



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:36 pm BST

PDB ID : 9H8I / pdb_00009h8i
Title : Crystallization of B. licheniformis levanase
Authors : Carr, S.; Cruz-Migoni, A.; Porras-Dominguez, J.R.; Van den Ende, W.; Lopez-Munguia Canales, A.
Deposited on : 2024-10-29
Resolution : 1.54 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

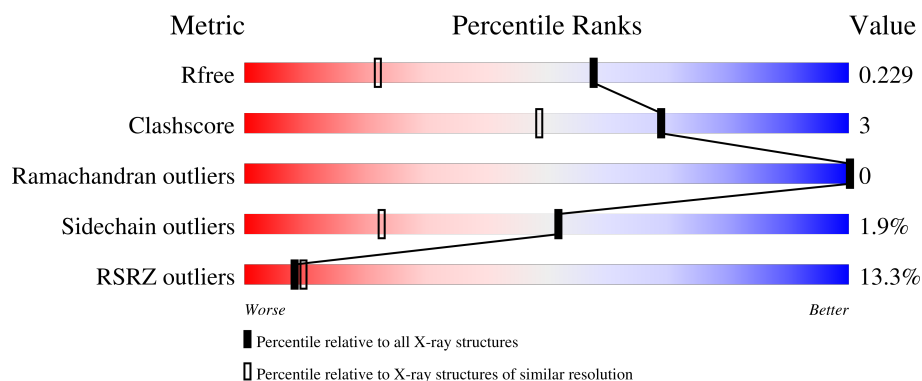
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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	486	<div> <div>12%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3860 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 Endolevansase LevB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	1	0
			3586	2276	603	702	5			

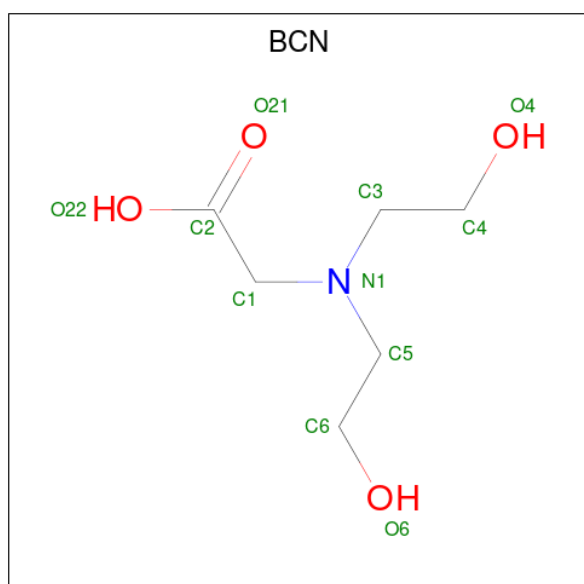
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	SER	ASP	conflict	UNP W8GV60
A	299	ASN	GLY	conflict	UNP W8GV60

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is BICINE (CCD ID: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

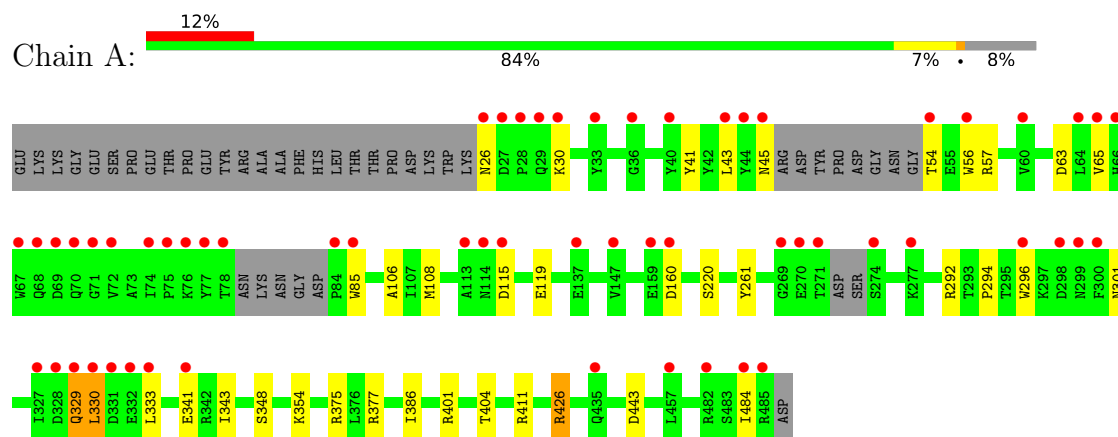
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		

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: Endolevansase LevB1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.59Å 82.59Å 171.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.38 – 1.54 74.37 – 1.54	Depositor EDS
% Data completeness (in resolution range)	96.8 (74.38-1.54) 96.8 (74.37-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.193 , 0.217 0.204 , 0.229	Depositor DCC
R_{free} test set	4284 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3860	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BCN, 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	0.58	0/3689	0.97	9/5008 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	375	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	375	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	377	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	401	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	411	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	119	GLU	CG-CD-OE2	-5.26	107.78	118.30
1	A	443	ASP	CB-CA-C	5.10	120.60	110.40
1	A	330	LEU	CB-CG-CD2	5.08	119.63	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3586	0	3333	24	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	20	0	0
4	A	8	0	12	0	0
5	A	242	0	0	1	0
All	All	3860	0	3365	24	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 3.

All (24) 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:45:ASN:HA	1:A:54:THR:CB	2.10	0.81
1:A:85:TRP:CZ3	1:A:108:MET:SD	2.86	0.68
1:A:63:ASP:O	1:A:329:GLN:OE1	2.14	0.66
1:A:354:LYS:HA	1:A:354:LYS:HE2	1.77	0.65
1:A:65:VAL:HG22	1:A:329:GLN:NE2	2.15	0.62
1:A:294:PRO:HB2	1:A:296:TRP:CZ3	2.41	0.55
1:A:85:TRP:HZ3	1:A:108:MET:CE	2.23	0.52
1:A:386:ILE:HG12	1:A:404:THR:HG21	1.91	0.51
1:A:85:TRP:CZ3	1:A:108:MET:CE	2.94	0.51
1:A:85:TRP:CE3	1:A:108:MET:SD	3.04	0.50
1:A:296:TRP:C	1:A:296:TRP:CD1	2.84	0.50
1:A:294:PRO:HB2	1:A:296:TRP:CE3	2.47	0.49
1:A:329:GLN:HG2	1:A:330:LEU:N	2.28	0.48
1:A:333:LEU:CD2	1:A:484:ILE:HD11	2.44	0.47
1:A:292:ARG:CD	1:A:296:TRP:CZ2	2.98	0.46
1:A:294:PRO:CB	1:A:296:TRP:CZ3	2.97	0.46
1:A:341:GLU:O	1:A:343:ILE:HG13	2.16	0.46
1:A:426:ARG:NH1	1:A:426:ARG:HB3	2.30	0.46
1:A:41:TYR:HA	1:A:57:ARG:O	2.17	0.45
1:A:106:ALA:HB1	1:A:108:MET:CE	2.47	0.44
1:A:26:ASN:HA	1:A:301:ASN:OD1	2.20	0.42
1:A:333:LEU:HD21	1:A:484:ILE:HD11	2.02	0.42
1:A:220:SER:HB3	1:A:261:TYR:CE1	2.56	0.41
1:A:30:LYS:NZ	5:A:610:HOH:O	2.53	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	438/486 (90%)	418 (95%)	20 (5%)	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	376/415 (91%)	369 (98%)	7 (2%)	52	23

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	56	TRP
1	A	115	ASP
1	A	160	ASP
1	A	329	GLN
1	A	348	SER
1	A	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS

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Mol	Chain	Res	Type
1	A	179	GLN
1	A	311	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	BCN	A	503	2	10,10,10	1.12	1 (10%)	11,11,11	1.10	2 (18%)
4	EDO	A	506	-	3,3,3	0.57	0	2,2,2	0.93	0
4	EDO	A	505	-	3,3,3	0.17	0	2,2,2	0.38	0
3	BCN	A	504	2	10,10,10	1.23	1 (10%)	11,11,11	0.82	0

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
3	BCN	A	503	2	-	0/10/10/10	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
3	BCN	A	504	2	-	0/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	BCN	O21-C2	3.01	1.32	1.22
3	A	503	BCN	O21-C2	2.19	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	BCN	O21-C2-C1	-2.15	113.76	122.31
3	A	503	BCN	O22-C2-O21	2.03	128.35	123.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	EDO	O1-C1-C2-O2

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 ⓘ

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	445/486 (91%)	0.56	59 (13%) 8 10	10, 20, 56, 79	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	7.2
1	A	78	THR	7.1
1	A	296	TRP	7.0
1	A	329	GLN	6.9
1	A	65	VAL	6.6
1	A	54	THR	6.2
1	A	45	ASN	6.0
1	A	44	TYR	5.5
1	A	28	PRO	5.5
1	A	271	THR	5.4
1	A	484	ILE	4.7
1	A	299	ASN	4.5
1	A	26	ASN	4.4
1	A	113	ALA	4.4
1	A	85	TRP	4.3
1	A	66	HIS	4.2
1	A	77	TYR	4.1
1	A	84	PRO	4.0
1	A	75	PRO	3.8
1	A	27	ASP	3.8
1	A	76	LYS	3.8
1	A	270	GLU	3.8
1	A	457	LEU	3.7
1	A	331	ASP	3.7
1	A	274	SER	3.6
1	A	30	LYS	3.4
1	A	328	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	482	ARG	3.3
1	A	72	VAL	3.2
1	A	68	GLN	3.2
1	A	298	ASP	3.2
1	A	67	TRP	3.2
1	A	43	LEU	3.1
1	A	56	TRP	3.1
1	A	69	ASP	2.9
1	A	114	ASN	2.8
1	A	64	LEU	2.7
1	A	40	TYR	2.6
1	A	36	GLY	2.5
1	A	332	GLU	2.5
1	A	115	ASP	2.5
1	A	435	GLN	2.4
1	A	159	GLU	2.4
1	A	269	GLY	2.4
1	A	485	ARG	2.3
1	A	70	GLN	2.3
1	A	160	ASP	2.3
1	A	29	GLN	2.2
1	A	333	LEU	2.2
1	A	74	ILE	2.2
1	A	327	ILE	2.2
1	A	147	VAL	2.2
1	A	341	GLU	2.1
1	A	33	TYR	2.1
1	A	300	PHE	2.1
1	A	71	GLY	2.1
1	A	277	LYS	2.0
1	A	60	VAL	2.0
1	A	137	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	505	4/4	0.92	0.11	26,26,28,38	0
4	EDO	A	506	4/4	0.95	0.12	18,26,29,30	0
3	BCN	A	503	11/11	0.98	0.04	10,11,12,14	0
3	BCN	A	504	11/11	0.98	0.05	11,12,13,15	0
2	CA	A	501	1/1	1.00	0.01	11,11,11,11	0
2	CA	A	502	1/1	1.00	0.02	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.