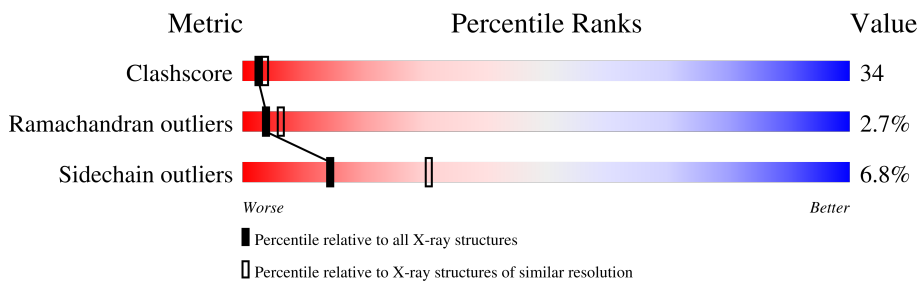
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	 57% 36% 5% ••
1	B	557	 41% 49% 8% •

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	3	-	-	X	-
2	SO4	A	5	-	-	X	-
2	SO4	A	7	-	-	X	-
2	SO4	A	8	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8586 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 FORMYLTETRAHYDROFOLATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4135	2618	716	780	21	0	0	0
1	B	548	4127	2614	715	777	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	GLU	ASP	conflict	UNP P21164
A	1225	LYS	ILE	conflict	UNP P21164
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	1174	GLU	ASP	conflict	UNP P21164
B	1225	LYS	ILE	conflict	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	71	Total	O	0	0
			71	71		

T1529	L1445	G1371	A1295	D1217
G1530	S1446	K1372	D1296	L1218
A1531	I1447	F1373	Y1297	K1219
I1532	K1448	G1374	V1298	E1220
M1533	D1449	V1375	V1299	R1221
T1534	K1450	P1376	T1300	F1222
M1535	I1451	A1377	E1301	S1223
P1536	I1454	V1378	A1302	R1224
G1537	A1455	V1379	G1303	K1225
K1540	I1458	A1380	F1304	V1226
R1541	I1459	I1381	E1311	V1227
P1542	I1460	A1382	K1312	V1236
A1543	G1461	F1383	F1313	Q1244
A1544	A1461	P1385	Y1314	L1250
C1545	D1462	T1386	D1315	D1253
M1546	Y1466	D1387	V1316	A1254
I1547	Y1466	T1388	R1319	I1255
D1548	K1472	E1389	Y1320	K1256
T1549	K1476	M1393	A1321	P1257
D1550	Y1477	L1394	P1325	N1258
A1551	E1478	L1398	D1326	L1259
D1552	E1478	C1399	V1329	V1260
G1553	S1479	A1400	I1330	Q1261
V1554	L1480	K1401	V1331	T1262
T1555	G1481	E1405	A1332	L1263
T1556	Y1482	L1408	T1333	E1264
LEU	G1483	S1409	V1334	N1265
PHE	N1484	W1412	R1335	T1266
	L1485	A1413	A1336	P1267
	P1486	K1414	A1337	A1268
	V1487	G1415	K1338	F1269
	M1488	G1416	M1339	I1270
	M1489	E1417	V1343	H1271
	A1490	G1418	P1344	G1272
	D1498	L1419	K1345	G1273
	P1506	L1420	F1275	P1274
	F1509	E1421	T1276	F1275
	T1510	L1422	A1276	N1277
	I1511	K1425	E1351	I1278
	H1512	V1426	M1352	A1279
	V1513	L1430	L1353	H1280
	R1514	E1431	L1356	G1281
	E1515	S1432	R1357	C1282
	V1516	R1433	F1360	N1283
	R1517	P1434	A1361	S1284
	L1518	S1435	M1362	I1285
	S1519	N1436	L1363	I1286
	A1520	F1437	E1364	A1287
	R1523	L1440	K1365	T1288
	L1524	L1443	H1366	K1289
	I1525	D1444	I1367	T1290
	V1526	L1443	E1368	A1291
	P1527	I1528	M1369	L1292
	I1528		I1370	K1293
				L1294

4 Data and refinement statistics

Xtrriage (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 – 2.50	Depositor
% Data completeness (in resolution range)	90.6 (19.99-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.253 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8586	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: 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	0.57	5/4203 (0.1%)	1.05	27/5691 (0.5%)
1	B	0.50	1/4195 (0.0%)	0.99	14/5680 (0.2%)
All	All	0.53	6/8398 (0.1%)	1.02	41/11371 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	ILE	CA-C	13.05	1.67	1.52
1	A	1008	ILE	N-CA	11.76	1.64	1.45
1	A	1007	ASP	CA-C	6.23	1.66	1.52
1	A	1007	ASP	C-N	5.58	1.42	1.33
1	A	1007	ASP	CA-CB	5.21	1.63	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	ILE	N-CA-C	-9.46	94.59	109.17
1	B	1015	LYS	N-CA-C	9.44	130.92	110.80
1	A	1008	ILE	CB-CA-C	-9.33	98.32	111.38
1	A	1007	ASP	CA-C-O	-8.81	105.83	120.80
1	A	1523	ARG	N-CA-C	8.45	118.20	108.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	ASP	Mainchain,Peptide

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	4135	0	4223	233	1
1	B	4127	0	4219	337	0
2	A	35	0	0	12	0
2	B	20	0	0	2	0
3	A	198	0	0	14	0
3	B	71	0	0	4	0
All	All	8586	0	8442	570	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 34.

The worst 5 of 570 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:1009:GLU:OE2	1:B:1111:ALA:HB2	1.33	1.27
1:A:1175:ARG:HD3	2:A:5:SO4:O3	1.55	1.07
1:A:1244:GLN:H	1:A:1244:GLN:NE2	1.55	1.03
1:B:1277:ASN:ND2	1:B:1278:ILE:H	1.59	1.01
1:B:1244:GLN:H	1:B:1244:GLN:NE2	1.59	0.99

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:1462:ASP:O	1:A:1462:ASP:O[12_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%)	485 (89%)	54 (10%)	8 (2%)	8	16
1	B	546/557 (98%)	444 (81%)	81 (15%)	21 (4%)	2	3
All	All	1093/1114 (98%)	929 (85%)	135 (12%)	29 (3%)	4	6

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1401	LYS
1	B	1015	LYS
1	A	1399	CYS
1	B	1065	ILE

5.3.2 Protein sidechains [i](#)

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%)	405 (94%)	27 (6%)	16	34
1	B	431/440 (98%)	399 (93%)	32 (7%)	13	27
All	All	863/880 (98%)	804 (93%)	59 (7%)	14	31

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1020	MET

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Mol	Chain	Res	Type
1	B	1526	VAL
1	B	1165	THR
1	B	1523	ARG
1	B	1382	ASN

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

Mol	Chain	Res	Type
1	B	1140	HIS
1	B	1158	ASN
1	B	1393	ASN
1	B	1150	HIS
1	B	1244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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	4	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	8	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	9	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	1	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	5	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	7	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	10	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	11	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	6	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	2	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	3	-	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.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	8	SO4	2	0
2	B	9	SO4	1	0
2	A	5	SO4	2	0
2	A	7	SO4	2	0
2	B	2	SO4	1	0
2	A	3	SO4	6	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.