Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:57 am BST

PDB ID	:	1ST2
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF BACILLUS AMYLOLIQUEFACIENS SUBTILISIN AT 1.8 ANGSTROMS AND AN ANALYSIS OF THE STRUCTURAL CONSEQUENCES OF PEROXIDE INACTIVATION
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Deposited on	:	1990-03-21
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 following versions of software and data (see references ⓘ) were used in the production of this report:

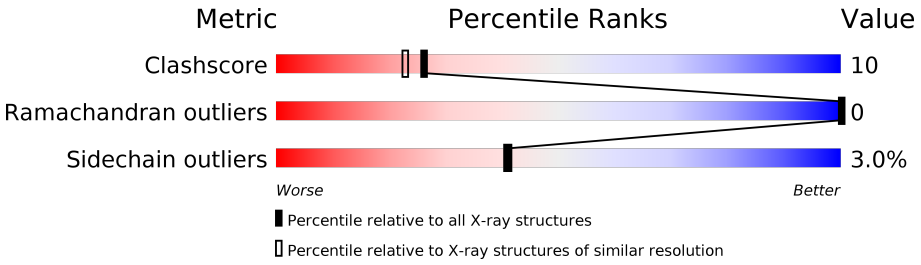
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 on 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	275	68% 27% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2064 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.

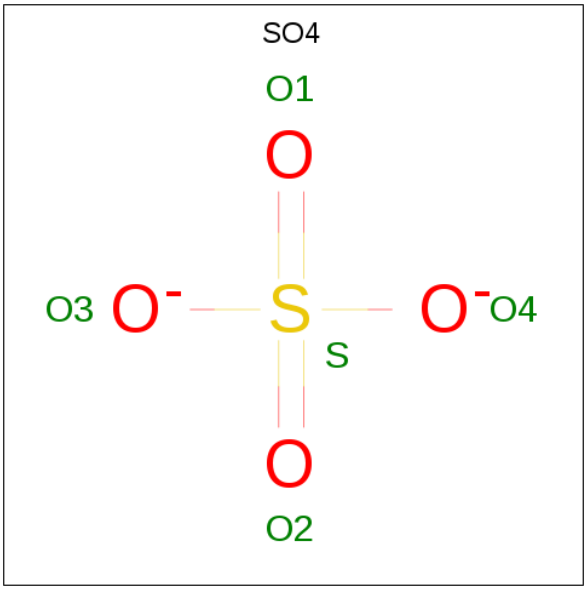
- Molecule 1 is a protein called SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	1941	1204	335	397	5	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	2	2	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		

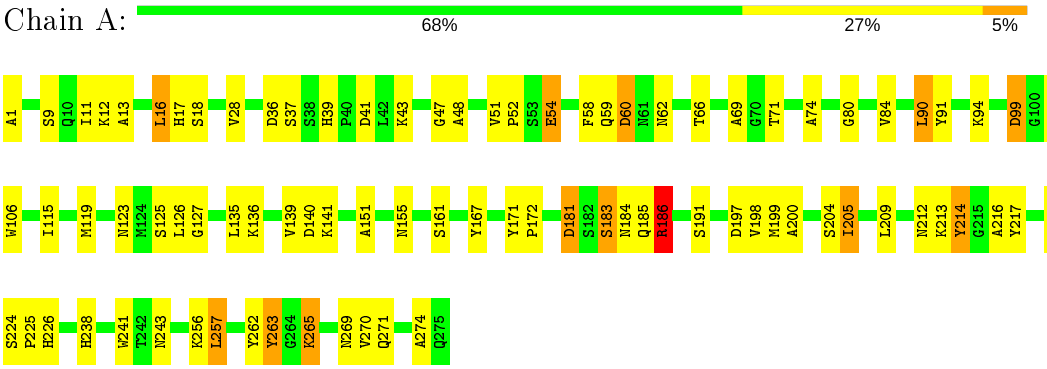
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: SUBTILISIN BPN'

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	39.30Å 72.80Å 75.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2064	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MHO, CA, 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	0.93	1/1949 (0.1%)	1.81	39/2658 (1.5%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	THR	N-CA	5.02	1.56	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	ASP	CB-CG-OD1	10.47	127.73	118.30
1	A	186	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	A	104	TYR	CB-CG-CD1	8.69	126.21	121.00
1	A	60	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	104	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	A	41	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	74	ALA	CB-CA-C	7.26	120.98	110.10
1	A	13	ALA	CB-CA-C	7.17	120.85	110.10
1	A	263	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	A	214	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	A	54	GLU	CG-CD-OE2	-6.98	104.34	118.30
1	A	186	ARG	CD-NE-CZ	-6.96	113.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	TYR	CB-CG-CD2	6.51	124.91	121.00
1	A	36	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	262	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	214	TYR	CB-CG-CD2	6.21	124.73	121.00
1	A	181	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	99	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	181	ASP	CB-CA-C	5.95	122.31	110.40
1	A	197	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	204	SER	N-CA-CB	5.90	119.35	110.50
1	A	265	LYS	CA-CB-CG	-5.89	100.44	113.40
1	A	185	GLN	O-C-N	-5.81	113.40	122.70
1	A	151	ALA	N-CA-CB	5.72	118.10	110.10
1	A	47	GLY	O-C-N	5.62	131.69	122.70
1	A	16	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	223	ALA	N-CA-CB	-5.56	102.31	110.10
1	A	28	VAL	CG1-CB-CG2	5.54	119.77	110.90
1	A	257	LEU	CA-C-N	5.51	127.22	116.20
1	A	200	ALA	CB-CA-C	5.50	118.34	110.10
1	A	54	GLU	CG-CD-OE1	5.49	129.28	118.30
1	A	48	ALA	CB-CA-C	5.36	118.13	110.10
1	A	198	VAL	CA-CB-CG1	5.23	118.75	110.90
1	A	217	TYR	CA-CB-CG	5.22	123.31	113.40
1	A	90	LEU	N-CA-CB	-5.19	100.03	110.40
1	A	9	SER	O-C-N	5.18	130.99	122.70
1	A	62	ASN	CB-CA-C	5.06	120.53	110.40
1	A	205	ILE	O-C-N	5.02	130.73	122.70
1	A	199	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain

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	1941	0	1897	40	1
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	116	0	0	4	0
All	All	2064	0	1897	40	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 10.

All (40) 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:135:LEU:O	1:A:139:VAL:HG23	1.75	0.86
1:A:205:ILE:O	1:A:216:ALA:HA	1.91	0.70
1:A:1:ALA:O	4:A:381:HOH:O	2.11	0.68
1:A:59:GLN:NE2	4:A:326:HOH:O	2.28	0.65
1:A:51:VAL:HG13	1:A:106:TRP:CZ3	2.33	0.64
1:A:136:LYS:NZ	1:A:140:ASP:OD2	2.32	0.63
1:A:181:ASP:OD1	1:A:183:SER:HB2	2.02	0.59
1:A:238:HIS:NE2	1:A:274:ALA:O	2.39	0.56
1:A:243:ASN:OD1	1:A:243:ASN:N	2.39	0.55
1:A:17:HIS:HE1	1:A:84:VAL:O	1.91	0.54
1:A:256:LYS:HD3	1:A:265:LYS:O	2.08	0.53
1:A:223:ALA:O	1:A:226:HIS:HB2	2.09	0.53
1:A:257:LEU:HB2	1:A:263:TYR:CD1	2.44	0.53
1:A:91:TYR:HB2	1:A:119:MHO:OD1	2.12	0.50
1:A:212:ASN:N	4:A:312:HOH:O	2.33	0.49
1:A:60:ASP:OD2	1:A:66:THR:OG1	2.20	0.49
1:A:123:ASN:ND2	1:A:125:SER:OG	2.38	0.48
1:A:37:SER:HB3	1:A:58:PHE:HB3	1.96	0.47
1:A:155:ASN:OD1	1:A:220:THR:N	2.32	0.47
1:A:224:SER:N	1:A:225:PRO:HD2	2.29	0.47
1:A:43:LYS:HE2	4:A:345:HOH:O	2.14	0.47
1:A:54:GLU:OE1	1:A:94:LYS:NZ	2.44	0.45
1:A:11:ILE:O	1:A:270:VAL:HG12	2.17	0.45
1:A:221:SER:O	1:A:225:PRO:CD	2.65	0.45
1:A:16:LEU:CD2	1:A:271:GLN:HA	2.46	0.45
1:A:238:HIS:HB3	1:A:241:TRP:CD1	2.52	0.45
1:A:171:TYR:HA	1:A:172:PRO:HD3	1.90	0.45
1:A:186:ARG:HD3	1:A:186:ARG:HH11	1.51	0.44
1:A:16:LEU:HD21	1:A:271:GLN:HA	2.00	0.43
1:A:126:LEU:HD12	1:A:126:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB3	1:A:225:PRO:HD3	2.01	0.43
1:A:69:ALA:HB1	1:A:90:LEU:HD21	2.00	0.42
1:A:184:ASN:HB3	1:A:257:LEU:HD22	2.01	0.42
1:A:126:LEU:HD12	1:A:126:LEU:O	2.20	0.42
1:A:39:HIS:HD2	1:A:209:LEU:O	2.04	0.41
1:A:51:VAL:HA	1:A:52:PRO:HD3	1.79	0.41
1:A:127:GLY:HA2	1:A:167:TYR:O	2.19	0.41
1:A:115:ILE:HD13	1:A:141:LYS:HG2	2.03	0.41
1:A:80:GLY:HA3	1:A:214:TYR:CZ	2.56	0.40
1:A:12:LYS:HD2	1:A:269:ASN:ND2	2.37	0.40

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:99:ASP:OD2	1:A:213:LYS:NZ[4_465]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	270/275 (98%)	260 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	202/202 (100%)	196 (97%)	6 (3%)	41 41

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	101	SER
1	A	104	TYR
1	A	161	SER
1	A	183	SER
1	A	191	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	25	ASN
1	A	123	ASN
1	A	206	GLN
1	A	271	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	MHO	A	119	1	7,8,9	1.46	1 (14%)	4,9,11	3.45	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MHO	A	222	1	7,8,9	1.56	1 (14%)	4,9,11	1.78	1 (25%)
1	MHO	A	124	1	7,8,9	1.32	1 (14%)	4,9,11	2.50	2 (50%)

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	MHO	A	119	1	-	2/6/7/9	-
1	MHO	A	222	1	-	4/6/7/9	-
1	MHO	A	124	1	-	1/6/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	MHO	OD1-SD	-3.62	1.40	1.50
1	A	119	MHO	OD1-SD	-3.01	1.42	1.50
1	A	124	MHO	OD1-SD	-2.98	1.42	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	MHO	OD1-SD-CE	5.59	117.57	106.25
1	A	124	MHO	OD1-SD-CE	4.20	114.76	106.25
1	A	119	MHO	CE-SD-CG	3.29	105.21	97.71
1	A	222	MHO	OD1-SD-CG	2.89	114.00	106.03
1	A	124	MHO	CE-SD-CG	2.52	103.44	97.71
1	A	119	MHO	OD1-SD-CG	-2.33	99.59	106.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	119	MHO	CB-CG-SD-OD1
1	A	222	MHO	O-C-CA-CB
1	A	222	MHO	CB-CG-SD-CE
1	A	222	MHO	CB-CG-SD-OD1
1	A	124	MHO	O-C-CA-CB
1	A	119	MHO	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
1	A	222	MHO	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	119	MHO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	278	-	4,4,4	0.66	0	6,6,6	0.39	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.