Full wwPDB X-ray Structure Validation Report (i)

Jul 6, 2022 – 04:08 am BST

PDB ID	:	7PJJ
Title	:	Structure of the Family-3 Glycosyl Hydrolase BcpE2 from Streptomyces scabies
Authors	:	Jadot, C.; Herman, R.; Deflandre, B.; Rigali, S.; Kerff, F.
Deposited on	:	2021-08-24
Resolution	:	3.09 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 (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 (i)) were used in the production of this report:

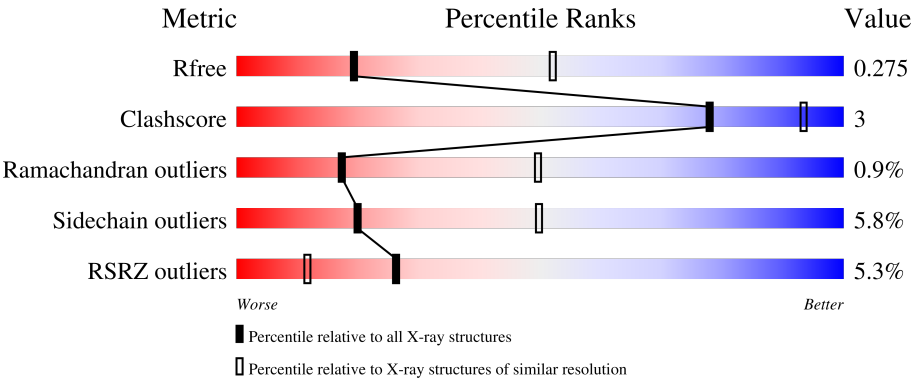
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	A	834	5% 83% 11% • 5%

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	GOL	A	901	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11733 atoms, of which 5815 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.

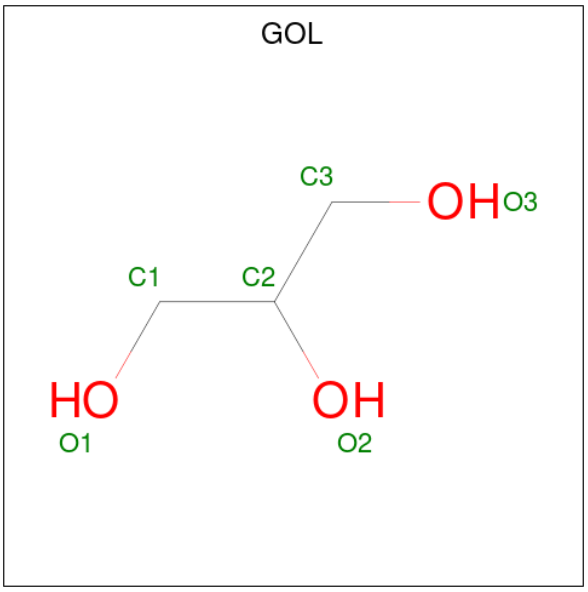
- Molecule 1 is a protein called Beta-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	791	11711	3710	5807	1042	1144	8	5807	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	822	LYS	-	expression tag	UNP C9ZDY4
A	823	LEU	-	expression tag	UNP C9ZDY4
A	824	ALA	-	expression tag	UNP C9ZDY4
A	825	ALA	-	expression tag	UNP C9ZDY4
A	826	ALA	-	expression tag	UNP C9ZDY4
A	827	LEU	-	expression tag	UNP C9ZDY4
A	828	GLU	-	expression tag	UNP C9ZDY4
A	829	HIS	-	expression tag	UNP C9ZDY4
A	830	HIS	-	expression tag	UNP C9ZDY4
A	831	HIS	-	expression tag	UNP C9ZDY4
A	832	HIS	-	expression tag	UNP C9ZDY4
A	833	HIS	-	expression tag	UNP C9ZDY4
A	834	HIS	-	expression tag	UNP C9ZDY4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	8	0
			14	3	8	3		

- Molecule 3 is water.

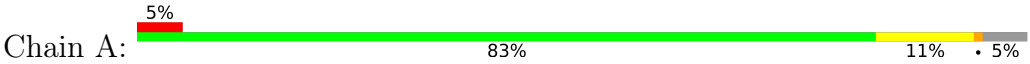
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		

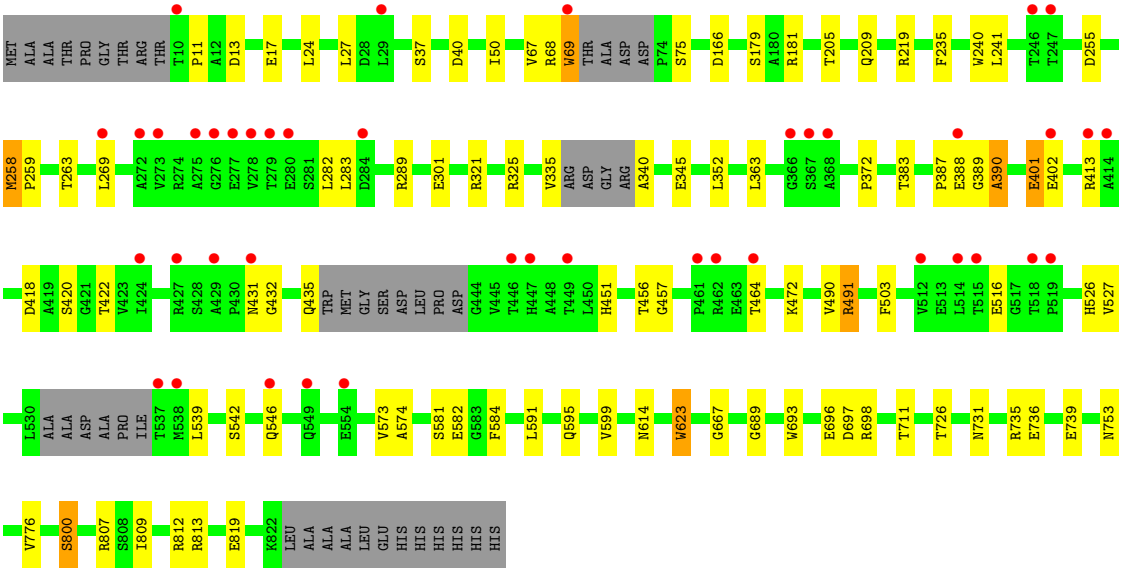
3 Residue-property plots (i)

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: Beta-glucosidase

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.62Å 109.62Å 164.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 3.09 47.41 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.41-3.09) 99.4 (47.41-3.09)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.223 , 0.270 0.217 , 0.275	Depositor DCC
R_{free} test set	1071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	90.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11733	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL

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	0.44	0/6030	0.62	0/8255

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

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	5904	5807	5803	34	0
2	A	6	8	8	0	0
3	A	8	0	0	0	0
All	All	5918	5815	5811	34	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 (34) 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:667:GLY:O	1:A:698:ARG:HD2	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:N	1:A:259:PRO:HD2	2.14	0.63
1:A:418:ASP:OD2	1:A:422:THR:HB	2.04	0.57
1:A:181:ARG:NH2	1:A:753:ASN:O	2.38	0.57
1:A:599:VAL:HG11	1:A:623:TRP:CD2	2.39	0.57
1:A:573:VAL:HG11	1:A:591:LEU:HD13	1.86	0.56
1:A:37:SER:HG	1:A:263:THR:HG1	1.53	0.55
1:A:255:ASP:OD1	1:A:289:ARG:NH1	2.41	0.53
1:A:689:GLY:O	1:A:693:TRP:HD1	1.91	0.52
1:A:711:THR:OG1	1:A:731:ASN:OD1	2.27	0.52
1:A:335:VAL:HA	1:A:340:ALA:N	2.25	0.52
1:A:739:GLU:OE2	1:A:807:ARG:HG2	2.10	0.52
1:A:75:SER:O	1:A:372:PRO:HA	2.11	0.51
1:A:389:GLY:O	1:A:390:ALA:O	2.29	0.50
1:A:451:HIS:CE1	1:A:527:VAL:HG13	2.49	0.48
1:A:696:GLU:O	1:A:697:ASP:HB3	2.15	0.46
1:A:27:LEU:HD12	1:A:50:ILE:HG21	1.99	0.45
1:A:420:SER:HG	1:A:422:THR:HG1	1.62	0.44
1:A:67:VAL:HG23	1:A:69:TRP:CD2	2.52	0.44
1:A:401:GLU:HG3	1:A:402:GLU:O	2.18	0.44
1:A:258:MET:N	1:A:259:PRO:CD	2.80	0.44
1:A:464:THR:HG22	1:A:516:GLU:H	1.83	0.43
1:A:800:SER:HB3	1:A:819:GLU:OE2	2.18	0.43
1:A:574:ALA:HB2	1:A:614:ASN:HB3	2.00	0.43
1:A:573:VAL:HG13	1:A:595:GLN:HB3	2.01	0.42
1:A:456:THR:HG22	1:A:457:GLY:N	2.34	0.42
1:A:68:ARG:HD3	1:A:435:GLN:OE1	2.19	0.42
1:A:269:LEU:HD21	1:A:283:LEU:HD13	2.01	0.42
1:A:451:HIS:CE1	1:A:527:VAL:CG1	3.02	0.42
1:A:490:VAL:HG12	1:A:491:ARG:N	2.34	0.41
1:A:726:THR:HG23	1:A:776:VAL:HG22	2.02	0.41
1:A:383:THR:HA	1:A:390:ALA:HB1	2.02	0.41
1:A:809:ILE:O	1:A:812:ARG:NH1	2.47	0.41
1:A:581:SER:HB3	1:A:584:PHE:CZ	2.56	0.41

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	781/834 (94%)	724 (93%)	50 (6%)	7 (1%)	17 49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ALA
1	A	11	PRO
1	A	241	LEU
1	A	432	GLY
1	A	431	ASN
1	A	387	PRO
1	A	258	MET

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	600/631 (95%)	565 (94%)	35 (6%)	20 50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	17	GLU
1	A	24	LEU
1	A	40	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	TRP
1	A	166	ASP
1	A	179	SER
1	A	205	THR
1	A	209	GLN
1	A	219	ARG
1	A	235	PHE
1	A	240	TRP
1	A	282	LEU
1	A	301	GLU
1	A	321	ARG
1	A	325	ARG
1	A	345	GLU
1	A	352	LEU
1	A	363	LEU
1	A	388	GLU
1	A	401	GLU
1	A	413	ARG
1	A	472	LYS
1	A	491	ARG
1	A	503	PHE
1	A	526	HIS
1	A	539	LEU
1	A	542	SER
1	A	546	GLN
1	A	582	GLU
1	A	623	TRP
1	A	735	ARG
1	A	736	GLU
1	A	800	SER
1	A	813	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	451	HIS

5.3.3 RNA

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)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	GOL	A	901	-	5,5,5	0.12	0	5,5,5	0.22	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
2	GOL	A	901	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-C3

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	791/834 (94%)	0.29	42 (5%) 26 12	65, 88, 120, 132	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	THR	6.1
1	A	273	VAL	4.7
1	A	447	HIS	3.8
1	A	464	THR	3.8
1	A	10	THR	3.7
1	A	246	THR	3.7
1	A	280	GLU	3.6
1	A	514	LEU	3.6
1	A	69	TRP	3.3
1	A	518	THR	3.3
1	A	449	THR	3.1
1	A	277	GLU	3.1
1	A	431	ASN	3.1
1	A	461	PRO	2.9
1	A	519	PRO	2.9
1	A	429	ALA	2.9
1	A	367	SER	2.8
1	A	538	MET	2.7
1	A	279	THR	2.7
1	A	413	ARG	2.7
1	A	276	GLY	2.5
1	A	275	ALA	2.4
1	A	272	ALA	2.4
1	A	388	GLU	2.4
1	A	427	ARG	2.4
1	A	554	GLU	2.4
1	A	284	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	2.3
1	A	278	VAL	2.3
1	A	462	ARG	2.3
1	A	512	VAL	2.3
1	A	546	GLN	2.3
1	A	549	GLN	2.3
1	A	515	THR	2.2
1	A	402	GLU	2.2
1	A	368	ALA	2.1
1	A	247	THR	2.1
1	A	29	LEU	2.1
1	A	366	GLY	2.0
1	A	424	ILE	2.0
1	A	537	THR	2.0
1	A	414	ALA	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	GOL	A	901	6/6	0.78	0.68	110,110,111,111	8

6.5 Other polymers (i)

There are no such residues in this entry.