



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:57 AM GMT

PDB ID : 3RST
Title : Crystal structure of Bacillus subtilis signal peptide peptidase A
Authors : Nam, S.E.; Paetzel, M.
Deposited on : 2011-05-02
Resolution : 2.37 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

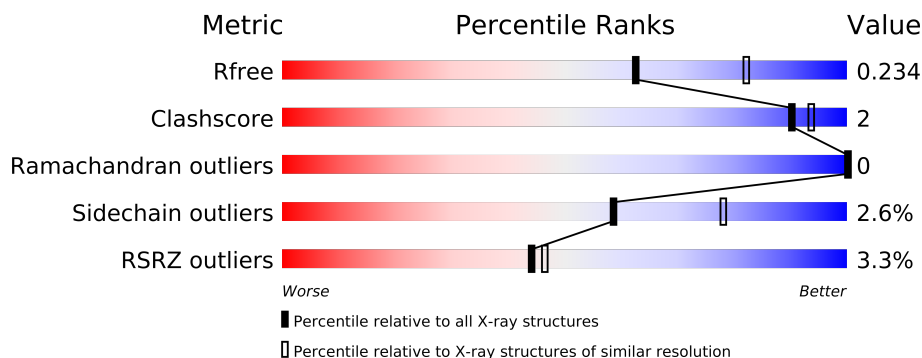
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.37 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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
1	B	240	
1	C	240	
1	D	240	
1	E	240	
1	F	240	
1	G	240	
1	H	240	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13957 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Signal peptide peptidase sppA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	1	0
			1726	1084	288	345	9			
1	B	223	Total	C	N	O	S	0	0	0
			1699	1069	286	335	9			
1	C	229	Total	C	N	O	S	0	0	0
			1740	1092	291	348	9			
1	D	223	Total	C	N	O	S	0	0	0
			1687	1058	282	338	9			
1	E	223	Total	C	N	O	S	12	1	0
			1701	1068	286	338	9			
1	F	226	Total	C	N	O	S	5	1	0
			1706	1071	282	343	10			
1	G	226	Total	C	N	O	S	7	1	0
			1714	1076	289	340	9			
1	H	226	Total	C	N	O	S	0	0	0
			1727	1086	290	342	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
B	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
C	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
D	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
E	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
F	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
G	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
H	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525

- Molecule 2 is water.

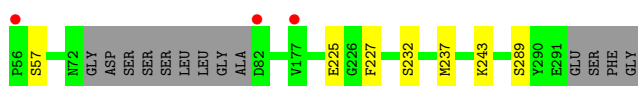
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total 45	O 45	0	0
2	B	18	Total 18	O 18	0	0
2	C	33	Total 33	O 33	0	0
2	D	23	Total 23	O 23	0	0
2	E	27	Total 27	O 27	0	0
2	F	46	Total 46	O 46	0	0
2	G	35	Total 35	O 35	0	0
2	H	30	Total 30	O 30	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Signal peptide peptidase sppA

Chain A: 



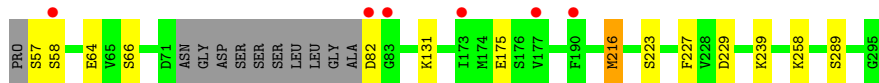
- Molecule 1: Signal peptide peptidase sppA

Chain B: 



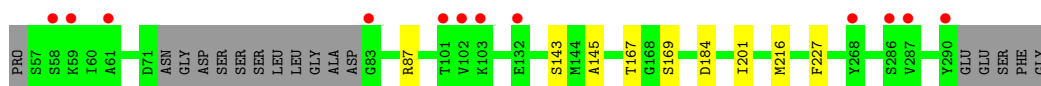
- Molecule 1: Signal peptide peptidase sppA

Chain C: 



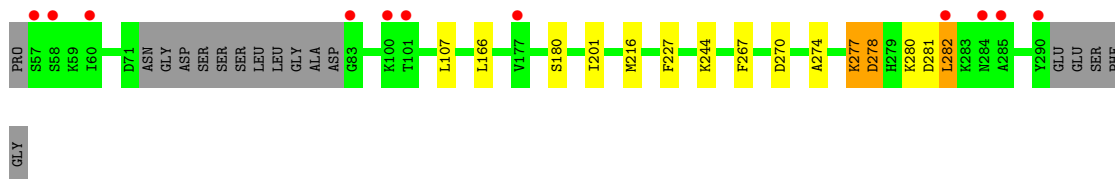
- Molecule 1: Signal peptide peptidase sppA

Chain D: 



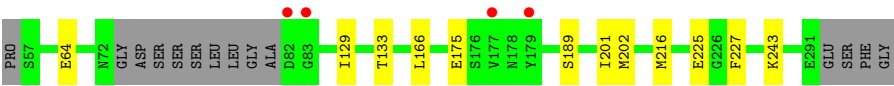
- Molecule 1: Signal peptide peptidase sppA

Chain E: 



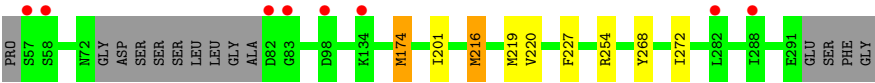
- Molecule 1: Signal peptide peptidase sppA

Chain F: 



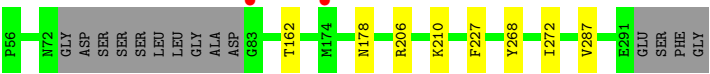
● Molecule 1: Signal peptide peptidase sppA

Chain G:



● Molecule 1: Signal peptide peptidase sppA

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.78Å 131.07Å 207.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.37 40.65 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.37) 98.2 (40.65-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.33 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.241 0.201 , 0.234	Depositor DCC
R_{free} test set	4806 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 96456 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13957	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.50	0/1752	0.59	0/2350
1	B	0.43	0/1721	0.55	0/2307
1	C	0.49	0/1763	0.57	0/2364
1	D	0.49	0/1709	0.55	0/2293
1	E	0.51	0/1729	0.56	0/2317
1	F	0.53	0/1733	0.58	0/2327
1	G	0.49	0/1743	0.59	0/2337
1	H	0.51	0/1750	0.59	0/2344
All	All	0.49	0/13900	0.57	0/18639

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	0	3	0
1	B	1699	0	0	3	0
1	C	1740	0	0	3	0
1	D	1687	0	0	3	0
1	E	1701	0	11	7	0
1	F	1706	0	9	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1714	0	9	4	0
1	H	1727	0	0	2	0
2	A	45	0	0	0	0
2	B	18	0	0	1	0
2	C	33	0	0	0	0
2	D	23	0	0	0	0
2	E	27	0	0	0	0
2	F	46	0	0	0	0
2	G	35	0	0	0	0
2	H	30	0	0	0	0
All	All	13957	0	29	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:281:ASP:C	1:E:282:LEU:CD2	2.14	1.15
1:G:201:ILE:CD1	1:G:216:MET:CE	2.46	0.93
1:E:282:LEU:N	1:E:282:LEU:CD2	2.34	0.87
1:E:281:ASP:O	1:E:282:LEU:CD2	2.33	0.76
1:A:225:GLU:OE2	1:A:243:LYS:NZ	2.36	0.59
1:E:277:LYS:CD	1:E:277:LYS:O	2.51	0.58
1:H:178:ASN:ND2	1:H:206:ARG:O	2.38	0.56
1:F:201:ILE:CD1	1:F:216:MET:CE	2.85	0.55
1:C:64:GLU:OE2	1:D:87:ARG:NH1	2.41	0.53
1:E:274:ALA:O	1:E:278:ASP:N	2.42	0.53
1:D:145:ALA:O	1:D:167:THR:OG1	2.29	0.51
1:G:174:MET:CE	1:G:220:VAL:CG2	2.90	0.50
1:F:225:GLU:OE2	1:F:243:LYS:NZ	2.46	0.49
1:F:166:LEU:CD1	1:G:219:MET:CE	2.91	0.48
1:C:229:ASP:OD1	1:C:239:LYS:NZ	2.46	0.48
1:B:147:SER:OG	2:B:307:HOH:O	2.20	0.48
1:E:201:ILE:CD1	1:E:216:MET:CE	2.92	0.47
1:C:216:MET:CE	1:C:216:MET:CA	2.92	0.47
1:G:268:TYR:CZ	1:G:272:ILE:CD1	2.97	0.47
1:D:201:ILE:CD1	1:D:216:MET:CE	2.93	0.46
1:A:232:SER:OG	1:A:237:MET:O	2.35	0.45
1:B:99:ASP:OD1	1:B:101:THR:OG1	2.36	0.43
1:B:229:ASP:OD1	1:B:239:LYS:NZ	2.52	0.42
1:E:267:PHE:N	1:E:270:ASP:OD2	2.53	0.41
1:A:57:SER:OG	1:A:57:SER:O	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:129:ILE:O	1:F:133:THR:OG1	2.39	0.40
1:H:268:TYR:CZ	1:H:272:ILE:CD1	3.05	0.40

There are no symmetry-related clashes.

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	224/240 (93%)	219 (98%)	5 (2%)	0	100	100
1	B	219/240 (91%)	212 (97%)	7 (3%)	0	100	100
1	C	225/240 (94%)	219 (97%)	6 (3%)	0	100	100
1	D	219/240 (91%)	213 (97%)	6 (3%)	0	100	100
1	E	220/240 (92%)	213 (97%)	7 (3%)	0	100	100
1	F	223/240 (93%)	218 (98%)	5 (2%)	0	100	100
1	G	223/240 (93%)	218 (98%)	5 (2%)	0	100	100
1	H	222/240 (92%)	215 (97%)	7 (3%)	0	100	100
All	All	1775/1920 (92%)	1727 (97%)	48 (3%)	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	185/201 (92%)	183 (99%)	2 (1%)	84	94
1	B	184/201 (92%)	183 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	188/201 (94%)	177 (94%)	11 (6%)	28	39
1	D	180/201 (90%)	176 (98%)	4 (2%)	64	83
1	E	184/201 (92%)	175 (95%)	9 (5%)	35	50
1	F	183/201 (91%)	179 (98%)	4 (2%)	64	83
1	G	184/201 (92%)	179 (97%)	5 (3%)	57	77
1	H	188/201 (94%)	184 (98%)	4 (2%)	66	84
All	All	1476/1608 (92%)	1436 (97%)	40 (3%)	59	77

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	PHE
1	A	289	SER
1	B	227	PHE
1	C	57	SER
1	C	58	SER
1	C	66	SER
1	C	82	ASP
1	C	131	LYS
1	C	175	GLU
1	C	216	MET
1	C	223	SER
1	C	227	PHE
1	C	258	LYS
1	C	289	SER
1	D	143	SER
1	D	169	SER
1	D	184	ASP
1	D	227	PHE
1	E	107	LEU
1	E	166	LEU
1	E	180	SER
1	E	227	PHE
1	E	244	LYS
1	E	277	LYS
1	E	278	ASP
1	E	280	LYS
1	E	282	LEU
1	F	64	GLU
1	F	175	GLU

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Mol	Chain	Res	Type
1	F	189	SER
1	F	227	PHE
1	G	174	MET
1	G	216	MET
1	G	227	PHE
1	G	254[A]	ARG
1	G	254[B]	ARG
1	H	162	THR
1	H	210	LYS
1	H	227	PHE
1	H	287	VAL

Some 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 chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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	227/240 (94%)	0.02	3 (1%) 74 77	26, 38, 60, 77	0
1	B	223/240 (92%)	0.18	13 (5%) 22 24	32, 50, 89, 105	0
1	C	229/240 (95%)	0.06	6 (2%) 53 55	29, 43, 63, 74	0
1	D	223/240 (92%)	0.31	12 (5%) 25 27	34, 55, 102, 112	0
1	E	223/240 (92%)	0.23	11 (4%) 28 30	27, 50, 111, 169	2 (0%)
1	F	226/240 (94%)	-0.13	4 (1%) 65 67	27, 40, 64, 81	1 (0%)
1	G	226/240 (94%)	-0.00	8 (3%) 42 44	27, 45, 81, 101	1 (0%)
1	H	226/240 (94%)	-0.08	2 (0%) 81 83	27, 43, 72, 84	0
All	All	1803/1920 (93%)	0.07	59 (3%) 44 46	26, 45, 82, 169	4 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	LEU	6.0
1	G	82	ASP	5.7
1	E	57	SER	5.0
1	D	83	GLY	4.6
1	D	287	VAL	4.4
1	G	58	SER	4.2
1	G	288	ILE	3.9
1	E	58	SER	3.8
1	F	82	ASP	3.8
1	B	280	LYS	3.7
1	D	58	SER	3.5
1	C	83	GLY	3.3
1	B	57	SER	3.2
1	D	101	THR	3.1
1	B	58	SER	3.1
1	E	284	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	3.1
1	D	290	TYR	3.0
1	B	281	ASP	3.0
1	E	285	ALA	3.0
1	E	290	TYR	2.9
1	B	134	LYS	2.9
1	D	102	VAL	2.8
1	C	82	ASP	2.7
1	C	58	SER	2.7
1	A	177	VAL	2.7
1	F	83	GLY	2.7
1	E	83	GLY	2.6
1	G	57	SER	2.6
1	B	101	THR	2.6
1	E	101	THR	2.5
1	A	56	PRO	2.5
1	B	284	ASN	2.5
1	G	83	GLY	2.4
1	H	83	GLY	2.4
1	A	82	ASP	2.4
1	G	134	LYS	2.4
1	F	177	VAL	2.4
1	H	174	MET	2.4
1	D	286	SER	2.3
1	D	59	LYS	2.3
1	E	100	LYS	2.3
1	E	177	VAL	2.3
1	B	131	LYS	2.3
1	F	179	TYR	2.2
1	E	60	ILE	2.2
1	B	100	LYS	2.2
1	B	177	VAL	2.2
1	C	177	VAL	2.2
1	C	173	ILE	2.1
1	G	98	ASP	2.1
1	C	190	PHE	2.1
1	B	190	PHE	2.1
1	G	282	LEU	2.1
1	B	236	GLY	2.1
1	D	103	LYS	2.1
1	D	61	ALA	2.1
1	D	268	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	132	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.