



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 07:24 PM EST

PDB ID : 4FGT
Title : Allosteric peptidic inhibitor of human thymidylate synthase that stabilizes inactive conformation of the enzyme.
Authors : Tochowicz, A.; Finer-Moore, J.; Stroud, R.M.; Costi, M.P.
Deposited on : 2012-06-04
Resolution : 2.00 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 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

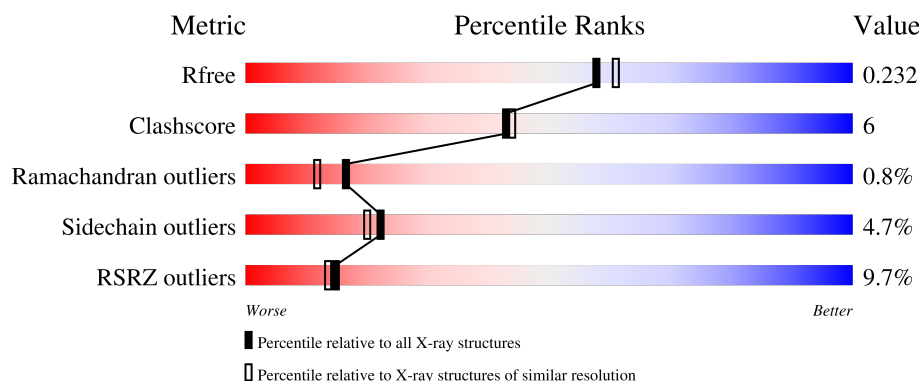
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	A	325	
2	D	4	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2326 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	A	267	2178	1394	378	391	15	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	LYS	engineered mutation	UNP P04818

- Molecule 2 is a protein called CG peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	4	41	27	6	7	1	0	1	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.81Å 95.81Å 83.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.76 – 2.00 27.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (27.76-2.00) 97.3 (27.76-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.229 0.209 , 0.232	Depositor DCC
R_{free} test set	1493 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2326	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 4.57% 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: CME, 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	1.27	7/2213 (0.3%)	1.03	3/2988 (0.1%)
2	D	0.92	0/44	1.76	1/58 (1.7%)
All	All	1.27	7/2257 (0.3%)	1.04	4/3046 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	TYR	CE2-CZ	6.49	1.47	1.38
1	A	178	ILE	CB-CG2	5.51	1.70	1.52
1	A	63	ALA	CA-CB	5.33	1.63	1.52
1	A	230	TYR	CE2-CZ	5.27	1.45	1.38
1	A	77	LYS	CD-CE	5.23	1.64	1.51
1	A	206	SER	CB-OG	5.15	1.49	1.42
1	A	135	TYR	CE2-CZ	5.11	1.45	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	MET	CG-SD-CE	-7.25	88.60	100.20
1	A	254	ASP	CB-CG-OD1	7.22	124.80	118.30
2	D	68	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	176	ARG	NE-CZ-NH1	-5.34	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2178	0	2160	26	1
2	D	41	0	39	2	1
3	A	15	0	0	0	0
4	A	92	0	0	0	0
All	All	2326	0	2199	27	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 6.

All (27) 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:195:CME:HB2	1:A:195:CME:HZ3	1.50	0.92
1:A:135:TYR:OH	1:A:196:HIS:ND1	2.07	0.87
1:A:186:ASP:HA	1:A:189:LEU:HD12	1.67	0.76
1:A:135:TYR:HH	1:A:196:HIS:HD1	1.32	0.75
1:A:195:CME:HE3	1:A:195:CME:H	1.54	0.71
1:A:152:ASP:OD2	1:A:154:SER:HB2	1.99	0.61
1:A:236:MET:HE3	1:A:291:PHE:CD2	2.35	0.60
1:A:195:CME:HB2	1:A:195:CME:CZ	2.27	0.60
1:A:260[A]:ASN:HD22	1:A:310:GLU:HB2	1.69	0.57
1:A:195:CME:H	1:A:195:CME:CE	2.19	0.55
1:A:236:MET:CE	1:A:291:PHE:CD2	2.90	0.54
1:A:102:SER:HA	1:A:106:VAL:O	2.09	0.53
1:A:142:PHE:CZ	2:D:67[B]:GLN:HB3	2.44	0.52
1:A:86:GLU:CD	1:A:104:LYS:HG2	2.31	0.51
1:A:148:ASP:HB3	1:A:151:SER:OG	2.13	0.48
1:A:148:ASP:CB	1:A:151:SER:OG	2.62	0.48
1:A:195:CME:HE3	1:A:195:CME:N	2.27	0.48
1:A:186:ASP:O	1:A:189:LEU:HB2	2.14	0.47
1:A:46:ARG:HD3	1:A:259:LEU:HD11	1.98	0.45
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.74	0.44
1:A:86:GLU:OE2	1:A:104:LYS:HG2	2.19	0.42
1:A:258:TYR:HB3	1:A:260[A]:ASN:OD1	2.19	0.42
1:A:260[A]:ASN:ND2	1:A:310:GLU:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD12	1:A:198:LEU:C	2.41	0.41
1:A:147:ARG:NH1	1:A:151:SER:HB3	2.36	0.41
1:A:236:MET:HE3	1:A:291:PHE:CG	2.56	0.41

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:144:ALA:O	2:D:69:TYR:OH[6_555]	2.17	0.03

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	262/325 (81%)	256 (98%)	5 (2%)	1 (0%)	30	27
2	D	3/4 (75%)	2 (67%)	0	1 (33%)	0	0
All	All	265/329 (80%)	258 (97%)	5 (2%)	2 (1%)	16	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
2	D	68	LEU

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	232/278 (84%)	223 (96%)	9 (4%)	27	27
2	D	5/4 (125%)	3 (60%)	2 (40%)	0	0
All	All	237/282 (84%)	226 (95%)	11 (5%)	22	21

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

Mol	Chain	Res	Type
1	A	82	LYS
1	A	104	LYS
1	A	107	LYS
1	A	126	ARG
1	A	148	ASP
1	A	150	GLU
1	A	154	SER
1	A	309	MET
1	A	311	MET
2	D	68	LEU
2	D	69	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	A	199	1	8,9,10	1.25	0	6,9,11	1.59	2 (33%)
1	CME	A	195	1	8,9,10	1.07	1 (12%)	6,9,11	1.23	1 (16%)

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	A	199	1	-	0/5/8/10	-
1	CME	A	195	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	CME	SD-SG	-2.25	1.87	2.03

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	CME	CZ-CE-SD	-2.37	105.48	113.39
1	A	195	CME	CE-SD-SG	2.28	113.45	103.46
1	A	199	CME	CB-CA-C	-2.06	105.20	110.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	195	CME	CZ-CE-SD-SG
1	A	195	CME	CE-SD-SG-CB
1	A	195	CME	SD-CE-CZ-OH

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	195	CME	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.41	0
3	SO4	A	402	-	4,4,4	0.39	0	6,6,6	0.42	0
3	SO4	A	401	-	4,4,4	0.48	0	6,6,6	1.18	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SO4	O4-S-O2	-2.22	97.97	109.56

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

6.1 Protein, DNA and RNA chains

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	265/325 (81%)	0.51	22 (8%) 19 17	27, 45, 91, 124	1 (0%)
2	D	4/4 (100%)	3.87	4 (100%) 0 0	58, 78, 101, 101	1 (25%)
All	All	269/329 (81%)	0.56	26 (9%) 15 13	27, 46, 93, 124	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	6.8
2	D	68	LEU	6.7
1	A	108	ILE	5.4
1	A	47	ALA	4.0
2	D	66	CYS	3.3
1	A	311	MET	3.2
2	D	69	TYR	3.1
1	A	154	SER	3.0
1	A	144	ALA	3.0
1	A	135	TYR	2.9
1	A	53	THR	2.9
1	A	48	ASP	2.7
1	A	106	VAL	2.7
1	A	143	GLY	2.7
1	A	189	LEU	2.7
1	A	109	TRP	2.5
1	A	152	ASP	2.5
2	D	67[A]	GLN	2.5
1	A	51	THR	2.4
1	A	156	GLN	2.4
1	A	126	ARG	2.3
1	A	310	GLU	2.2
1	A	188	PRO	2.2
1	A	102	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	2.0
1	A	147	ARG	2.0

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	A	199	10/11	0.86	0.14	28,31,43,45	0
1	CME	A	195	10/11	0.92	0.13	33,37,79,86	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(Å ²)	Q<0.9
3	SO4	A	402	5/5	0.83	0.10	75,76,78,78	0
3	SO4	A	403	5/5	0.87	0.09	79,80,82,83	0
3	SO4	A	401	5/5	0.93	0.11	59,59,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.