



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 01:11 pm BST

PDB ID : 7ZAO
Title : Structure of BPP43_05035 of *Brachyspira pilosicoli*
Authors : Rajan, A.; Gallego, P.; Pelaseyed, T.
Deposited on : 2022-03-22
Resolution : 2.20 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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

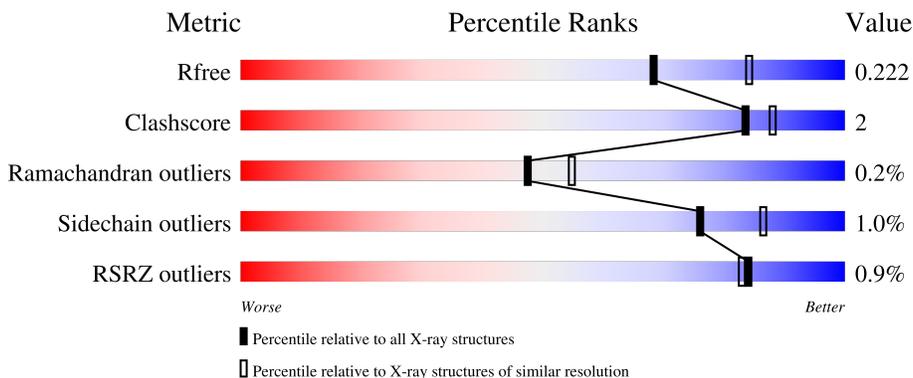
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	462	
1	B	462	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	502	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6734 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 Sialidase (Neuraminidase) family protein-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3216	2007	538	664	7	0	1	0
1	B	429	3216	2007	538	664	7	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP A0A3B6VYW6
A	2	HIS	-	expression tag	UNP A0A3B6VYW6
A	3	HIS	-	expression tag	UNP A0A3B6VYW6
A	4	HIS	-	expression tag	UNP A0A3B6VYW6
A	5	HIS	-	expression tag	UNP A0A3B6VYW6
A	6	HIS	-	expression tag	UNP A0A3B6VYW6
A	7	LEU	-	expression tag	UNP A0A3B6VYW6
A	8	VAL	-	expression tag	UNP A0A3B6VYW6
A	9	PRO	-	expression tag	UNP A0A3B6VYW6
A	10	ARG	-	expression tag	UNP A0A3B6VYW6
A	11	GLY	-	expression tag	UNP A0A3B6VYW6
A	12	SER	-	expression tag	UNP A0A3B6VYW6
A	454	TYR	-	expression tag	UNP A0A3B6VYW6
A	455	PRO	-	expression tag	UNP A0A3B6VYW6
A	456	TYR	-	expression tag	UNP A0A3B6VYW6
A	457	ASP	-	expression tag	UNP A0A3B6VYW6
A	458	VAL	-	expression tag	UNP A0A3B6VYW6
A	459	PRO	-	expression tag	UNP A0A3B6VYW6
A	460	ASP	-	expression tag	UNP A0A3B6VYW6
A	461	TYR	-	expression tag	UNP A0A3B6VYW6
A	462	ALA	-	expression tag	UNP A0A3B6VYW6
B	1	HIS	-	expression tag	UNP A0A3B6VYW6
B	2	HIS	-	expression tag	UNP A0A3B6VYW6
B	3	HIS	-	expression tag	UNP A0A3B6VYW6
B	4	HIS	-	expression tag	UNP A0A3B6VYW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP A0A3B6VYW6
B	6	HIS	-	expression tag	UNP A0A3B6VYW6
B	7	LEU	-	expression tag	UNP A0A3B6VYW6
B	8	VAL	-	expression tag	UNP A0A3B6VYW6
B	9	PRO	-	expression tag	UNP A0A3B6VYW6
B	10	ARG	-	expression tag	UNP A0A3B6VYW6
B	11	GLY	-	expression tag	UNP A0A3B6VYW6
B	12	SER	-	expression tag	UNP A0A3B6VYW6
B	454	TYR	-	expression tag	UNP A0A3B6VYW6
B	455	PRO	-	expression tag	UNP A0A3B6VYW6
B	456	TYR	-	expression tag	UNP A0A3B6VYW6
B	457	ASP	-	expression tag	UNP A0A3B6VYW6
B	458	VAL	-	expression tag	UNP A0A3B6VYW6
B	459	PRO	-	expression tag	UNP A0A3B6VYW6
B	460	ASP	-	expression tag	UNP A0A3B6VYW6
B	461	TYR	-	expression tag	UNP A0A3B6VYW6
B	462	ALA	-	expression tag	UNP A0A3B6VYW6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

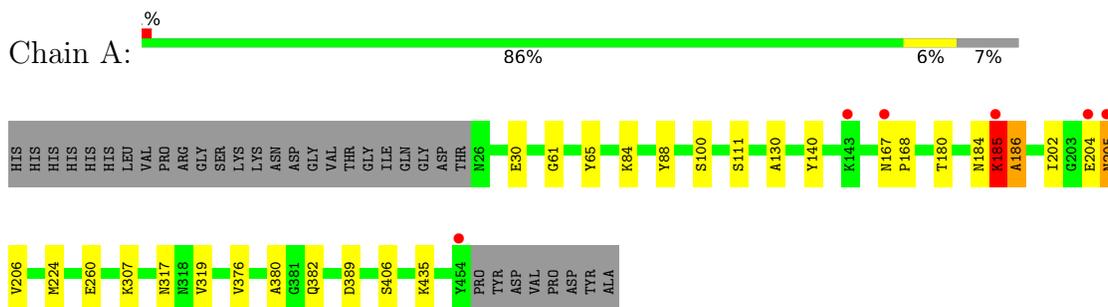
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	157	Total O 157 157	0	0
3	B	141	Total O 141 141	0	0

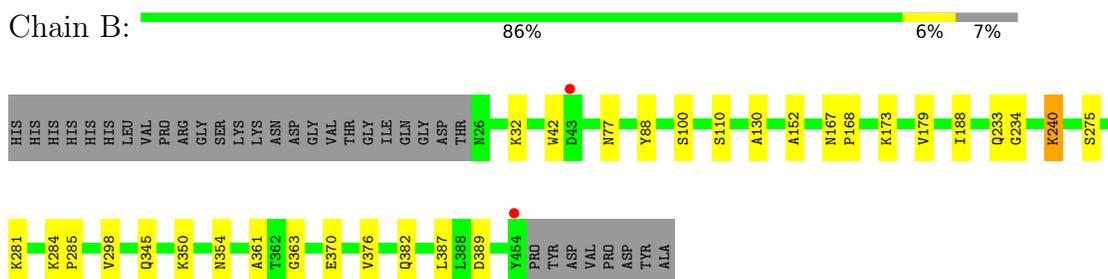
3 Residue-property plots [i](#)

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 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: Sialidase (Neuraminidase) family protein-like protein



- Molecule 1: Sialidase (Neuraminidase) family protein-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.91Å 101.36Å 154.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.20 48.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.17-2.20) 97.0 (48.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.223 0.181 , 0.222	Depositor DCC
R_{free} test set	3033 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.48	0/3276	0.73	7/4435 (0.2%)
1	B	0.47	0/3276	0.64	2/4435 (0.0%)
All	All	0.47	0/6552	0.69	9/8870 (0.1%)

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASN	CB-CA-C	-11.06	88.27	110.40
1	A	205	ASN	N-CA-C	8.18	133.08	111.00
1	A	185	LYS	CA-CB-CG	7.59	130.11	113.40
1	A	205	ASN	N-CA-CB	6.93	123.08	110.60
1	A	205	ASN	C-N-CA	-6.50	105.44	121.70
1	B	240	LYS	CA-CB-CG	6.22	127.09	113.40
1	A	205	ASN	CA-C-N	5.83	130.03	117.20
1	B	240	LYS	CB-CG-CD	5.68	126.38	111.60
1	A	184	ASN	C-N-CA	-5.49	107.99	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLU	Peptide

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	3216	0	3128	16	0
1	B	3216	0	3128	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	157	0	0	1	0
3	B	141	0	0	0	0
All	All	6734	0	6256	31	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 2.

All (31) 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:111:SER:HB2	1:A:185:LYS:HB2	1.55	0.89
1:A:111:SER:OG	1:A:185:LYS:NZ	2.20	0.74
1:A:111:SER:CB	1:A:185:LYS:HB2	2.21	0.71
1:A:30:GLU:OE1	1:B:32:LYS:HE3	1.91	0.70
1:A:100:SER:HA	1:A:130:ALA:HB2	1.82	0.62
1:B:234:GLY:N	1:B:240:LYS:HB2	2.15	0.61
1:B:100:SER:HA	1:B:130:ALA:HB2	1.82	0.61
1:B:42:TRP:CG	1:B:345:GLN:HG3	2.42	0.55
1:A:202:ILE:CG2	1:A:206:VAL:HB	2.37	0.54
1:B:179:VAL:HG22	1:B:188:ILE:HG12	1.89	0.54
1:B:233:GLN:C	1:B:240:LYS:HB2	2.28	0.53
1:A:180:THR:O	1:A:186:ALA:HA	2.11	0.51
1:A:167:ASN:HB3	1:A:168:PRO:HD3	1.92	0.51
1:B:152:ALA:HB1	1:B:173:LYS:HE2	1.93	0.51
1:B:350:LYS:HE3	1:B:363:GLY:O	2.15	0.47
1:A:376:VAL:HA	1:A:382:GLN:O	2.16	0.46
1:B:167:ASN:HB3	1:B:168:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:OD1	1:A:319:VAL:HG12	2.17	0.45
1:A:380:ALA:HA	1:A:406:SER:O	2.16	0.45
1:B:370:GLU:HG3	1:B:387:LEU:HD22	1.98	0.44
1:B:152:ALA:CB	1:B:173:LYS:HE2	2.47	0.44
1:B:345:GLN:NE2	1:B:361:ALA:HA	2.33	0.43
1:A:260:GLU:HG3	3:A:742:HOH:O	2.19	0.43
1:B:77:ASN:HA	1:B:110:SER:O	2.18	0.43
1:A:140:TYR:CE2	1:A:224:MET:HB3	2.54	0.43
1:A:61:GLY:O	1:A:435:LYS:NZ	2.52	0.42
1:A:65:TYR:OH	1:A:84:LYS:HE3	2.19	0.42
1:B:284:LYS:HA	1:B:285:PRO:HD3	1.97	0.42
1:A:307:LYS:HA	1:A:307:LYS:HD3	1.95	0.40
1:B:281:LYS:HB2	1:B:298:VAL:HG23	2.04	0.40
1:B:376:VAL:HA	1:B:382:GLN:O	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	428/462 (93%)	402 (94%)	24 (6%)	2 (0%)	29	31
1	B	428/462 (93%)	402 (94%)	26 (6%)	0	100	100
All	All	856/924 (93%)	804 (94%)	50 (6%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
1	A	205	ASN

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	347/374 (93%)	344 (99%)	3 (1%)	78	88
1	B	347/374 (93%)	343 (99%)	4 (1%)	71	83
All	All	694/748 (93%)	687 (99%)	7 (1%)	76	86

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

Mol	Chain	Res	Type
1	A	88	TYR
1	A	185	LYS
1	A	389	ASP
1	B	88	TYR
1	B	275	SER
1	B	354	ASN
1	B	389	ASP

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	391	GLN
1	B	290	ASN
1	B	354	ASN
1	B	357	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	429/462 (92%)	-0.41	6 (1%) 75 73	20, 30, 44, 76	0
1	B	429/462 (92%)	-0.51	2 (0%) 91 90	21, 31, 47, 76	0
All	All	858/924 (92%)	-0.46	8 (0%) 84 83	20, 30, 47, 76	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	TYR	4.7
1	A	185	LYS	4.1
1	B	454	TYR	3.2
1	A	167	ASN	2.8
1	A	143	LYS	2.7
1	B	43	ASP	2.3
1	A	204	GLU	2.2
1	A	205	ASN	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 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
2	MG	B	502	1/1	0.66	0.82	65,65,65,65	0
2	MG	A	502	1/1	0.93	0.05	34,34,34,34	0
2	MG	A	501	1/1	0.97	0.08	31,31,31,31	0
2	MG	B	501	1/1	0.98	0.10	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.