



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2020 – 12:13 PM JST

PDB ID : 7C11
Title : Formate--tetrahydrofolate ligase from Methylobacterium extorquens CM4 strain
Authors : Kim, K.-J.; Kim, S.; Seo, H.; Lee, S.
Deposited on : 2020-05-02
Resolution : 2.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

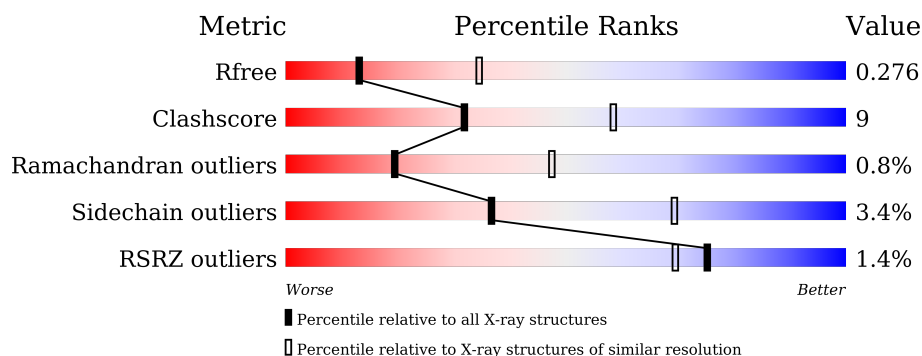
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



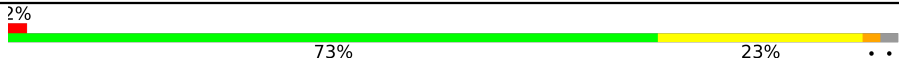

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	568	
1	B	568	
1	C	568	
1	D	568	
1	M	568	
1	N	568	

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Mol	Chain	Length	Quality of chain
1	O	568	
1	P	568	

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
4	FLC	N	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33673 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	557	Total	C	N	O	S	0	1	0
			4184	2637	745	781	21			
1	B	558	Total	C	N	O	S	0	0	0
			4181	2634	745	781	21			
1	C	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	D	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	M	552	Total	C	N	O	S	0	0	0
			4139	2609	738	772	20			
1	N	555	Total	C	N	O	S	0	0	0
			4159	2621	741	777	20			
1	O	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	P	547	Total	C	N	O	S	0	0	0
			4099	2583	731	765	20			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	-	expression tag	UNP B7L0A5
A	559	ALA	-	expression tag	UNP B7L0A5
A	560	ALA	-	expression tag	UNP B7L0A5
A	561	LEU	-	expression tag	UNP B7L0A5
A	562	GLU	-	expression tag	UNP B7L0A5
A	563	HIS	-	expression tag	UNP B7L0A5
A	564	HIS	-	expression tag	UNP B7L0A5
A	565	HIS	-	expression tag	UNP B7L0A5
A	566	HIS	-	expression tag	UNP B7L0A5
A	567	HIS	-	expression tag	UNP B7L0A5
A	568	HIS	-	expression tag	UNP B7L0A5
B	558	ALA	-	expression tag	UNP B7L0A5
B	559	ALA	-	expression tag	UNP B7L0A5

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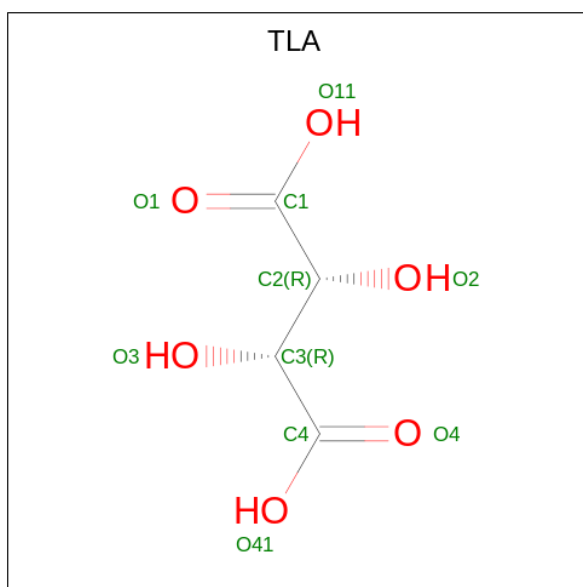
Chain	Residue	Modelled	Actual	Comment	Reference
B	560	ALA	-	expression tag	UNP B7L0A5
B	561	LEU	-	expression tag	UNP B7L0A5
B	562	GLU	-	expression tag	UNP B7L0A5
B	563	HIS	-	expression tag	UNP B7L0A5
B	564	HIS	-	expression tag	UNP B7L0A5
B	565	HIS	-	expression tag	UNP B7L0A5
B	566	HIS	-	expression tag	UNP B7L0A5
B	567	HIS	-	expression tag	UNP B7L0A5
B	568	HIS	-	expression tag	UNP B7L0A5
C	558	ALA	-	expression tag	UNP B7L0A5
C	559	ALA	-	expression tag	UNP B7L0A5
C	560	ALA	-	expression tag	UNP B7L0A5
C	561	LEU	-	expression tag	UNP B7L0A5
C	562	GLU	-	expression tag	UNP B7L0A5
C	563	HIS	-	expression tag	UNP B7L0A5
C	564	HIS	-	expression tag	UNP B7L0A5
C	565	HIS	-	expression tag	UNP B7L0A5
C	566	HIS	-	expression tag	UNP B7L0A5
C	567	HIS	-	expression tag	UNP B7L0A5
C	568	HIS	-	expression tag	UNP B7L0A5
D	558	ALA	-	expression tag	UNP B7L0A5
D	559	ALA	-	expression tag	UNP B7L0A5
D	560	ALA	-	expression tag	UNP B7L0A5
D	561	LEU	-	expression tag	UNP B7L0A5
D	562	GLU	-	expression tag	UNP B7L0A5
D	563	HIS	-	expression tag	UNP B7L0A5
D	564	HIS	-	expression tag	UNP B7L0A5
D	565	HIS	-	expression tag	UNP B7L0A5
D	566	HIS	-	expression tag	UNP B7L0A5
D	567	HIS	-	expression tag	UNP B7L0A5
D	568	HIS	-	expression tag	UNP B7L0A5
M	558	ALA	-	expression tag	UNP B7L0A5
M	559	ALA	-	expression tag	UNP B7L0A5
M	560	ALA	-	expression tag	UNP B7L0A5
M	561	LEU	-	expression tag	UNP B7L0A5
M	562	GLU	-	expression tag	UNP B7L0A5
M	563	HIS	-	expression tag	UNP B7L0A5
M	564	HIS	-	expression tag	UNP B7L0A5
M	565	HIS	-	expression tag	UNP B7L0A5
M	566	HIS	-	expression tag	UNP B7L0A5
M	567	HIS	-	expression tag	UNP B7L0A5
M	568	HIS	-	expression tag	UNP B7L0A5

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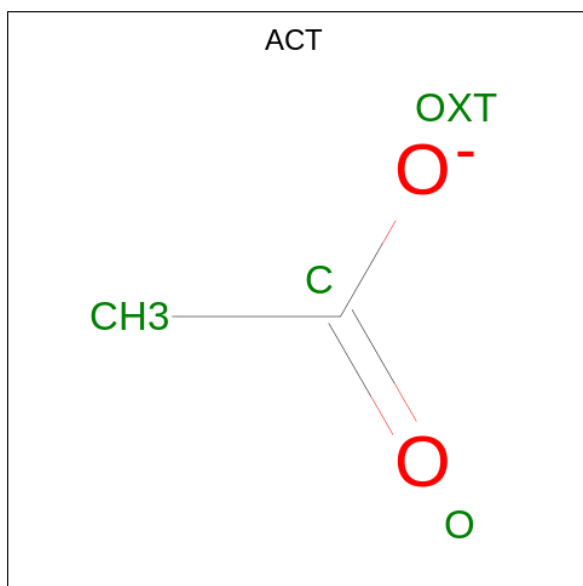
Chain	Residue	Modelled	Actual	Comment	Reference
N	558	ALA	-	expression tag	UNP B7L0A5
N	559	ALA	-	expression tag	UNP B7L0A5
N	560	ALA	-	expression tag	UNP B7L0A5
N	561	LEU	-	expression tag	UNP B7L0A5
N	562	GLU	-	expression tag	UNP B7L0A5
N	563	HIS	-	expression tag	UNP B7L0A5
N	564	HIS	-	expression tag	UNP B7L0A5
N	565	HIS	-	expression tag	UNP B7L0A5
N	566	HIS	-	expression tag	UNP B7L0A5
N	567	HIS	-	expression tag	UNP B7L0A5
N	568	HIS	-	expression tag	UNP B7L0A5
O	558	ALA	-	expression tag	UNP B7L0A5
O	559	ALA	-	expression tag	UNP B7L0A5
O	560	ALA	-	expression tag	UNP B7L0A5
O	561	LEU	-	expression tag	UNP B7L0A5
O	562	GLU	-	expression tag	UNP B7L0A5
O	563	HIS	-	expression tag	UNP B7L0A5
O	564	HIS	-	expression tag	UNP B7L0A5
O	565	HIS	-	expression tag	UNP B7L0A5
O	566	HIS	-	expression tag	UNP B7L0A5
O	567	HIS	-	expression tag	UNP B7L0A5
O	568	HIS	-	expression tag	UNP B7L0A5
P	558	ALA	-	expression tag	UNP B7L0A5
P	559	ALA	-	expression tag	UNP B7L0A5
P	560	ALA	-	expression tag	UNP B7L0A5
P	561	LEU	-	expression tag	UNP B7L0A5
P	562	GLU	-	expression tag	UNP B7L0A5
P	563	HIS	-	expression tag	UNP B7L0A5
P	564	HIS	-	expression tag	UNP B7L0A5
P	565	HIS	-	expression tag	UNP B7L0A5
P	566	HIS	-	expression tag	UNP B7L0A5
P	567	HIS	-	expression tag	UNP B7L0A5
P	568	HIS	-	expression tag	UNP B7L0A5

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



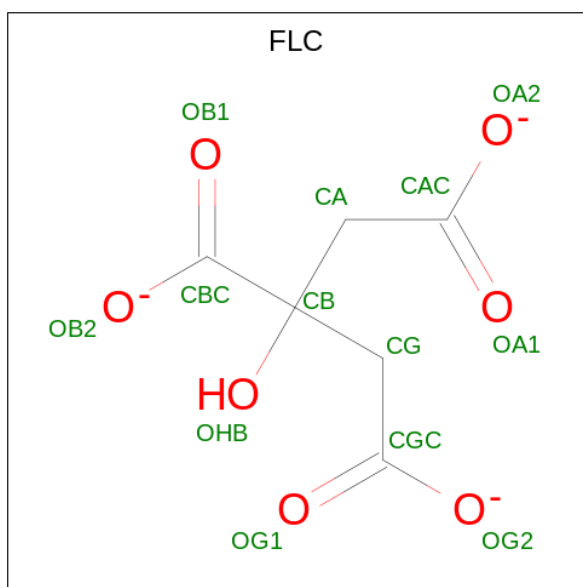
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	C	O	0	0
			13	6	7		

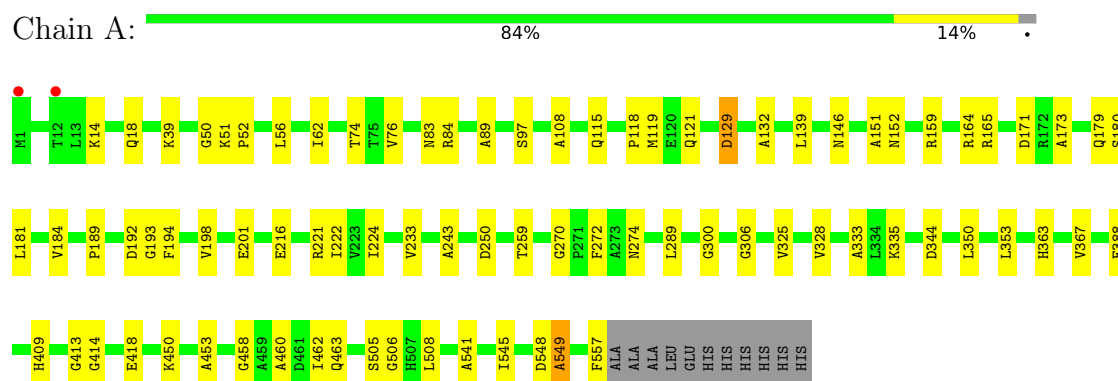
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	73	Total	O	0	0
			73	73		
5	C	51	Total	O	0	0
			51	51		
5	D	58	Total	O	0	0
			58	58		
5	M	37	Total	O	0	0
			37	37		
5	N	42	Total	O	0	0
			42	42		
5	O	31	Total	O	0	0
			31	31		
5	P	21	Total	O	0	0
			21	21		

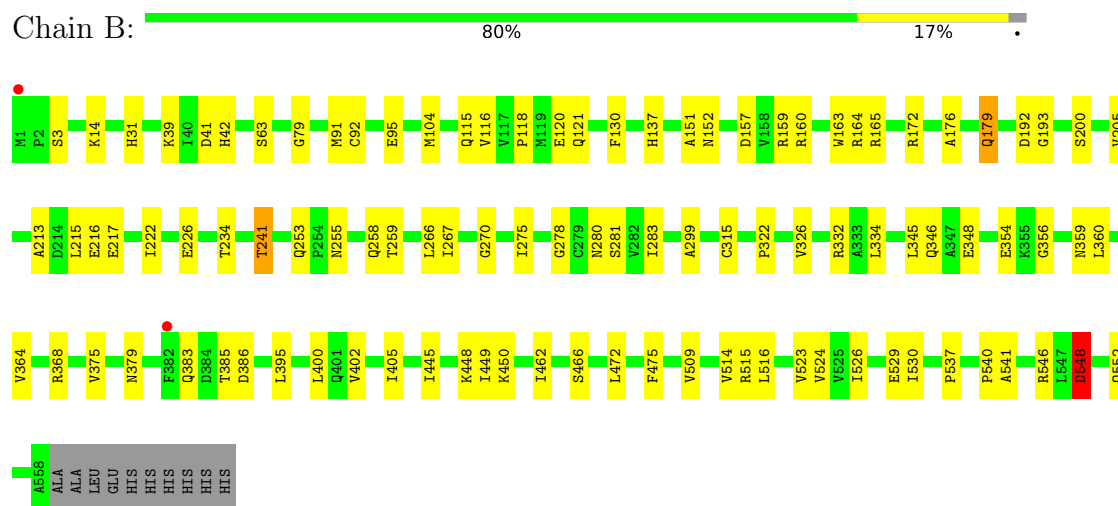
3 Residue-property plots

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 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.

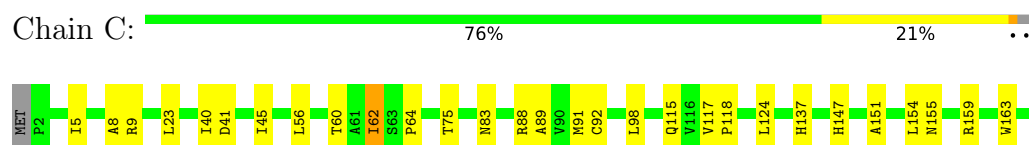
• Molecule 1: Formate-tetrahydrofolate ligase

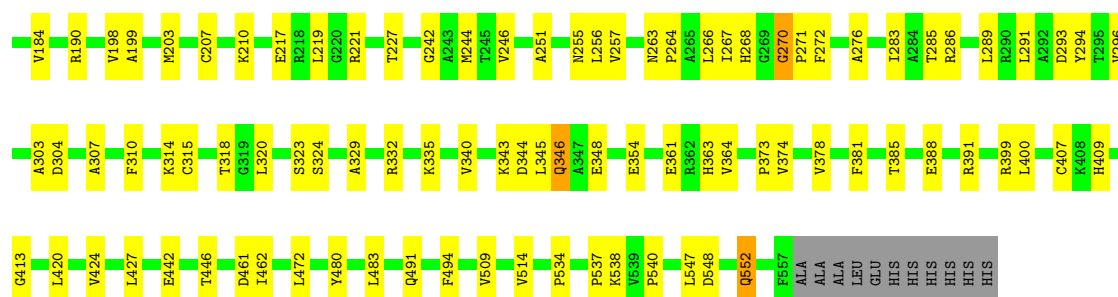


• Molecule 1: Formate-tetrahydrofolate ligase



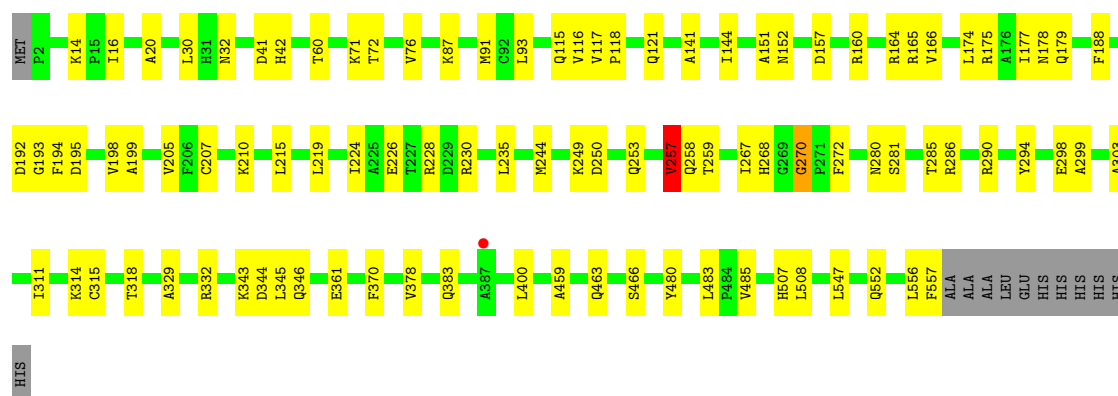
• Molecule 1: Formate-tetrahydrofolate ligase





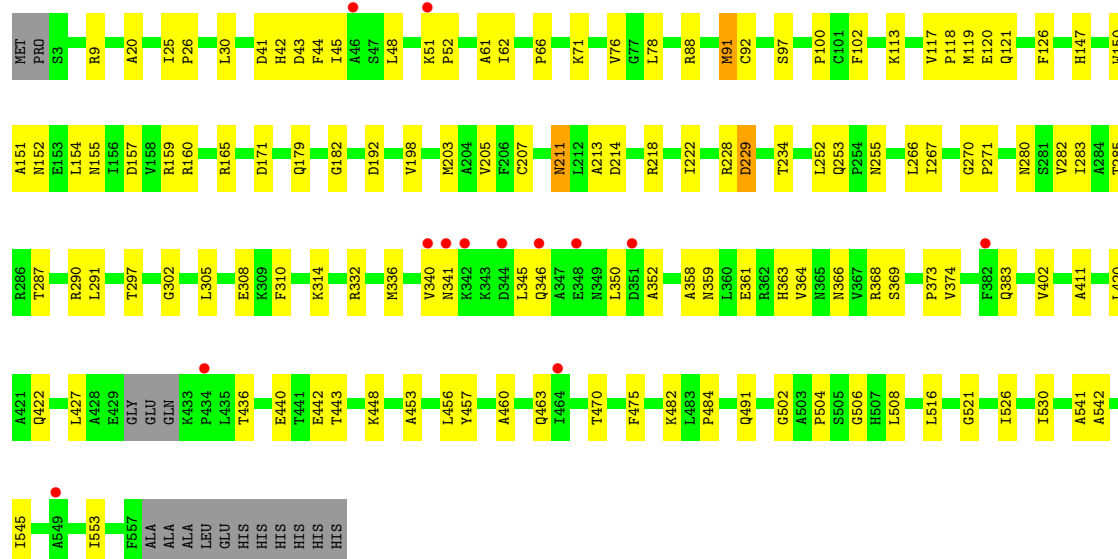
• Molecule 1: Formate-tetrahydrofolate ligase

Chain D: 81% 17%



• Molecule 1: Formate-tetrahydrofolate ligase

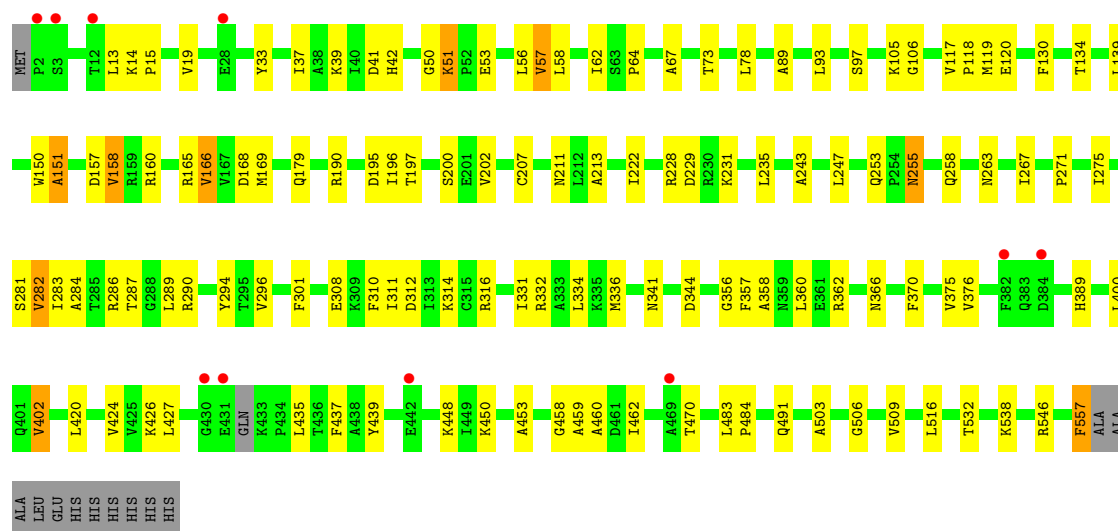
Chain M: 2% 74% 22%



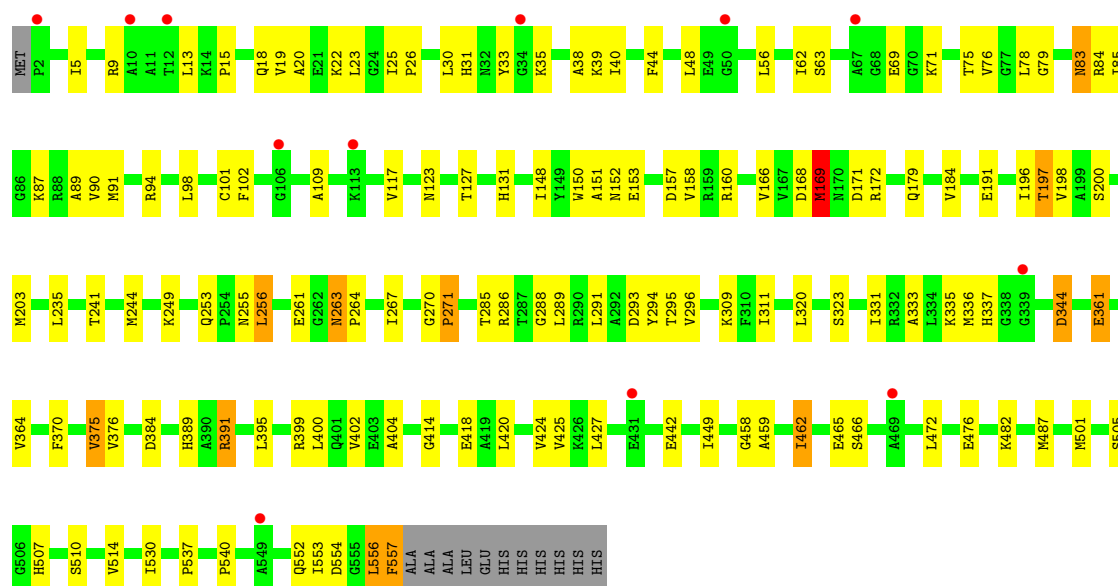
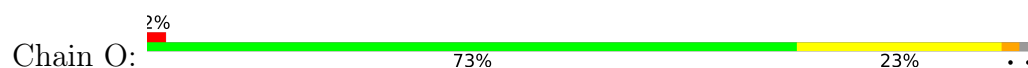
• Molecule 1: Formate-tetrahydrofolate ligase

Chain N: 2% 76% 21%



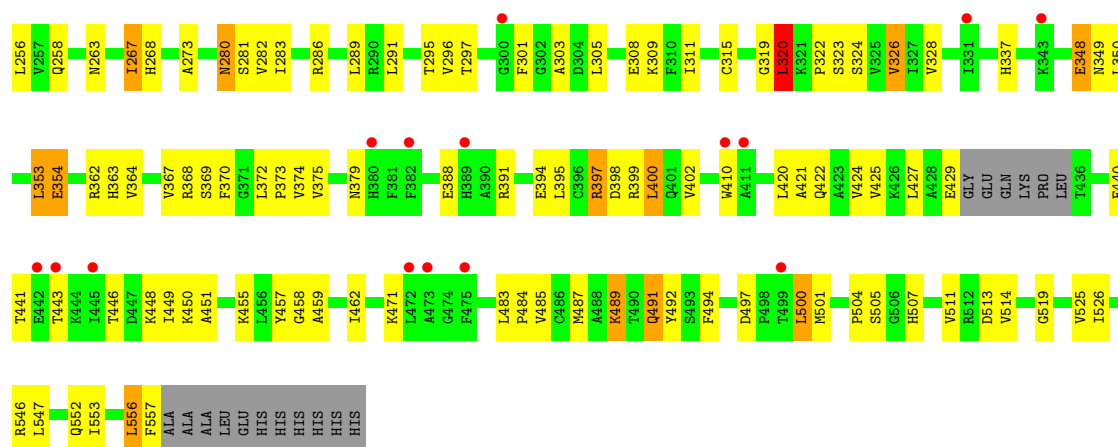


• Molecule 1: Formate-tetrahydrofolate ligase



• Molecule 1: Formate-tetrahydrofolate ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 168.74Å 126.99Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	36.60 – 2.81 36.58 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.60-2.81) 97.5 (36.58-2.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.180 , 0.276 0.183 , 0.276	Depositor DCC
R_{free} test set	5124 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33673	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, FLC, ACT

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	0.75	0/4254	0.92	1/5759 (0.0%)
1	B	0.76	0/4251	0.91	0/5755
1	C	0.76	0/4238	0.92	2/5737 (0.0%)
1	D	0.74	0/4238	0.91	0/5737
1	M	0.73	0/4207	0.87	0/5694
1	N	0.74	0/4228	0.88	0/5722
1	O	0.72	0/4238	0.89	0/5737
1	P	0.72	0/4166	0.87	1/5638 (0.0%)
All	All	0.74	0/33820	0.90	4/45779 (0.0%)

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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	ASP	CB-CA-C	-5.71	98.99	110.40
1	C	190	ARG	CB-CA-C	-5.57	99.27	110.40
1	P	165	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	221	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	GLY	Peptide

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	4184	0	4262	48	0
1	B	4181	0	4257	66	0
1	C	4168	0	4241	80	0
1	D	4168	0	4241	65	0
1	M	4139	0	4215	78	0
1	N	4159	0	4232	87	0
1	O	4168	0	4241	86	0
1	P	4099	0	4167	110	0
2	D	10	0	4	0	0
3	D	4	0	3	0	0
4	N	13	0	5	4	0
5	A	67	0	0	0	0
5	B	73	0	0	2	0
5	C	51	0	0	0	0
5	D	58	0	0	1	0
5	M	37	0	0	0	0
5	N	42	0	0	0	0
5	O	31	0	0	0	0
5	P	21	0	0	0	0
All	All	33673	0	33868	597	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 9.

The worst 5 of 597 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:O:78:LEU:HD13	1:O:420:LEU:HD23	1.53	0.89
1:N:53:GLU:OE2	1:N:286:ARG:NH2	2.04	0.89
1:N:420:LEU:O	1:N:424:VAL:HG23	1.73	0.88
1:A:83:ASN:HD21	1:A:89:ALA:H	1.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:229:ASP:HB2	1:N:231:LYS:HE3	1.60	0.84

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	556/568 (98%)	527 (95%)	26 (5%)	3 (0%)	29	59
1	B	556/568 (98%)	516 (93%)	36 (6%)	4 (1%)	22	51
1	C	554/568 (98%)	513 (93%)	38 (7%)	3 (0%)	29	59
1	D	554/568 (98%)	522 (94%)	30 (5%)	2 (0%)	34	64
1	M	548/568 (96%)	498 (91%)	48 (9%)	2 (0%)	34	64
1	N	551/568 (97%)	473 (86%)	71 (13%)	7 (1%)	12	34
1	O	554/568 (98%)	507 (92%)	43 (8%)	4 (1%)	22	51
1	P	541/568 (95%)	484 (90%)	48 (9%)	9 (2%)	9	27
All	All	4414/4544 (97%)	4040 (92%)	340 (8%)	34 (1%)	19	47

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ASP
1	P	18	GLN
1	P	320	LEU
1	A	151	ALA
1	A	549	ALA

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	434/441 (98%)	429 (99%)	5 (1%)	71	91
1	B	433/441 (98%)	424 (98%)	9 (2%)	53	82
1	C	432/441 (98%)	424 (98%)	8 (2%)	57	84
1	D	432/441 (98%)	425 (98%)	7 (2%)	62	87
1	M	429/441 (97%)	418 (97%)	11 (3%)	46	78
1	N	431/441 (98%)	416 (96%)	15 (4%)	36	68
1	O	432/441 (98%)	405 (94%)	27 (6%)	18	44
1	P	425/441 (96%)	390 (92%)	35 (8%)	11	31
All	All	3448/3528 (98%)	3331 (97%)	117 (3%)	37	69

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	516	LEU
1	O	263	ASN
1	P	398	ASP
1	N	557	PHE
1	O	169	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	GLN
1	M	211	ASN
1	O	432	GLN
1	D	253	GLN
1	M	147	HIS

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
4	FLC	N	601	-	3,12,12	0.36	0	3,17,17	2.16	1 (33%)
2	TLA	D	601	-	3,9,9	0.79	0	6,12,12	1.92	2 (33%)
3	ACT	D	602	-	1,3,3	5.18	1 (100%)	0,3,3	0.00	-

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
4	FLC	N	601	-	-	2/6/16/16	-
2	TLA	D	601	-	-	4/4/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	ACT	CH3-C	5.18	1.55	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	601	FLC	CB-CA-CAC	3.31	120.29	114.98
2	D	601	TLA	C4-C3-C2	3.08	119.74	113.11
2	D	601	TLA	C1-C2-C3	-2.19	108.40	113.11

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	TLA	C1-C2-C3-C4
2	D	601	TLA	O2-C2-C3-O3
2	D	601	TLA	O2-C2-C3-C4
2	D	601	TLA	C1-C2-C3-O3
4	N	601	FLC	CA-CB-CG-CGC

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	601	FLC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/568 (98%)	-0.55	2 (0%) 92 91	17, 28, 48, 84	0
1	B	558/568 (98%)	-0.43	2 (0%) 92 91	18, 29, 46, 76	0
1	C	556/568 (97%)	-0.31	0 100 100	18, 33, 55, 71	0
1	D	556/568 (97%)	-0.41	1 (0%) 95 94	18, 30, 49, 69	0
1	M	552/568 (97%)	-0.06	13 (2%) 59 49	21, 51, 75, 97	0
1	N	555/568 (97%)	-0.02	10 (1%) 68 61	24, 55, 79, 95	0
1	O	556/568 (97%)	-0.13	12 (2%) 62 52	23, 49, 73, 92	0
1	P	547/568 (96%)	0.16	20 (3%) 41 31	23, 59, 83, 112	0
All	All	4437/4544 (97%)	-0.22	60 (1%) 75 69	17, 39, 74, 112	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	2	PRO	4.2
1	P	499	THR	4.1
1	M	341	ASN	3.8
1	N	469	ALA	3.7
1	P	389	HIS	3.7

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	D	602	4/4	0.81	0.51	52,55,60,61	0
2	TLA	D	601	10/10	0.89	0.17	41,46,47,50	0
4	FLC	N	601	13/13	0.93	0.17	39,46,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.