



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 01:51 PM EDT

PDB ID : 3EGY
Title : Crystal Structure of Human Thymidylate Synthase A191K with Loop 181-197 stabilized in the inactive conformation
Authors : Lovelace, L.L.; Gibson, L.M.; Johnson, S.R.; Berger, S.H.; Lebioda, L.
Deposited on : 2008-09-11
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	2.23.2
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)	:	2.23.2

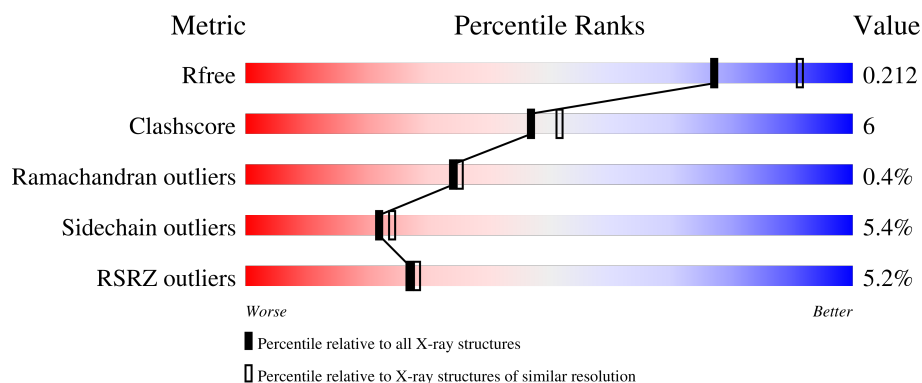
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 $\leq 5\%$. 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	X	313	

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
1	CME	X	195	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2066 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	234	1927	1243	336	333	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	191	LYS	ALA	engineered mutation	UNP P04818

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	X	1	5	4	1	0	0
2	X	1	5	4	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	125	Total	O	0	0
			125	125		

i

- Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.87Å 95.87Å 82.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.18 41.51 – 2.18	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.18) 92.2 (41.51-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.207 0.184 , 0.212	Depositor DCC
R_{free} test set	1114 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2066	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 4.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CME, EDO

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	X	0.82	1/1934 (0.1%)	0.84	3/2609 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	196	HIS	N-CA	5.75	1.57	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	252	LEU	CB-CG-CD1	6.49	122.03	111.00
1	X	198	LEU	CA-CB-CG	5.54	128.03	115.30
1	X	64	ARG	NE-CZ-NH1	-5.40	117.60	120.30

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	X	1927	0	1934	24	0
2	X	10	0	0	0	0
3	X	4	0	6	2	0
4	X	125	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2066	0	1940	24	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 6.

All (24) 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:X:195:CME:O	1:X:196:HIS:CB	1.76	1.21
1:X:195:CME:O	1:X:196:HIS:HB3	1.17	0.97
1:X:195:CME:HH	1:X:213:TYR:HD1	1.16	0.92
1:X:195:CME:OH	1:X:213:TYR:HD1	1.53	0.91
1:X:195:CME:OH	1:X:213:TYR:CD1	2.29	0.85
1:X:196:HIS:HA	1:X:215:ARG:HD3	1.65	0.79
1:X:239:HIS:HE1	1:X:285:VAL:H	1.37	0.70
1:X:135:TYR:OH	1:X:196:HIS:CD2	2.58	0.57
1:X:195:CME:O	1:X:196:HIS:HB2	1.96	0.54
1:X:160:GLN:HB3	1:X:179:MET:HG3	1.91	0.53
1:X:164:VAL:HG21	1:X:179:MET:HE2	1.90	0.53
1:X:135:TYR:HH	1:X:196:HIS:CD2	2.28	0.51
1:X:252:LEU:HD22	3:X:314:EDO:H12	1.92	0.51
1:X:195:CME:HZ3	1:X:215:ARG:HB3	1.96	0.47
1:X:252:LEU:HD22	3:X:314:EDO:C1	2.45	0.47
1:X:140:ARG:NH1	1:X:159:ASP:OD2	2.47	0.47
1:X:134:VAL:HG12	1:X:135:TYR:H	1.80	0.46
1:X:179:MET:HE2	1:X:179:MET:HB2	1.82	0.44
1:X:138:GLN:O	1:X:142:PHE:HB2	2.19	0.42
1:X:244:LYS:HE3	1:X:244:LYS:HB2	1.92	0.42
1:X:140:ARG:NH2	1:X:289:ASP:OD1	2.52	0.41
1:X:195:CME:HZ2	1:X:196:HIS:C	2.41	0.41
1:X:221:LEU:HG	1:X:309:MET:HB2	2.03	0.41
1:X:274:ARG:HB3	1:X:275:PRO:HD2	2.01	0.41

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	X	224/313 (72%)	219 (98%)	4 (2%)	1 (0%)	34	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	196	HIS

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	X	204/268 (76%)	193 (95%)	11 (5%)	22	24

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	82	LYS
1	X	95	SER
1	X	135	TYR
1	X	179	MET
1	X	240	ILE
1	X	252	LEU
1	X	259	LEU
1	X	263	GLU
1	X	274	ARG
1	X	280	ARG

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Mol	Chain	Res	Type
1	X	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	171	ASN
1	X	196	HIS
1	X	205	ASN
1	X	211	GLN
1	X	226	ASN
1	X	239	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	X	180	1	8,9,10	0.87	0	5,9,11	1.62	2 (40%)
1	CME	X	43	1	8,9,10	0.75	0	5,9,11	0.70	0
1	CME	X	195	1	8,9,10	1.15	0	5,9,11	1.94	2 (40%)
1	CME	X	199	1	8,9,10	1.05	1 (12%)	5,9,11	1.17	1 (20%)

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
1	CME	X	180	1	-	1/5/8/10	-
1	CME	X	43	1	-	2/5/8/10	-
1	CME	X	195	1	-	3/5/8/10	-
1	CME	X	199	1	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	199	CME	CB-SG	-2.43	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	195	CME	CB-SG-SD	-3.13	95.72	103.82
1	X	180	CME	CZ-CE-SD	-2.79	103.68	113.37
1	X	199	CME	CE-SD-SG	2.27	113.93	103.45
1	X	180	CME	CB-SG-SD	2.20	109.53	103.82
1	X	195	CME	CZ-CE-SD	-2.07	106.18	113.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	X	43	CME	SD-CE-CZ-OH
1	X	195	CME	CE-SD-SG-CB
1	X	180	CME	SD-CE-CZ-OH
1	X	43	CME	CE-SD-SG-CB
1	X	195	CME	SD-CE-CZ-OH
1	X	195	CME	CZ-CE-SD-SG
1	X	199	CME	CA-CB-SG-SD

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	X	195	CME	8	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
3	EDO	X	314	-	3,3,3	0.51	0	2,2,2	0.36	0
2	SO4	X	417	-	4,4,4	0.26	0	6,6,6	0.47	0
2	SO4	X	416	-	4,4,4	0.28	0	6,6,6	0.34	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
3	EDO	X	314	-	-	0/1/1/1	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	314	EDO	2	0

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 [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	X	230/313 (73%)	0.29	12 (5%) 27 28	32, 38, 58, 76	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	95	SER	5.3
1	X	282	LEU	5.2
1	X	26	PRO	5.1
1	X	96	THR	4.4
1	X	94	GLY	3.5
1	X	134	VAL	3.2
1	X	284	LYS	3.0
1	X	135	TYR	2.9
1	X	252	LEU	2.6
1	X	90	TRP	2.6
1	X	137	PHE	2.5
1	X	198	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CME	X	195	10/11	0.93	0.20	40,46,68,72	0
1	CME	X	43	10/11	0.95	0.11	45,46,63,63	0
1	CME	X	199	10/11	0.95	0.15	35,38,50,51	0
1	CME	X	180	10/11	0.97	0.16	41,44,67,74	0

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	EDO	X	314	4/4	0.96	0.10	38,38,38,40	0
2	SO4	X	417	5/5	0.97	0.06	66,71,72,73	0
2	SO4	X	416	5/5	0.98	0.11	51,55,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.