

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 09:33 AM EDT

PDB ID	:	1VZE
Title	:	L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q TERNARY COM-
		PLEX WITH DUMP AND CB3717
Authors	:	Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.
Deposited on		
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

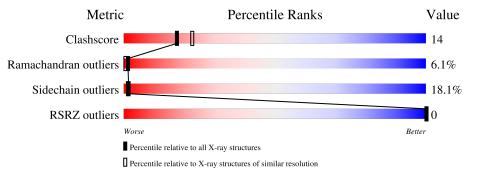
MolProbity		
		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.30 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	Quali	ty of chain		
1	A	316	47%	34%	16% •	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3896 atoms, of which 1013 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.

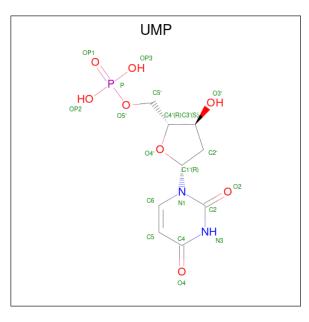
• Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	А	316	Total 3122	C 1677	Н 532	N 439	O 466	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	GLN	GLU	engineered mutation	UNP P00469
А	111	ALA	ASP	conflict	UNP P00469

• Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).

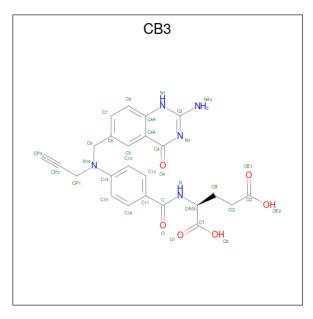


Mol	Chain	Residues		A	ton	ns			ZeroOcc	AltConf
2	А	1	Total 21	_		N 2	_	Р 1	0	0

• Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3)



(formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues		Ato	\mathbf{pms}			ZeroOcc	AltConf
2	Δ	1	Total	С	Η	Ν	0	0	0
5	A	1	39	24	4	5	6	0	0

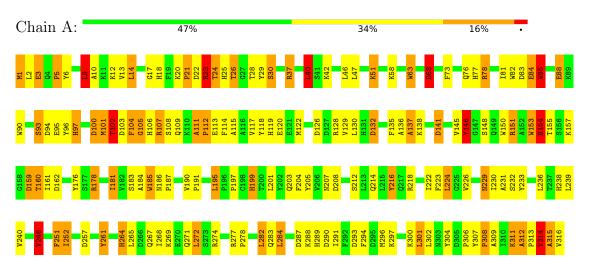
• Molecule 4 is water.

Mol	Chain	Residues	Α	toms		ZeroOcc	AltConf
4	А	238	Total 714	Н 476	O 238	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 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: THYMIDYLATE SYNTHASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	78.90Å 78.90Å 230.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 - 2.30	Depositor
Resolution (A)	65.52 - 2.18	EDS
% Data completeness	(Not available) $(15.00-2.30)$	Depositor
(in resolution range)	54.9(65.52-2.18)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 2.18 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D.	0.186 , (Not available)	Depositor
R, R_{free}	0.190 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	22.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 902.7	EDS
L-test for twinning ²	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: UMP, $\mathrm{CB3}$

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	Bo	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.16	5/2674~(0.2%)	2.04	94/3634~(2.6%)

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	А	0	4

 All (5) bond length outliers are listed below:

 Mol
 Chain
 Res
 Type
 Atoms
 Z
 Observed(Å)
 Ideal(Å)

10101	Cham	ICCS	- TADC	11001115	-		iucai(11)
1	А	84	GLU	CG-CD	5.43	1.60	1.51
1	А	63	TRP	CD1-NE1	-5.30	1.28	1.38
1	А	153	TRP	CG-CD2	-5.22	1.34	1.43
1	А	82	TRP	CG-CD2	-5.08	1.35	1.43
1	А	183	SER	CA-CB	-5.03	1.45	1.52

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	277	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	А	23	ARG	CA-CB-CG	10.12	135.66	113.40
1	А	201	LEU	CA-CB-CG	9.42	136.96	115.30
1	А	115	ALA	N-CA-C	-9.28	85.95	111.00
1	А	226	VAL	CG1-CB-CG2	-9.09	96.36	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	154	HIS	Sidechain
1	А	205	TYR	Sidechain
1	А	216	TYR	Sidechain
1	А	312	ALA	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	А	2590	532	2500	71	0
2	А	20	1	10	1	0
3	А	35	4	21	0	0
4	А	238	476	0	1	0
All	All	2883	1013	2531	71	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 14.

The worst 5 of 71 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:A:108:SER:HA	1:A:114:PHE:HB3	1.52	0.91
1:A:51:LYS:HB2	1:A:309:ALA:HB2	1.52	0.91
1:A:101:MET:SD	1:A:118:TYR:HA	2.13	0.88
1:A:24:THR:HB	1:A:316:VAL:HB	1.63	0.79
1:A:85:TRP:HZ2	1:A:195:LEU:HB2	1.48	0.77

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	А	314/316~(99%)	255 (81%)	40 (13%)	19 (6%)	1 0	

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	25	HIS
1	А	104	PHE
1	А	105	GLY
1	А	112	PRO
1	А	137	ALA

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 Outliers		
1	А	277/277~(100%)	227~(82%)	50 (18%)	1 1

5 of 50 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	181	ILE
1	А	229	ASN
1	А	311	LYS
1	А	195	LEU
1	А	212	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	76	GLN
1	А	174	HIS
1	А	207	ASN
1	А	303	ASN



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)

2 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	Chain	Chain	Chain	Chain	Res	Link	В	ond leng	gths	B	ond ang	gles
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2				
2	UMP	А	317	1	18,21,21	<mark>3.69</mark>	6 (33%)	21,31,31	1.66	3 (14%)				
3	CB3	А	318	-	30,37,37	2.18	10 (33%)	38,51,51	2.80	12 (31%)				

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
2	UMP	А	317	1	-	4/7/22/22	0/2/2/2
3	CB3	А	318	-	-	11/21/28/28	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	317	UMP	C6-N1	11.47	1.50	1.35

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
2	А	317	UMP	C6-C5	6.38	1.52	1.38
3	А	318	CB3	O4-C4	6.16	1.40	1.24
2	А	317	UMP	C4-N3	5.93	1.43	1.33
3	А	318	CB3	CP1-N10	4.63	1.50	1.46

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The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	А	318	CB3	C4A-C8A-N1	-9.97	118.18	123.60
3	А	318	CB3	C4A-C4-N3	-8.22	118.67	124.40
3	А	318	CB3	N1-C2-N3	-5.21	120.28	127.22
2	А	317	UMP	C6-N1-C2	-4.45	114.12	121.20
3	А	318	CB3	C4-N3-C2	3.87	122.08	115.93

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	317	UMP	O4'-C1'-N1-C6
3	А	318	CB3	CP2-CP1-N10-C9
3	А	318	CB3	C11-C-N-CA
3	А	318	CB3	CT-CA-N-C
3	А	318	CB3	O-C-C11-C12

There are no ring outliers.

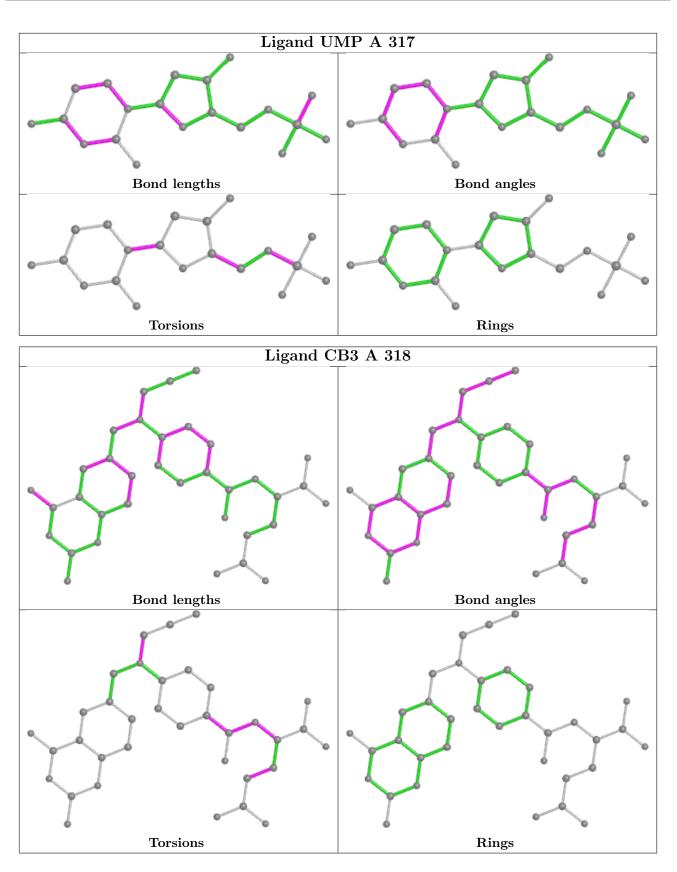
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	317	UMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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, 95^{th} 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	А	316/316~(100%)	-0.80	0 100 100	7, 15, 24, 30	0

There are no RSRZ outliers to report.

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.

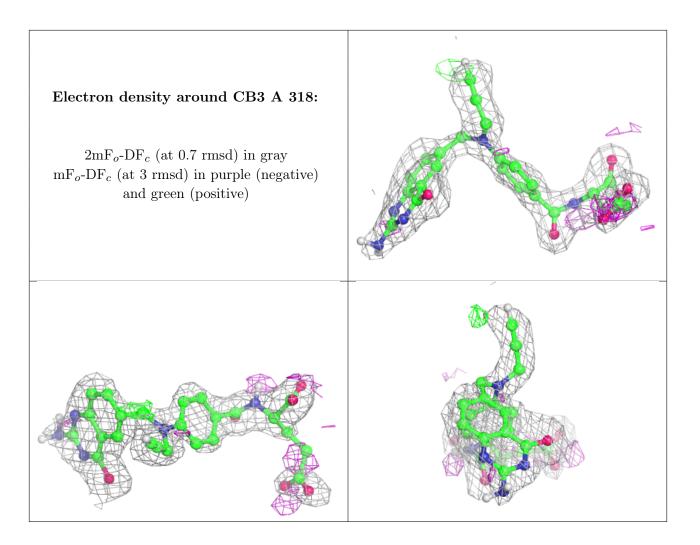
6.4 Ligands (i)

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, 95^{th} 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.

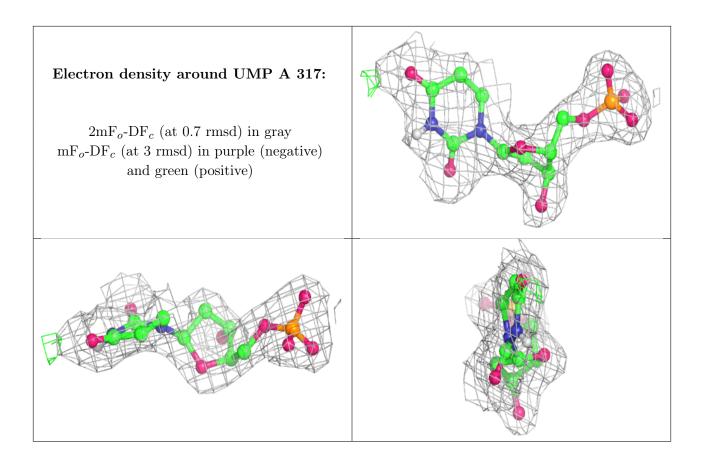
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	CB3	А	318	35/35	0.87	0.18	15,29,34,34	0
2	UMP	А	317	20/20	0.96	0.09	15,19,21,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers (i)

There are no such residues in this entry.

