



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1Q5P / pdb_00001q5p
Title : S156E/S166D variant of Bacillus lentus subtilisin
Authors : Bott, R.R.; Chan, G.; Domingo, B.; Ganshaw, G.; Hsia, C.Y.; Knapp, M.;
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Deposited on : 2003-08-08
Resolution : 1.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

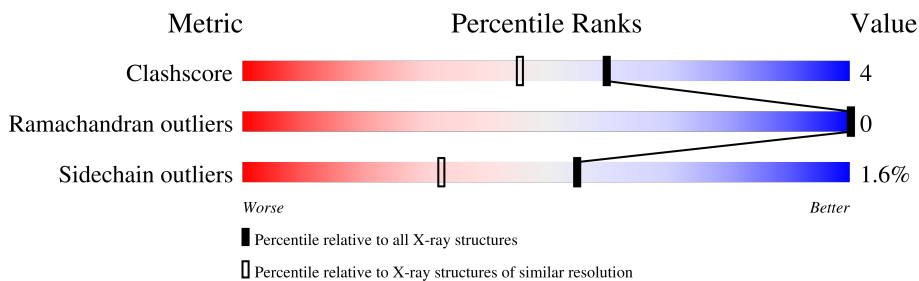
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2005 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 Serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	1895	1161	346	384	4	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

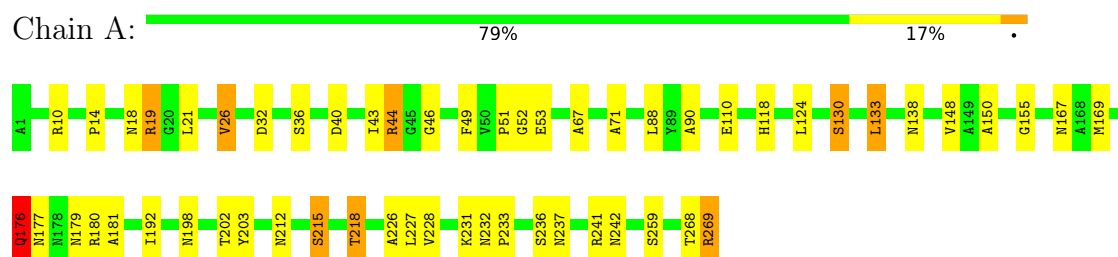
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total 103	O 103	0	0

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: Serine protease



4 Data and refinement statistics

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	53.45Å 61.50Å 75.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	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	2005	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: SO4, SEB, CA

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	1.18	1/1912 (0.1%)	2.09	61/2610 (2.3%)

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	218	THR	CA-CB	6.93	1.60	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	CD-NE-CZ	21.48	154.47	124.40
1	A	180	ARG	NE-CZ-NH1	11.66	133.16	121.50
1	A	18	ASN	CB-CG-ND2	10.59	132.29	116.40
1	A	19	ARG	NE-CZ-NH2	-9.27	110.86	119.20
1	A	198	ASN	CA-C-O	-8.84	111.31	121.65
1	A	179	ASN	OD1-CG-ND2	8.43	131.03	122.60
1	A	138	ASN	OD1-CG-ND2	8.09	130.69	122.60
1	A	52	GLY	CA-C-N	7.92	131.56	122.85
1	A	52	GLY	C-N-CA	7.92	131.56	122.85
1	A	180	ARG	NH1-CZ-NH2	-7.29	109.82	119.30
1	A	259	SER	CA-CB-OG	-7.21	96.68	111.10
1	A	232	ASN	O-C-N	7.11	127.77	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLN	CB-CG-CD	6.78	124.12	112.60
1	A	43	ILE	CA-C-O	-6.29	113.08	120.75
1	A	236	SER	CA-C-N	6.26	128.99	120.54
1	A	236	SER	C-N-CA	6.26	128.99	120.54
1	A	242	ASN	CB-CG-ND2	-6.23	107.06	116.40
1	A	44	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	14	PRO	CA-C-N	6.20	128.58	120.28
1	A	14	PRO	C-N-CA	6.20	128.58	120.28
1	A	237	ASN	CA-CB-CG	6.16	118.76	112.60
1	A	155	GLY	CA-C-N	6.16	131.61	121.39
1	A	155	GLY	C-N-CA	6.16	131.61	121.39
1	A	130	SER	CA-C-O	-6.03	112.84	120.20
1	A	10	ARG	NH1-CZ-NH2	-5.95	111.57	119.30
1	A	36	SER	CA-CB-OG	-5.94	99.22	111.10
1	A	19	ARG	NH1-CZ-NH2	5.89	126.96	119.30
1	A	26	VAL	CA-C-O	-5.87	114.26	120.48
1	A	241	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	A	242	ASN	OD1-CG-ND2	5.76	128.36	122.60
1	A	192	ILE	N-CA-CB	-5.69	101.84	111.23
1	A	49	PHE	O-C-N	5.68	129.60	122.22
1	A	71	ALA	N-CA-C	5.65	119.28	111.71
1	A	228	VAL	CA-C-O	-5.61	115.12	120.95
1	A	53	GLU	N-CA-CB	5.59	118.06	110.79
1	A	181	ALA	CB-CA-C	5.55	119.15	109.65
1	A	10	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	198	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	169	MET	CA-C-N	5.49	129.72	122.30
1	A	169	MET	C-N-CA	5.49	129.72	122.30
1	A	198	ASN	O-C-N	5.47	129.15	122.58
1	A	202	THR	CA-C-O	5.46	127.51	121.56
1	A	18	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	32	ASP	N-CA-CB	-5.44	103.96	109.51
1	A	44	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	A	242	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	118	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	212	ASN	O-C-N	5.23	129.65	123.27
1	A	177	ASN	O-C-N	5.23	129.58	122.37
1	A	167	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	227	LEU	CA-C-O	-5.20	115.36	120.82
1	A	51	PRO	CA-C-N	-5.17	114.39	122.51
1	A	51	PRO	C-N-CA	-5.17	114.39	122.51
1	A	71	ALA	N-CA-CB	-5.15	103.62	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLU	CB-CA-C	-5.15	103.70	111.27
1	A	10	ARG	O-C-N	5.13	127.36	122.07
1	A	18	ASN	CB-CG-OD1	-5.12	110.56	120.80
1	A	269	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	133	LEU	N-CA-CB	-5.07	102.66	110.01
1	A	203	TYR	O-C-N	5.05	125.38	121.85
1	A	40	ASP	CA-CB-CG	-5.02	107.58	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	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	1895	0	1843	16	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	103	0	0	2	0
All	All	2005	0	1843	16	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 (16) 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:SEB:HJ	4:A:339:HOH:O	1.27	1.29
1:A:176:GLN:HE21	1:A:176:GLN:H	1.26	0.83
1:A:215:SEB:OG	1:A:215:SEB:HH1	1.80	0.78
1:A:176:GLN:H	1:A:176:GLN:NE2	1.94	0.61
1:A:130:SER:HB3	1:A:133:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG12	1:A:218:THR:HG23	1.85	0.58
1:A:150:ALA:HB3	1:A:215:SEB:HI1	1.87	0.56
1:A:215:SEB:CJ	4:A:339:HOH:O	2.12	0.51
1:A:21:LEU:CD1	1:A:268:THR:HB	2.41	0.49
1:A:231:LYS:HE3	1:A:268:THR:O	2.12	0.49
1:A:26:VAL:HG11	1:A:226:ALA:HA	1.97	0.47
1:A:46:GLY:HA3	1:A:90:ALA:O	2.15	0.45
1:A:44:ARG:HH21	1:A:44:ARG:HD2	1.41	0.43
1:A:67:ALA:HB1	1:A:88:LEU:HD21	2.00	0.43
1:A:124:LEU:C	1:A:124:LEU:HD12	2.45	0.42
1:A:231:LYS:C	1:A:233:PRO:HD3	2.45	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	266/269 (99%)	258 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	192/192 (100%)	189 (98%)	3 (2%)	55 33

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	110	GLU
1	A	176	GLN

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

Mol	Chain	Res	Type
1	A	115	ASN
1	A	138	ASN
1	A	167	ASN
1	A	176	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	SEB	A	215	1	15,16,17	1.67	1 (6%)	16,21,23	4.65	12 (75%)

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	SEB	A	215	1	-	3/10/13/15	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	SEB	CJ-CI2	5.00	1.49	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	SEB	CE-CZ-CH1	-7.27	111.79	120.56
1	A	215	SEB	CI1-CJ-CI2	7.22	129.75	119.87
1	A	215	SEB	CH1-CZ-CH2	7.19	128.92	118.23
1	A	215	SEB	OG-CB-CA	7.06	116.27	107.63
1	A	215	SEB	CJ-CI2-CH2	-5.36	113.62	120.24
1	A	215	SEB	CJ-CI1-CH1	-5.15	113.88	120.24
1	A	215	SEB	CB-OG-SD	-4.97	108.60	119.30
1	A	215	SEB	OD2-SD-CE	-4.38	99.04	108.71
1	A	215	SEB	OG-SD-CE	3.57	114.01	104.18
1	A	215	SEB	CI2-CH2-CZ	-3.37	115.87	120.61
1	A	215	SEB	OD1-SD-CE	2.77	114.82	108.71
1	A	215	SEB	CI1-CH1-CZ	-2.11	117.65	120.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	215	SEB	SD-CE-CZ-CH1
1	A	215	SEB	CB-OG-SD-OD1
1	A	215	SEB	SD-CE-CZ-CH2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	215	SEB	4	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
2	SO4	A	270	-	4,4,4	0.77	0	6,6,6	0.19	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 [i](#)

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.