Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 08:46 AM EDT

PDB ID	:	1BQ2
Title	:	E. COLI THYMIDYLATE SYNTHASE MUTANT N177A
Authors	:	Reyes, C.L.; Sage, C.R.; Rutenber, E.E.; Finer-Moore, J.S.; Stroud, R.M.
Deposited on	:	1998-08-20
Resolution	:	2.20 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 (i)) were used in the production of this report:

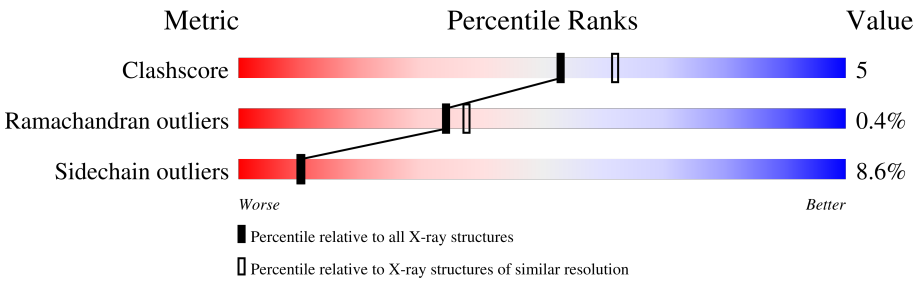
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	77% 19% •

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
2	PO4	A	603	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2803 atoms, of which 589 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.

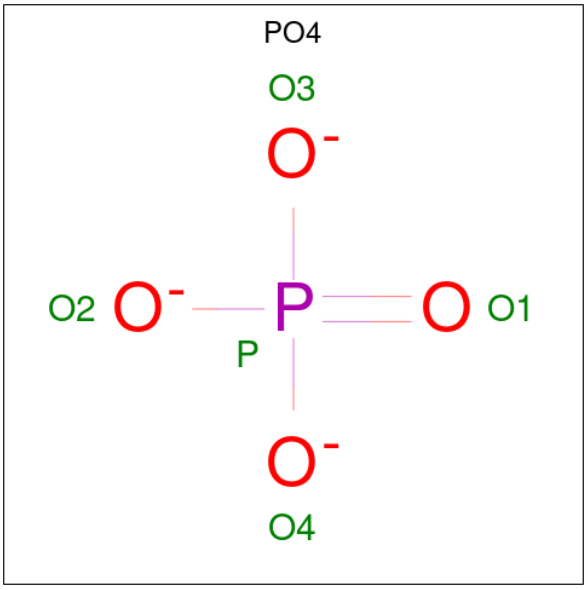
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	264	2612	1373	465	370	392	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	ALA	ASN	engineered mutation	UNP P0A884

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	62	186	124	62	0	0

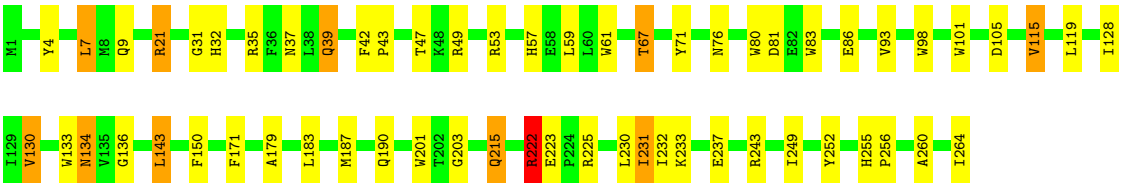
3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE

Chain A: 77% 19% •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	133.06Å 133.06Å 133.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.5 (8.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.172 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2803	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

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: PO4

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	0.87	0/2207	1.55	33/2996 (1.1%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	A	80	TRP	CD1-CG-CD2	8.53	113.13	106.30
1	A	133	TRP	CE2-CD2-CG	-8.28	100.68	107.30
1	A	61	TRP	CD1-CG-CD2	8.24	112.90	106.30
1	A	35	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	21	ARG	CA-CB-CG	8.12	131.27	113.40
1	A	80	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	101	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	98	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	201	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	201	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	61	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	83	TRP	CD1-CG-CD2	6.91	111.82	106.30
1	A	83	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	A	21	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	252	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	A	98	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	115	VAL	CG1-CB-CG2	-6.15	101.06	110.90
1	A	143	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	101	TRP	CG-CD2-CE3	6.06	139.35	133.90
1	A	101	TRP	CD1-CG-CD2	5.86	110.98	106.30
1	A	53	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	201	TRP	CG-CD2-CE3	5.76	139.09	133.90
1	A	222	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	4	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	A	243	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	243	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	21	ARG	CA-C-N	-5.34	105.45	117.20
1	A	230	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	61	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	187	MET	CG-SD-CE	5.16	108.45	100.20
1	A	67	THR	N-CA-CB	-5.08	100.64	110.30

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	A	2147	465	2081	23	0
2	A	5	0	0	0	0
3	A	62	124	0	3	0
All	All	2214	589	2081	23	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 5.

All (23) 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:215:GLN:HE21	1:A:215:GLN:H	1.42	0.65
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.64	0.62
1:A:134:ASN:HD22	1:A:136:GLY:N	2.06	0.53
1:A:115:VAL:HG21	1:A:130:VAL:HG12	1.93	0.50
1:A:86:GLU:H	1:A:86:GLU:CD	2.16	0.49
1:A:231:ILE:HD11	1:A:233:LYS:HG3	1.96	0.48
1:A:134:ASN:ND2	1:A:136:GLY:N	2.62	0.48
1:A:171:PHE:CE2	1:A:260:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HG2	1:A:255:HIS:CD2	2.48	0.48
1:A:190:GLN:HE22	1:A:232:ILE:HG21	1.78	0.47
1:A:119:LEU:HD23	1:A:128:ILE:HD13	1.96	0.47
1:A:42:PHE:HA	1:A:43:PRO:HD3	1.82	0.46
1:A:31:GLY:HA2	1:A:203:GLY:O	2.16	0.45
1:A:134:ASN:HD22	1:A:134:ASN:C	2.21	0.44
1:A:59:LEU:HD23	1:A:183:LEU:HD23	1.99	0.44
1:A:223:GLU:O	1:A:255:HIS:HE1	2.01	0.43
1:A:43:PRO:HD2	3:A:633:HOH:O	2.19	0.43
1:A:7:LEU:HG	1:A:32:HIS:CD2	2.54	0.43
1:A:179:ALA:HA	3:A:633:HOH:O	2.20	0.42
1:A:215:GLN:HE21	1:A:215:GLN:N	2.15	0.42
1:A:57:HIS:O	1:A:71:TYR:HE2	2.03	0.41
1:A:130:VAL:HG13	1:A:150:PHE:CE2	2.55	0.41
1:A:256:PRO:HB2	3:A:617:HOH:O	2.21	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	A	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	34 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL

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	232/232 (100%)	212 (91%)	20 (9%)	10 10

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	GLN
1	A	21	ARG
1	A	39	GLN
1	A	47	THR
1	A	49	ARG
1	A	67	THR
1	A	76	ASN
1	A	81	ASP
1	A	105	ASP
1	A	130	VAL
1	A	134	ASN
1	A	143	LEU
1	A	215	GLN
1	A	222	ARG
1	A	225	ARG
1	A	231	ILE
1	A	237	GLU
1	A	249	ILE
1	A	264	ILE

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

Mol	Chain	Res	Type
1	A	37	ASN
1	A	39	GLN
1	A	134	ASN
1	A	190	GLN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	255	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)

1 ligand is 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	$\#\|Z\| > 2$
2	PO4	A	603	-	4,4,4	2.64	2 (50%)	6,6,6	2.26	2 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	PO4	P-O1	4.14	1.60	1.50
2	A	603	PO4	P-O4	-2.08	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	603	PO4	O2-P-O1	-3.35	98.65	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	603	PO4	O3-P-O2	2.70	116.65	107.97

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.