



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1X7F / pdb_00001x7f
Title : Crystal structure of an uncharacterized B. cereus protein
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Deposited on : 2004-08-13
Resolution : 2.30 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

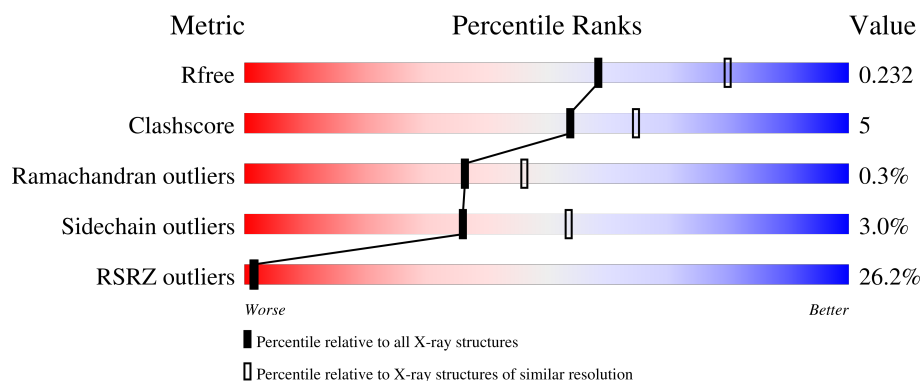
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	385	24% 78% 11% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3285 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 outer surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	13	0
			2909	1847	494	556	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q81HJ5
A	-22	HIS	-	expression tag	UNP Q81HJ5
A	-21	HIS	-	expression tag	UNP Q81HJ5
A	-20	HIS	-	expression tag	UNP Q81HJ5
A	-19	HIS	-	expression tag	UNP Q81HJ5
A	-18	HIS	-	expression tag	UNP Q81HJ5
A	-17	HIS	-	expression tag	UNP Q81HJ5
A	-16	SER	-	expression tag	UNP Q81HJ5
A	-15	SER	-	expression tag	UNP Q81HJ5
A	-14	GLY	-	expression tag	UNP Q81HJ5
A	-13	VAL	-	expression tag	UNP Q81HJ5
A	-12	ASP	-	expression tag	UNP Q81HJ5
A	-11	LEU	-	expression tag	UNP Q81HJ5
A	-10	GLY	-	expression tag	UNP Q81HJ5
A	-9	THR	-	expression tag	UNP Q81HJ5
A	-8	GLU	-	expression tag	UNP Q81HJ5
A	-7	ASN	-	expression tag	UNP Q81HJ5
A	-6	LEU	-	expression tag	UNP Q81HJ5
A	-5	TYR	-	expression tag	UNP Q81HJ5
A	-4	PHE	-	expression tag	UNP Q81HJ5
A	-3	GLN	-	expression tag	UNP Q81HJ5
A	-2	SER	-	expression tag	UNP Q81HJ5
A	-1	ASN	-	expression tag	UNP Q81HJ5
A	0	ALA	-	expression tag	UNP Q81HJ5

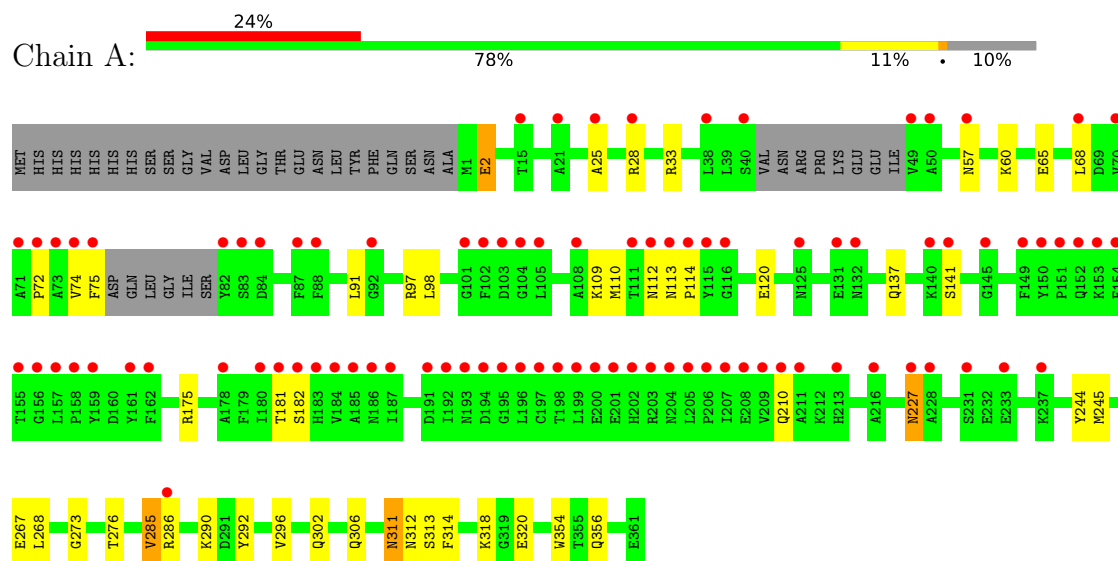
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	359	Total 376	O 376	0	48

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 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: outer surface protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	141.68Å 141.68Å 141.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.30) 99.8 (25.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.171 , 0.232 0.170 , 0.232	Depositor DCC
R_{free} test set	1132 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3285	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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	0.62	1/2965 (0.0%)	0.86	0/3998

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	ASN	CG-OD1	7.06	1.36	1.23

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	2909	0	2840	28	0
2	A	376	0	0	1	0
All	All	3285	0	2840	28	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 5.

All (28) 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:182:SER:H	1:A:227:ASN:HD21	1.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:H	1:A:210:GLN:HE22	1.30	0.77
1:A:33:ARG:NH2	1:A:120:GLU:OE1	2.20	0.74
1:A:227:ASN:HD22	1:A:227:ASN:H	1.34	0.74
1:A:311:ASN:HD22	1:A:313:SER:H	1.40	0.68
1:A:227:ASN:H	1:A:227:ASN:ND2	1.98	0.62
1:A:311:ASN:HD22	1:A:311:ASN:C	2.08	0.62
1:A:311:ASN:ND2	1:A:313:SER:H	1.99	0.60
1:A:68:LEU:HD11	1:A:91:LEU:HD12	1.84	0.59
1:A:268:LEU:HD11	1:A:356:GLN:HB3	1.84	0.59
1:A:296:VAL:HG13	2:A:662:HOH:O	2.05	0.57
1:A:302:GLN:HA	1:A:306:GLN:HE22	1.69	0.56
1:A:65:GLU:OE1	1:A:175:ARG:NH2	2.27	0.54
1:A:98:LEU:HD21	1:A:110:MET:HE1	1.90	0.53
1:A:286[A]:ARG:HD3	1:A:320:GLU:HB2	1.90	0.53
1:A:72:PRO:HA	1:A:75:PHE:CE2	2.45	0.52
1:A:273:GLY:HA3	1:A:354:TRP:CE2	2.48	0.49
1:A:312:ASN:HA	1:A:318:LYS:HD2	1.93	0.49
1:A:97:ARG:HD2	1:A:120:GLU:OE2	2.14	0.48
1:A:28[B]:ARG:HH11	1:A:28[B]:ARG:HB2	1.81	0.45
1:A:2:GLU:HA	1:A:244[B]:TYR:OH	2.17	0.43
1:A:25:ALA:O	1:A:28[B]:ARG:HG2	2.18	0.43
1:A:113:ASN:HA	1:A:114:PRO:HD3	1.88	0.43
1:A:286[A]:ARG:O	1:A:290:LYS:HB3	2.19	0.43
1:A:57:ASN:O	1:A:60:LYS:HG2	2.19	0.42
1:A:267:GLU:HG3	1:A:285:VAL:HG22	2.03	0.41
1:A:292:TYR:O	1:A:318:LYS:HE3	2.21	0.40
1:A:245:MET:HE2	1:A:245:MET:HB3	1.63	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	354/385 (92%)	342 (97%)	11 (3%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	VAL

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	313/334 (94%)	304 (97%)	9 (3%)	37	55

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	109	LYS
1	A	137	GLN
1	A	141	SER
1	A	227	ASN
1	A	276	THR
1	A	285	VAL
1	A	311	ASN
1	A	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	148	ASN
1	A	210	GLN
1	A	227	ASN
1	A	306	GLN
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	335	ASN

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 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 ⓘ

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	347/385 (90%)	1.36	91 (26%) ⓘ ⓘ	17, 37, 50, 66	13 (3%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	4.8
1	A	156	GLY	4.7
1	A	154	PHE	4.7
1	A	155	THR	4.6
1	A	192	ILE	4.6
1	A	202	HIS	4.5
1	A	152	GLN	4.3
1	A	157	LEU	4.0
1	A	49	VAL	4.0
1	A	206	PRO	4.0
1	A	82	TYR	4.0
1	A	196	LEU	3.9
1	A	70	VAL	3.9
1	A	75	PHE	3.8
1	A	153	LYS	3.8
1	A	205	LEU	3.6
1	A	38	LEU	3.6
1	A	199	LEU	3.6
1	A	200	GLU	3.6
1	A	194	ASP	3.6
1	A	72	PRO	3.5
1	A	207	ILE	3.5
1	A	40	SER	3.5
1	A	187	ILE	3.5
1	A	116	GLY	3.4
1	A	132	ASN	3.4
1	A	209	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	TYR	3.3
1	A	197	CYS	3.3
1	A	103	ASP	3.3
1	A	151	PRO	3.3
1	A	204	ASN	3.2
1	A	198	THR	3.2
1	A	68	LEU	3.2
1	A	162	PHE	3.1
1	A	158	PRO	3.1
1	A	84	ASP	3.1
1	A	71	ALA	3.1
1	A	141	SER	3.1
1	A	181	THR	3.0
1	A	15	THR	2.9
1	A	105	LEU	2.9
1	A	185	ALA	2.9
1	A	25	ALA	2.9
1	A	203	ARG	2.8
1	A	182	SER	2.8
1	A	114	PRO	2.8
1	A	201	GLU	2.7
1	A	73	ALA	2.7
1	A	28[A]	ARG	2.7
1	A	87	PHE	2.7
1	A	112	ASN	2.7
1	A	150	TYR	2.6
1	A	74	VAL	2.6
1	A	210	GLN	2.6
1	A	88	PHE	2.6
1	A	228	ALA	2.6
1	A	233[A]	GLU	2.6
1	A	216	ALA	2.6
1	A	149	PHE	2.6
1	A	184	VAL	2.6
1	A	211	ALA	2.5
1	A	227	ASN	2.5
1	A	115	TYR	2.5
1	A	125[A]	ASN	2.4
1	A	213	HIS	2.4
1	A	193	ASN	2.4
1	A	231	SER	2.4
1	A	131[A]	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	2.3
1	A	21	ALA	2.3
1	A	286[A]	ARG	2.3
1	A	57	ASN	2.3
1	A	50	ALA	2.3
1	A	186	ASN	2.2
1	A	92	GLY	2.2
1	A	104	GLY	2.2
1	A	111	THR	2.2
1	A	180	ILE	2.2
1	A	161	TYR	2.2
1	A	101	GLY	2.2
1	A	102	PHE	2.1
1	A	140	LYS	2.1
1	A	83	SER	2.1
1	A	178	ALA	2.1
1	A	237	LYS	2.1
1	A	108	ALA	2.1
1	A	183	HIS	2.1
1	A	145	GLY	2.1
1	A	208	GLU	2.0
1	A	113	ASN	2.0

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.