

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 01:42 PM EDT

PDB ID : 3EDW

Title : Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Prop-

erties and Intracellular Stability

Authors: Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Pena, M.M.; Berger, F.G.;

Berger, S.H.

Deposited on : 2008-09-03

Resolution : 1.75 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 (i) symbol.

The following versions of software and data (see references (1)) 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)

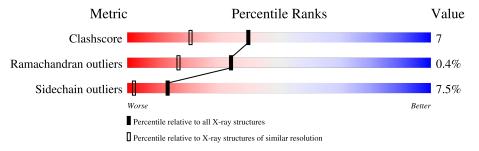
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.75 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\AA))$
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 <=5%

Mol	Chain	Length	Quality of chain					
1	X	313	65%	13%		17%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2255 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.

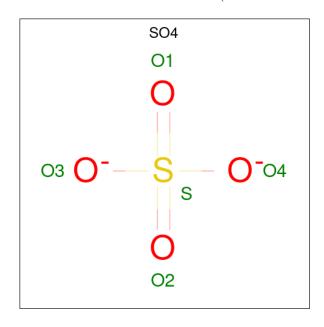
• Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	v	260	Total	С	N	О	S	0	0	0
1	Λ	200	2116	1356	370	379	11	0	U	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	3	PHE	VAL	engineered mutation	UNP P04818

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



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



• Molecule 3 is water.

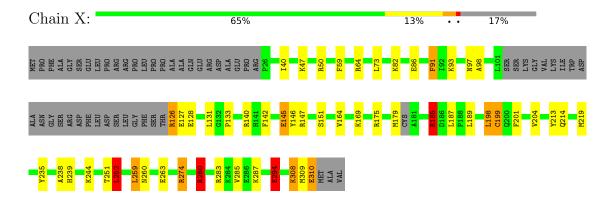
Mol	Chain	Residues	Atoms		Atoms		Atoms		Atoms		ZeroOcc	AltConf
3	X	124	Total C 124 12	4	0	0						



3 Residue-property plots (i)

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.

• Molecule 1: Thymidylate synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	96.02Å 96.02Å 80.72Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 - 1.75	Depositor
rtesolution (A)	48.01 - 1.85	EDS
% Data completeness	85.9 (50.00-1.75)	Depositor
(in resolution range)	86.0 (48.01-1.85)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.60 (at 1.86Å)	Xtriage
Refinement program	REFMAC	Depositor
Ρ. Р.	0.229 , 0.268	Depositor
R, R_{free}	0.305 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 49.0	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2255	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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		Bo	nd lengths	Bond angles		
			RMSZ	# Z > 5	RMSZ	# Z >5	
	1	X	1.34	$13/2170 \ (0.6\%)$	1.17	12/2933 (0.4%)	

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(Å)
1	X	235	TYR	CG-CD2	7.15	1.48	1.39
1	X	213	TYR	CD1-CE1	7.11	1.50	1.39
1	X	294	GLU	CG-CD	6.88	1.62	1.51
1	X	91	PHE	CE1-CZ	6.75	1.50	1.37
1	X	199	CYS	CB-SG	6.36	1.93	1.82
1	X	64	ARG	CG-CD	6.12	1.67	1.51
1	X	251	THR	CB-CG2	6.06	1.72	1.52
1	X	145	GLU	CG-CD	5.77	1.60	1.51
1	X	164	VAL	CB-CG2	5.73	1.64	1.52
1	X	59	PHE	CE1-CZ	5.55	1.48	1.37
1	X	238	ALA	CA-CB	-5.53	1.40	1.52
1	X	252	LEU	N-CA	-5.27	1.35	1.46
1	X	91	PHE	CG-CD2	5.23	1.46	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type			$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	X	274	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	X	274	ARG	NE-CZ-NH1	-9.45	115.57	120.30
1	X	198	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	X	140	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	X	280	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	X	260	ASN	CB-CA-C	-5.81	98.78	110.40
1	X	73	LEU	CB-CG-CD1	5.58	120.49	111.00
1	X	175	ARG	NE-CZ-NH1	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms Z		$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	X	283	ARG	NE-CZ-NH2 5.45		123.03	120.30
1	X	47	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	X	175	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	X	185	ARG	NE-CZ-NH1	5.27	122.94	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	2116	0	2094	30	0
2	X	15	0	0	0	0
3	X	124	0	0	4	0
All	All	2255	0	2094	30	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 7.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:X:280:ARG:HH21	1:X:280:ARG:HB2	1.02	1.12	
1:X:294:GLU:N	1:X:294:GLU:OE1	1.91	1.02	
1:X:239:HIS:HE1	1:X:285:VAL:H	1.11	0.95	
1:X:126:ARG:HD3	1:X:128:GLU:CG	1.99	0.91	
1:X:126:ARG:HD3	1:X:128:GLU:HG3	1.48	0.91	
1:X:280:ARG:HB2	1:X:280:ARG:NH2	1.88	0.89	
1:X:280:ARG:HH21	1:X:280:ARG:CB	1.92	0.77	
1:X:294:GLU:H	1:X:294:GLU:CD	1.89	0.76	
1:X:179:MET:C	3:X:415:HOH:O	2.23	0.75	
1:X:93:LYS:HE3	3:X:405:HOH:O	1.94	0.67	
1:X:239:HIS:CE1	1:X:285:VAL:H	2.04	0.61	
1:X:263:GLU:HG3	3:X:418:HOH:O	2.02	0.58	
1:X:126:ARG:HD3	1:X:128:GLU:HG2	1.82	0.57	

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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)	
1:X:98:ALA:HB2	1:X:131:LEU:HD21	1.87	0.56	
1:X:169:LYS:HD2	3:X:439:HOH:O	2.06	0.55	
1:X:126:ARG:CD	1:X:128:GLU:HG3	2.33	0.51	
1:X:50:ARG:HD2	1:X:185:ARG:CZ	2.41	0.50	
1:X:50:ARG:HD2	1:X:185:ARG:NH2	2.27	0.48	
1:X:133:PRO:HB3	1:X:146:TYR:HB2	1.98	0.46	
1:X:40:ILE:CD1	1:X:219:MET:HG3	2.47	0.45	
1:X:308:LYS:HE2	1:X:308:LYS:HB3	1.70	0.44	
1:X:214:GLN:HB2	1:X:252:LEU:HD12	2.00	0.43	
1:X:259:LEU:HD12	1:X:259:LEU:HA	1.76	0.43	
1:X:244:LYS:HD3	1:X:244:LYS:HA	1.87	0.42	
1:X:147:ARG:NH2	1:X:151:SER:HB3	2.35	0.42	
1:X:187:LEU:HA	1:X:187:LEU:HD23	1.79	0.41	
1:X:199:CYS:SG	1:X:201:PHE:CZ	3.13	0.41	
1:X:309:MET:O	1:X:310:GLU:C	2.60	0.41	
1:X:142:PHE:CD2	1:X:142:PHE:C	2.95	0.40	
1:X:198:LEU:C	1:X:198:LEU:HD12	2.42	0.40	

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	254/313 (81%)	241 (95%)	12 (5%)	1 (0%)	34 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	127	GLU



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	Analysed Rotameric		Percentiles		
1	X	228/271 (84%)	211 (92%)	17 (8%)	13 2		

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	82	LYS
1	X	86	GLU
1	X	91	PHE
1	X	97	ASN
1	X	126	ARG
1	X	145	GLU
1	X	185	ARG
1	X	189	LEU
1	X	204	VAL
1	X	252	LEU
1	X	259	LEU
1	X	274	ARG
1	X	280	ARG
1	X	287	LYS
1	X	294	GLU
1	X	308	LYS
1	X	310	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	97	ASN
1	X	171	ASN
1	X	239	HIS

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 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	Res Link	Bond lengths			Bond angles			
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	X	315	-	4,4,4	0.33	0	6,6,6	0.83	0
2	SO4	X	318	-	4,4,4	0.44	0	6,6,6	0.97	0
2	SO4	X	317	-	4,4,4	0.55	0	6,6,6	1.17	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.

No monomer is involved in short contacts.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

