

wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 06:35 AM EDT

PDB ID	:	7LHA
Title	:	Structure of the Exo-L-galactose-6-sulfatase BuS1_11 from Bacteroides
		uniformis
Authors	:	Robb, C.S.; Boraston, A.B.
Deposited on	:	2021-01-21
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

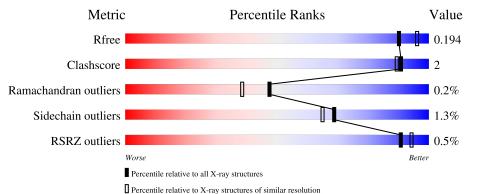
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	А	533	89%	5% 6%
1	В	533	88%	5% 6%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9126 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 Exo-L-galactose-6-sulfatase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	501	Total 4104	C 2617	N 699	0 762	S 26	0	1	0
1	В	499	Total 4074	C 2597	1,	0 761	S 26	0	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	3	MET	-	initiating methionine	UNP A0A4Y1VMZ7
А	4	GLY	-	expression tag	UNP A0A4Y1VMZ7
А	5	SER	-	expression tag	UNP A0A4Y1VMZ7
А	6	SER	-	expression tag	UNP A0A4Y1VMZ7
А	7	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	8	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	9	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	10	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	11	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	12	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	13	SER	-	expression tag	UNP A0A4Y1VMZ7
А	14	SER	-	expression tag	UNP A0A4Y1VMZ7
А	15	GLY	-	expression tag	UNP A0A4Y1VMZ7
А	16	LEU	-	expression tag	UNP A0A4Y1VMZ7
А	17	VAL	-	expression tag	UNP A0A4Y1VMZ7
А	18	PRO	-	expression tag	UNP A0A4Y1VMZ7
А	19	ARG	-	expression tag	UNP A0A4Y1VMZ7
А	20	GLY	-	expression tag	UNP A0A4Y1VMZ7
А	21	SER	-	expression tag	UNP A0A4Y1VMZ7
А	22	HIS	-	expression tag	UNP A0A4Y1VMZ7
А	23	MET	-	expression tag	UNP A0A4Y1VMZ7
А	24	ALA	-	expression tag	UNP A0A4Y1VMZ7
А	25	GLN	-	expression tag	UNP A0A4Y1VMZ7
А	26	GLU	-	expression tag	UNP A0A4Y1VMZ7
А	27	LYS	-	expression tag	UNP A0A4Y1VMZ7

There are 66 discrepancies between the modelled and reference sequences:

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Residue	N /T 1 11 1			Continued from previous page Comment Reference Chain Residue Modelled Actual Comment Reference							
ittosiaao	Modelled	Actual	Comment	Reference							
28	PRO	-	expression tag	UNP A0A4Y1VMZ7							
29	MET	-	expression tag	UNP A0A4Y1VMZ7							
30	ASN	-	expression tag	UNP A0A4Y1VMZ7							
31	VAL	-	expression tag	UNP A0A4Y1VMZ7							
32	ILE	-	expression tag	UNP A0A4Y1VMZ7							
33	PHE	-	expression tag	UNP A0A4Y1VMZ7							
34	ILE	-	expression tag	UNP A0A4Y1VMZ7							
392	LYS	GLU	conflict	UNP A0A4Y1VMZ7							
3	MET	-	initiating methionine	UNP A0A4Y1VMZ7							
4	GLY	-	expression tag	UNP A0A4Y1VMZ7							
5	SER	-	expression tag	UNP A0A4Y1VMZ7							
6	SER	-	expression tag	UNP A0A4Y1VMZ7							
7	HIS	-	expression tag	UNP A0A4Y1VMZ7							
8	HIS	_	expression tag	UNP A0A4Y1VMZ7							
9	HIS	_	expression tag	UNP A0A4Y1VMZ7							
10	HIS	-	expression tag	UNP A0A4Y1VMZ7							
11	HIS	-	expression tag	UNP A0A4Y1VMZ7							
12	HIS	-	expression tag	UNP A0A4Y1VMZ7							
13	SER	-	expression tag	UNP A0A4Y1VMZ7							
14	SER	-	expression tag	UNP A0A4Y1VMZ7							
15	GLY	-	expression tag	UNP A0A4Y1VMZ7							
16	LEU	-	expression tag	UNP A0A4Y1VMZ7							
17	VAL	-	expression tag	UNP A0A4Y1VMZ7							
18	PRO	-	expression tag	UNP A0A4Y1VMZ7							
19	ARG	-	expression tag	UNP A0A4Y1VMZ7							
20	GLY	-	expression tag	UNP A0A4Y1VMZ7							
21	SER	-	expression tag	UNP A0A4Y1VMZ7							
22	HIS	-	expression tag	UNP A0A4Y1VMZ7							
23	MET	-	expression tag	UNP A0A4Y1VMZ7							
24	ALA	-	expression tag	UNP A0A4Y1VMZ7							
25	GLN	-	expression tag	UNP A0A4Y1VMZ7							
26	GLU	-	expression tag	UNP A0A4Y1VMZ7							
27	LYS	-	expression tag	UNP A0A4Y1VMZ7							
28	PRO	-	expression tag	UNP A0A4Y1VMZ7							
29	MET	-	expression tag	UNP A0A4Y1VMZ7							
30	ASN	-	expression tag	UNP A0A4Y1VMZ7							
31	VAL	-	expression tag	UNP A0A4Y1VMZ7							
32	ILE	_	expression tag	UNP A0A4Y1VMZ7							
33	PHE	_	expression tag	UNP A0A4Y1VMZ7							
34	ILE	_	• •	UNP A0A4Y1VMZ7							
392	LYS	GLU	conflict	UNP A0A4Y1VMZ7							
	29 30 31 32 33 34 392 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34	29 MET 30 ASN 31 VAL 32 ILE 33 PHE 34 ILE 392 LYS 3 MET 4 GLY 5 SER 6 SER 7 HIS 8 HIS 9 HIS 10 HIS 11 HIS 12 HIS 13 SER 14 SER 15 GLY 16 LEU 17 VAL 18 PRO 19 ARG 20 GLY 21 SER 22 HIS 23 MET 24 ALA 25 GLN 26 GLU 27 LYS 28 PRO 29 MET 30 ASN 31 VAL 32 <td>29 MET - 30 ASN - 31 VAL - 32 ILE - 33 PHE - 34 ILE - 392 LYS GLU 3 MET - 392 LYS GLU 3 MET - 4 GLY - 5 SER - 6 SER - 7 HIS - 8 HIS - 9 HIS - 10 HIS - 11 HIS - 12 HIS - 13 SER - 14 SER - 15 GLY - 16 LEU - 17 VAL - 18 PRO - 20 GLY - 21 SER - 22 HIS -</td> <td>29MET-expression tag30ASN-expression tag31VAL-expression tag32ILE-expression tag33PHE-expression tag34ILE-expression tag392LYSGLUconflict3MET-initiating methionine4GLY-expression tag5SER-expression tag6SER-expression tag7HIS-expression tag9HIS-expression tag10HIS-expression tag11HIS-expression tag12HIS-expression tag13SER-expression tag14SER-expression tag15GLY-expression tag16LEU-expression tag17VAL-expression tag18PRO-expression tag20GLY-expression tag21SER-expression tag22HIS-expression tag23MET-expression tag24ALA-expression tag25GLN-expression tag26GLU-expression tag27LYS-expression tag28PRO-expression tag31VAL<!--</td--></td>	29 MET - 30 ASN - 31 VAL - 32 ILE - 33 PHE - 34 ILE - 392 LYS GLU 3 MET - 392 LYS GLU 3 MET - 4 GLY - 5 SER - 6 SER - 7 HIS - 8 HIS - 9 HIS - 10 HIS - 11 HIS - 12 HIS - 13 SER - 14 SER - 15 GLY - 16 LEU - 17 VAL - 18 PRO - 20 GLY - 21 SER - 22 HIS -	29MET-expression tag30ASN-expression tag31VAL-expression tag32ILE-expression tag33PHE-expression tag34ILE-expression tag392LYSGLUconflict3MET-initiating methionine4GLY-expression tag5SER-expression tag6SER-expression tag7HIS-expression tag9HIS-expression tag10HIS-expression tag11HIS-expression tag12HIS-expression tag13SER-expression tag14SER-expression tag15GLY-expression tag16LEU-expression tag17VAL-expression tag18PRO-expression tag20GLY-expression tag21SER-expression tag22HIS-expression tag23MET-expression tag24ALA-expression tag25GLN-expression tag26GLU-expression tag27LYS-expression tag28PRO-expression tag31VAL </td							

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• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Ni 2 2	0	0
3	В	2	Total Ni 2 2	0	0

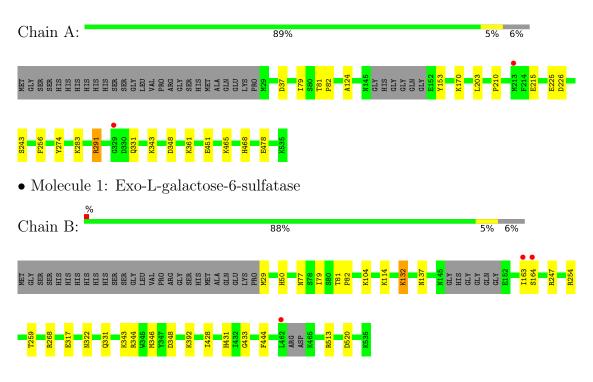
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	493	Total O 493 493	0	0
4	В	449	Total O 449 449	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: Exo-L-galactose-6-sulfatase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	89.41Å 89.41Å 264.79Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.60 - 1.95	Depositor
Resolution (A)	40.60 - 1.95	EDS
% Data completeness	$100.0 \ (40.60-1.95)$	Depositor
(in resolution range)	$100.0 \ (40.60-1.95)$	EDS
R _{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.44 (at 1.95 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D D.	0.148 , 0.194	Depositor
R, R_{free}	0.148 , 0.194	DCC
R_{free} test set	3978 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 51.3	EDS
L-test for twinning ²	$ \langle L \rangle = 0.46, \langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CA, NI

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		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/4214	0.59	0/5700	
1	В	0.44	0/4183	0.59	0/5663	
All	All	0.46	0/8397	0.59	0/11363	

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	А	4104	0	3935	15	0
1	В	4074	0	3874	12	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
4	А	493	0	0	4	0
4	В	449	0	0	0	0
All	All	9126	0	7809	27	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.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MET:HE2	1:B:322:ASN:HA	1.54	0.89
1:A:170:LYS:NZ	4:A:708:HOH:O	2.36	0.58
1:A:283:LYS:NZ	4:A:714:HOH:O	2.39	0.54
1:A:225:GLU:HG3	1:A:226:ASP:N	2.24	0.51
1:A:451:GLU:OE2	4:A:701:HOH:O	2.20	0.49

The worst 5 of 27 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	entiles
1	А	498/533~(93%)	483~(97%)	15 (3%)	0	100	100
1	В	494/533~(93%)	480 (97%)	12 (2%)	2~(0%)	34	22
All	All	992/1066~(93%)	963~(97%)	27 (3%)	2~(0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	132	LYS
1	В	77	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	А	439/475~(92%)	434 (99%)	5(1%)	73 71	
1	В	434/475~(91%)	428 (99%)	6 (1%)	67 62	
All	All	873/950~(92%)	862~(99%)	11 (1%)	69 65	

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	331	GLN
1	В	343	LYS
1	В	392	LYS
1	В	348	ASP
1	А	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 6 ligands modelled in this entry, 6 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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	501/533~(93%)	-0.37	2 (0%) 92 95	6, 13, 31, 49	0
1	В	499/533~(93%)	-0.27	3 (0%) 89 93	6, 15, 33, 60	0
All	All	1000/1066~(93%)	-0.32	5 (0%) 91 94	6, 14, 32, 60	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	163	ILE	3.2
1	А	329	GLY	2.1
1	А	213	MET	2.1
1	В	164	SER	2.1
1	В	462	LEU	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, 95^{th} 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	CA	А	601	1/1	0.99	0.05	$25,\!25,\!25,\!25$	0
2	CA	В	601	1/1	0.99	0.12	24,24,24,24	0
3	NI	А	602	1/1	1.00	0.04	22,22,22,22	0
3	NI	А	603	1/1	1.00	0.05	27,27,27,27	0
3	NI	В	602	1/1	1.00	0.06	24,24,24,24	0
3	NI	В	603	1/1	1.00	0.05	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.

