Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 12:44 AM EDT

PDB ID	:	1BKP
Title	:	THERMOSTABLE THYMIDYLATE SYNTHASE A FROM BACILLUS SUBTILIS
Authors	:	Stout, T.J.; Schellenberger, U.; Santi, D.V.; Stroud, R.M.
Deposited on	:	1998-07-09
Resolution	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

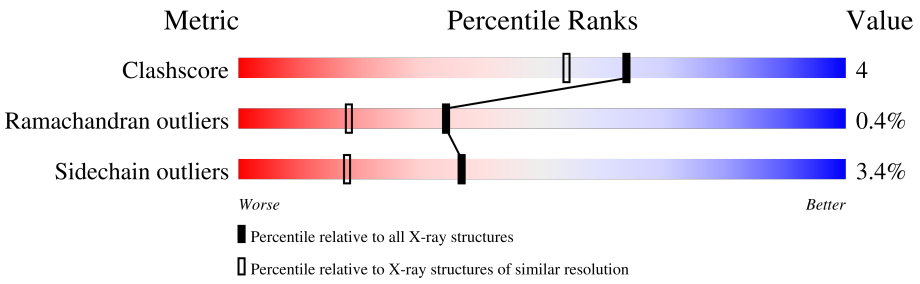
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	278	88% 9% •
1	B	278	86% 13% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4963 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	2307	1474	391	431	11	0	1	0
1	B	278	2307	1474	393	430	10	6	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	177	177	177	0	0
2	B	172	172	172	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.

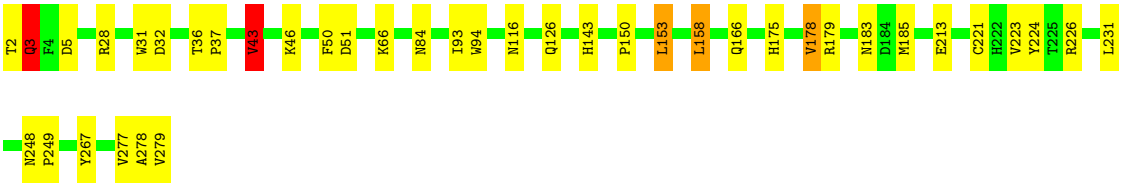
Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE A

Chain A:

• Molecule 1: THYMIDYLATE SYNTHASE A

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.94Å 81.63Å 64.79Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	48.30 – 1.70	Depositor
% Data completeness (in resolution range)	88.9 (48.30-1.70)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.151 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4963	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.19	9/2365 (0.4%)	1.16	7/3204 (0.2%)
1	B	1.18	3/2365 (0.1%)	1.08	7/3203 (0.2%)
All	All	1.19	12/4730 (0.3%)	1.12	14/6407 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	VAL	CB-CG2	-7.41	1.37	1.52
1	A	3	GLN	CB-CG	6.97	1.71	1.52
1	A	54	GLU	CB-CG	-6.74	1.39	1.52
1	B	267	TYR	CD1-CE1	6.41	1.49	1.39
1	A	221[A]	CYS	CB-SG	-6.23	1.71	1.82
1	A	221[B]	CYS	CB-SG	-6.23	1.71	1.82
1	A	216	PHE	CE1-CZ	5.64	1.48	1.37
1	A	276	GLU	CG-CD	5.51	1.60	1.51
1	A	236	GLU	CG-CD	5.50	1.60	1.51
1	A	276	GLU	CB-CG	5.11	1.61	1.52
1	A	257	PHE	CE2-CZ	5.08	1.47	1.37
1	B	3	GLN	CG-CD	5.06	1.62	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ARG	NE-CZ-NH1	21.14	130.87	120.30
1	A	237	ARG	NE-CZ-NH2	-16.88	111.86	120.30
1	A	124	VAL	CG1-CB-CG2	7.53	122.94	110.90
1	B	3	GLN	N-CA-C	7.28	130.66	111.00
1	B	43	VAL	CG1-CB-CG2	7.13	122.31	110.90
1	B	51	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	179	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	14	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	226	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	179	ARG	NE-CZ-NH2	-5.70	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	237	ARG	CD-NE-CZ	5.63	131.48	123.60
1	A	124	VAL	N-CA-CB	-5.49	99.43	111.50
1	B	158	LEU	CA-CB-CG	5.19	127.23	115.30

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	2307	0	2230	16	0
1	B	2307	0	2237	22	0
2	A	177	0	0	2	0
2	B	172	0	0	8	0
All	All	4963	0	4467	38	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 4.

All (38) 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:B:2:THR:HG21	2:B:559:HOH:O	1.78	0.83
1:B:46:LYS:HE2	2:B:543:HOH:O	1.82	0.79
1:A:3:GLN:HE21	1:A:5:ASP:H	1.43	0.67
1:A:93:ILE:HG13	1:A:94:TRP:CD1	2.30	0.66
1:B:175:HIS:CD2	1:B:213:GLU:H	2.18	0.62
1:B:93:ILE:HG13	1:B:94:TRP:CD1	2.41	0.56
1:B:126:GLN:HG3	2:B:484:HOH:O	2.06	0.55
1:B:3:GLN:NE2	2:B:657:HOH:O	2.39	0.54
1:B:2:THR:HG22	1:B:50:PHE:HD2	1.73	0.53
1:A:158:LEU:H	1:A:158:LEU:HD12	1.75	0.52
1:A:183:ASN:HD21	1:A:192:ASN:HD22	1.57	0.51
1:A:2:THR:O	1:A:3:GLN:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:HIS:HD2	1:B:213:GLU:H	1.60	0.50
1:B:185:MET:HB2	1:B:223:VAL:HG12	1.93	0.49
1:A:158:LEU:HD12	1:A:158:LEU:N	2.28	0.49
1:B:32:ASP:OD1	1:B:277:VAL:HB	2.13	0.48
1:A:237:ARG:HD2	2:A:595:HOH:O	2.12	0.48
1:B:3:GLN:HG3	1:B:5:ASP:H	1.79	0.47
1:A:126:GLN:HG3	2:A:429:HOH:O	2.15	0.46
1:A:93:ILE:HG13	1:A:94:TRP:HD1	1.77	0.46
1:A:276:GLU:H	1:A:276:GLU:CD	2.19	0.46
1:B:150:PRO:HA	1:B:153:LEU:HD22	1.99	0.45
1:A:171:HIS:HE1	2:B:507:HOH:O	2.00	0.45
1:B:278:ALA:O	1:B:279:VAL:C	2.55	0.44
1:B:175:HIS:HE1	2:B:663:HOH:O	2.01	0.44
1:B:31:TRP:CH2	1:B:224:TYR:HB3	2.53	0.44
1:B:36:THR:HB	1:B:37:PRO:HD2	2.00	0.43
1:B:43:VAL:HG12	1:B:221:CYS:HB2	2.00	0.43
1:B:248:ASN:HA	1:B:249:PRO:HD3	1.74	0.43
1:B:143:HIS:HD2	2:B:623:HOH:O	2.02	0.43
1:A:185:MET:HB2	1:A:223:VAL:HG12	2.01	0.42
1:A:43:VAL:HG21	1:A:46:LYS:HE3	2.01	0.42
1:B:3:GLN:HG3	1:B:5:ASP:N	2.33	0.42
1:A:129:TYR:CE2	1:A:133:GLN:HG3	2.56	0.41
1:A:248:ASN:HA	1:A:249:PRO:HD3	1.88	0.41
1:B:84:ASN:HB3	2:B:578:HOH:O	2.20	0.41
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.93	0.40
1:B:143:HIS:O	1:B:166:GLN:HA	2.22	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	A	277/278 (100%)	270 (98%)	6 (2%)	1 (0%)	34	18
1	B	276/278 (99%)	269 (98%)	6 (2%)	1 (0%)	34	18
All	All	553/556 (100%)	539 (98%)	12 (2%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	A	45	SER

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	253/253 (100%)	246 (97%)	7 (3%)	43	25
1	B	253/253 (100%)	243 (96%)	10 (4%)	31	13
All	All	506/506 (100%)	489 (97%)	17 (3%)	37	18

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	96	GLN
1	A	124	VAL
1	A	158	LEU
1	A	183	ASN
1	A	263	LYS
1	A	277	VAL
1	B	3	GLN
1	B	28	ARG
1	B	43	VAL
1	B	66	LYS
1	B	116	ASN
1	B	153	LEU
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	178	VAL
1	B	183	ASN
1	B	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	133	GLN
1	A	137	ASN
1	A	192	ASN
1	A	195	GLN
1	A	222	HIS
1	B	99	GLN
1	B	116	ASN
1	B	120	ASN
1	B	132	HIS
1	B	133	GLN
1	B	137	ASN
1	B	143	HIS
1	B	171	HIS
1	B	175	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)

There are no ligands in this entry.

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.