



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:40 AM UTC

PDB ID : 7DD0 / pdb_00007dd0
Title : Crystal structure of the N-terminal domain of TagH from Bacillus subtilis
Authors : Ko, T.P.; Yang, C.S.; Wang, Y.C.; Chen, Y.
Deposited on : 2020-10-27
Resolution : 2.70 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 ⓘ 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

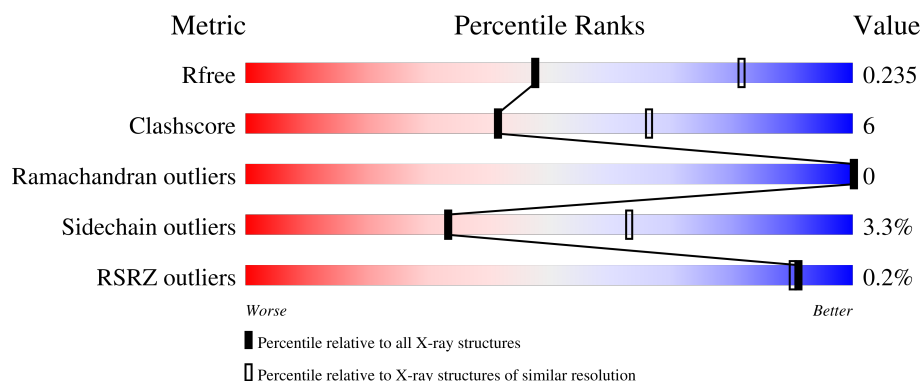
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	 71% 16% 13%
1	B	280	 74% 19% 7%
1	C	280	 69% 20% 10%
1	D	280	 71% 15% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8314 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 Teichoic acids export ATP-binding protein TagH.

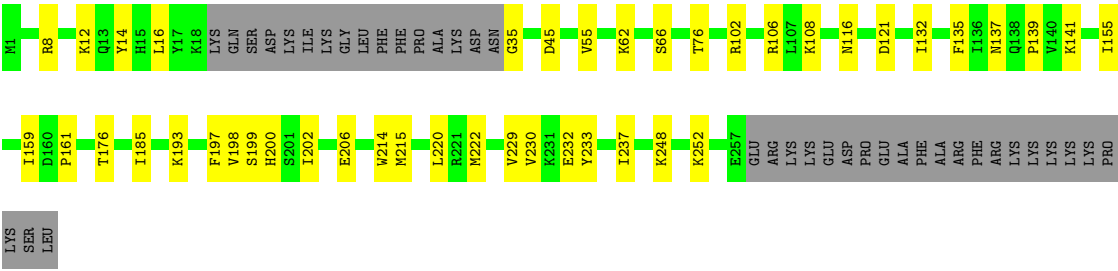
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1954	1245	329	367	13			
1	B	260	Total	C	N	O	S	0	0	0
			2088	1335	351	390	12			
1	C	252	Total	C	N	O	S	0	0	0
			2022	1290	339	380	13			
1	D	241	Total	C	N	O	S	0	0	0
			1929	1233	321	362	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total	O	0	0
			104	104		
2	B	69	Total	O	0	0
			69	69		
2	C	80	Total	O	0	0
			80	80		
2	D	68	Total	O	0	0
			68	68		

- Molecule 1: Teichoic acids export ATP-binding protein TagH





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.73Å 90.67Å 91.21Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	19.73 – 2.70 19.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.73-2.70) 98.3 (19.73-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.71Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.186 , 0.235 0.186 , 0.235	Depositor DCC
R_{free} test set	1986 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k 0.016 for -h,-l,-k 0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8314	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.18	0/1988	0.45	0/2663
1	B	0.18	0/2127	0.49	0/2849
1	C	0.19	0/2059	0.46	0/2759
1	D	0.21	0/1964	0.46	0/2633
All	All	0.19	0/8138	0.47	0/10904

There are no bond length outliers.

There are no bond angle outliers.

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	1954	0	1964	23	0
1	B	2088	0	2103	26	0
1	C	2022	0	2022	32	0
1	D	1929	0	1935	24	0
2	A	104	0	0	0	0
2	B	69	0	0	4	0
2	C	80	0	0	2	0
2	D	68	0	0	0	0
All	All	8314	0	8024	103	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 6.

All (103) 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:C:9:ASN:OD1	1:C:41:ASN:ND2	2.18	0.76
1:C:106:ARG:HG3	1:C:119:ILE:HG21	1.70	0.72
1:A:108:LYS:HE2	1:A:112:MET:HE3	1.71	0.71
1:A:59:GLY:O	1:A:259:ARG:NH2	2.28	0.65
1:C:59:GLY:O	1:C:259:ARG:NH2	2.22	0.64
1:C:222:MET:HE1	1:C:232:GLU:HG2	1.82	0.61
1:C:215:MET:HE2	1:C:220:LEU:HD13	1.83	0.61
1:B:40:ARG:HH22	1:B:261:LYS:HG3	1.64	0.61
1:B:239:TRP:HA	1:B:242:LYS:HZ1	1.65	0.60
1:D:215:MET:HE2	1:D:220:LEU:HD13	1.84	0.60
1:B:215:MET:HE2	1:B:220:LEU:HD13	1.85	0.58
1:D:8:ARG:NH2	1:D:45:ASP:OD1	2.33	0.58
1:B:109:CYS:HB3	1:B:114:LEU:HD12	1.86	0.57
1:C:106:ARG:NH1	1:C:120:ASP:OD1	2.35	0.56
1:A:155:ILE:O	1:A:159:ILE:HG12	2.06	0.56
1:B:141:LYS:NZ	2:B:302:HOH:O	2.37	0.56
1:C:237:ILE:O	1:C:241:ASN:ND2	2.30	0.56
1:B:239:TRP:HA	1:B:242:LYS:NZ	2.21	0.55
1:A:124:ASP:HA	1:A:127:VAL:HG22	1.88	0.55
1:B:132:ILE:O	1:B:135:PHE:HB2	2.06	0.55
1:D:66:SER:HB2	1:D:198:VAL:HG21	1.89	0.55
1:C:258:GLU:O	1:C:261:LYS:HG3	2.06	0.55
1:C:225:GLU:OE1	1:C:228:THR:N	2.35	0.54
1:C:131:GLU:O	1:C:150:ARG:NH1	2.41	0.54
1:B:161:PRO:O	1:B:193:LYS:HD2	2.08	0.54
1:C:181:CYS:O	1:C:185:ILE:HG12	2.09	0.53
1:D:155:ILE:O	1:D:159:ILE:HG12	2.09	0.53
1:D:214:TRP:HZ3	1:D:232:GLU:HG3	1.74	0.53
1:A:42:VAL:HG21	1:A:65:MET:HE3	1.89	0.53
1:A:45:ASP:O	1:A:211:ARG:NH1	2.39	0.53
1:B:10:VAL:HG13	1:B:75:PRO:HB3	1.91	0.52
1:C:263:ASP:HB3	1:C:269:ARG:HH12	1.74	0.52
1:A:215:MET:HE2	1:A:220:LEU:HD13	1.92	0.52
1:D:233:TYR:O	1:D:237:ILE:HG12	2.11	0.51
1:D:161:PRO:O	1:D:193:LYS:HD2	2.11	0.50
1:A:254:GLU:O	1:A:258:GLU:HG2	2.12	0.50
1:A:66:SER:HB2	1:A:198:VAL:HG21	1.94	0.50
1:D:12:LYS:HD2	1:D:76:THR:HG23	1.93	0.50
1:C:39:VAL:HG11	1:C:65:MET:HE3	1.94	0.49
1:A:40:ARG:NH1	1:A:261:LYS:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD21	1:A:6:SER:HB2	1.95	0.49
1:A:174:ASP:OD1	1:A:176:THR:OG1	2.19	0.48
1:B:2:LYS:N	2:B:304:HOH:O	2.46	0.48
1:D:202:ILE:HG13	1:D:206:GLU:HG3	1.95	0.48
1:D:214:TRP:CZ3	1:D:232:GLU:HG3	2.49	0.48
1:A:40:ARG:HH12	1:A:261:LYS:HD3	1.79	0.48
1:A:238:ASP:OD1	1:A:242:LYS:NZ	2.44	0.48
1:C:132:ILE:O	1:C:135:PHE:HB2	2.14	0.47
1:C:114:LEU:HB2	1:C:119:ILE:HD11	1.96	0.47
1:B:102:ARG:NE	2:B:305:HOH:O	2.48	0.47
1:D:132:ILE:O	1:D:135:PHE:HB2	2.14	0.47
1:C:115:THR:O	1:C:119:ILE:HG12	2.15	0.46
1:C:150:ARG:NH2	2:C:306:HOH:O	2.48	0.46
1:B:42:VAL:HG21	1:B:65:MET:CE	2.44	0.46
1:B:155:ILE:O	1:B:159:ILE:HG12	2.16	0.46
1:C:1:MET:HA	2:C:331:HOH:O	2.16	0.46
1:A:38:ALA:HA	1:A:259:ARG:HH11	1.79	0.46
1:B:240:PHE:CE2	1:D:176:THR:HG21	2.51	0.46
1:A:160:ASP:OD1	1:A:193:LYS:NZ	2.38	0.46
1:C:161:PRO:O	1:C:193:LYS:HD2	2.16	0.46
1:D:206:GLU:OE2	1:D:230:VAL:HG11	2.16	0.45
1:C:65:MET:HE2	1:C:68:LEU:HD12	1.98	0.45
1:C:226:THR:O	1:C:230:VAL:HG23	2.17	0.45
1:A:102:ARG:NH2	1:A:106:ARG:HD2	2.32	0.45
1:B:211:ARG:HG3	1:B:224:ASP:O	2.16	0.45
1:A:132:ILE:O	1:A:135:PHE:HB2	2.17	0.45
1:A:7:PHE:O	1:A:43:SER:HA	2.18	0.44
1:A:115:THR:O	1:A:119:ILE:HG13	2.17	0.44
1:C:174:ASP:OD1	1:C:176:THR:HB	2.17	0.44
1:D:222:MET:HG2	1:D:229:VAL:HG22	1.99	0.44
1:A:143:TYR:HB3	1:A:147:MET:HB2	2.00	0.43
1:D:14:TYR:O	1:D:35:GLY:HA2	2.18	0.43
1:C:109:CYS:HB3	1:C:114:LEU:HD12	2.00	0.43
1:D:106:ARG:NH2	1:D:116:ASN:OD1	2.51	0.43
1:D:185:ILE:HD13	1:D:197:PHE:HZ	1.84	0.43
1:A:238:ASP:CG	1:A:242:LYS:HZ3	2.27	0.43
1:C:150:ARG:HG2	1:C:177:PHE:CE2	2.54	0.43
1:B:185:ILE:HD13	1:B:197:PHE:CZ	2.54	0.43
1:D:139:PRO:HB2	1:D:141:LYS:HG2	2.01	0.43
1:C:155:ILE:O	1:C:159:ILE:HG12	2.19	0.42
1:D:55:VAL:HA	1:D:199:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LYS:HE3	1:D:200:HIS:HB3	2.01	0.42
1:B:66:SER:HB2	1:B:198:VAL:HG21	2.02	0.42
1:C:118:GLU:O	1:C:122:MET:HG2	2.20	0.42
1:B:115:THR:O	1:B:119:ILE:HG13	2.20	0.42
1:C:239:TRP:CH2	1:C:243:LEU:HD11	2.55	0.42
1:B:242:LYS:HB2	1:B:242:LYS:HZ3	1.84	0.42
1:C:54:PHE:HE2	1:C:215:MET:HE3	1.85	0.42
1:D:248:LYS:HE3	1:D:248:LYS:HB2	1.89	0.42
1:A:14:TYR:O	1:A:35:GLY:HA3	2.20	0.41
1:B:240:PHE:CD2	1:D:176:THR:HG21	2.55	0.41
1:C:51:THR:HG23	1:C:195:ILE:HB	2.02	0.41
1:B:44:PHE:HB2	1:B:223:PHE:CE2	2.55	0.41
1:D:102:ARG:HH21	1:D:137:ASN:ND2	2.19	0.41
1:C:67:ASN:HB3	1:C:73:ILE:HG12	2.02	0.41
1:B:225:GLU:OE2	1:B:227:LYS:HG2	2.20	0.41
1:D:248:LYS:HG2	1:D:252:LYS:HE3	2.03	0.41
1:B:8:ARG:HB2	1:B:79:GLU:HG2	2.02	0.41
1:B:101:GLY:O	1:B:105:VAL:HG23	2.21	0.40
1:B:123:TYR:OH	2:B:301:HOH:O	2.22	0.40
1:C:10:VAL:HG13	1:C:75:PRO:HB3	2.04	0.40
1:B:67:ASN:HB3	1:B:73:ILE:HG12	2.02	0.40
1:C:245:LYS:O	1:C:249:GLU:HG2	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	240/280 (86%)	235 (98%)	5 (2%)	0	100	100
1	B	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	C	248/280 (89%)	243 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	237/280 (85%)	231 (98%)	6 (2%)	0	100	100
All	All	983/1120 (88%)	959 (98%)	24 (2%)	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	216/248 (87%)	213 (99%)	3 (1%)	59	82
1	B	230/248 (93%)	215 (94%)	15 (6%)	15	37
1	C	222/248 (90%)	214 (96%)	8 (4%)	31	60
1	D	213/248 (86%)	210 (99%)	3 (1%)	59	82
All	All	881/992 (89%)	852 (97%)	29 (3%)	33	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	SER
1	A	221	ARG
1	A	257	GLU
1	B	18	LYS
1	B	19	LYS
1	B	20	GLN
1	B	23	LYS
1	B	24	ILE
1	B	25	LYS
1	B	33	ASP
1	B	34	ASN
1	B	108	LYS
1	B	145	SER
1	B	211	ARG
1	B	231	LYS
1	B	232	GLU

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Mol	Chain	Res	Type
1	B	260	LYS
1	B	261	LYS
1	C	1	MET
1	C	16	LEU
1	C	145	SER
1	C	190	LYS
1	C	211	ARG
1	C	259	ARG
1	C	261	LYS
1	C	262	GLU
1	D	16	LEU
1	D	108	LYS
1	D	121	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	138	GLN
1	A	204	GLN
1	A	216	HIS
1	A	255	GLN
1	B	15	HIS
1	B	97	ASN
1	B	204	GLN
1	B	241	ASN
1	B	255	GLN
1	C	204	GLN
1	D	137	ASN
1	D	142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides 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](#)

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	244/280 (87%)	-0.55	0 100 100	39, 54, 82, 109	0
1	B	260/280 (92%)	-0.31	1 (0%) 88 87	46, 67, 128, 154	0
1	C	252/280 (90%)	-0.26	1 (0%) 88 87	40, 63, 106, 127	0
1	D	241/280 (86%)	-0.41	0 100 100	43, 63, 115, 141	0
All	All	997/1120 (89%)	-0.38	2 (0%) 91 90	39, 62, 106, 154	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	PHE	3.6
1	C	235	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.