wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 11:41 PM EDT

PDB ID	:	6D8K
Title	:	Bacteroides multiple species beta-glucuronidase
Authors	:	Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-04-26
Resolution	:	2.65 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 (i)) were used in the production of this report:

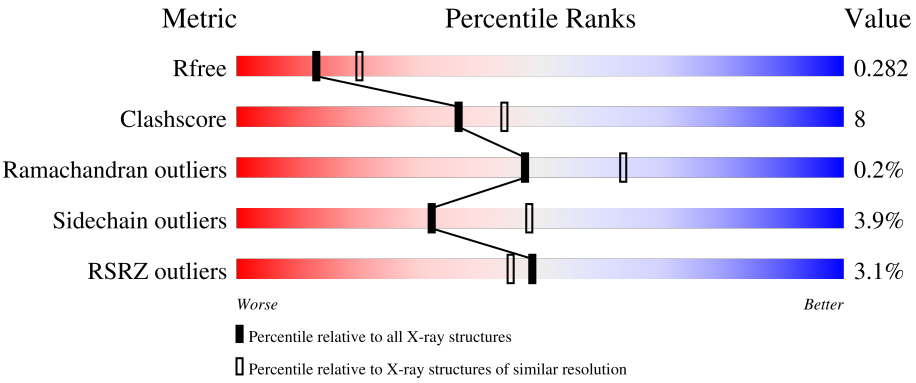
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

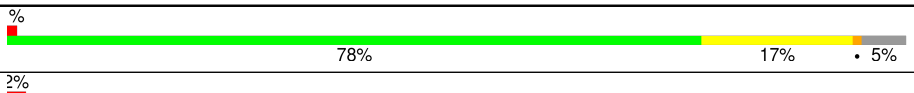
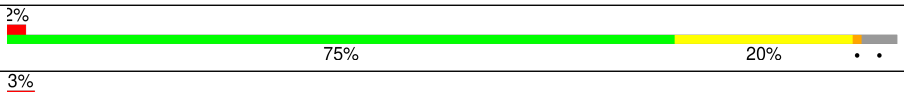
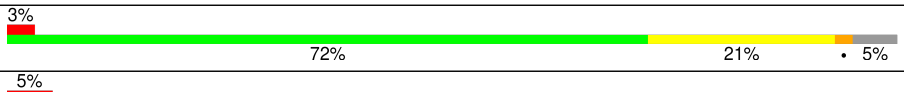
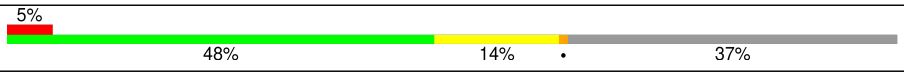
The reported resolution of this entry is 2.65 Å.

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	597	
1	B	597	
1	C	597	
1	D	597	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17233 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 Glycosyl hydrolase family 2, sugar binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4676	2979	813	866	18			
1	B	571	Total	C	N	O	S	0	0	0
			4687	2988	814	867	18			
1	C	569	Total	C	N	O	S	0	0	0
			4667	2974	811	864	18			
1	D	375	Total	C	N	O	S	0	0	0
			3093	1967	546	569	11			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A139KTC9
A	2	GLN	-	expression tag	UNP A0A139KTC9
A	3	ILE	-	expression tag	UNP A0A139KTC9
A	4	ARG	-	expression tag	UNP A0A139KTC9
A	5	LYS	-	expression tag	UNP A0A139KTC9
A	6	LYS	-	expression tag	UNP A0A139KTC9
A	7	THR	-	expression tag	UNP A0A139KTC9
A	8	ILE	-	expression tag	UNP A0A139KTC9
A	9	VAL	-	expression tag	UNP A0A139KTC9
A	10	CYS	-	expression tag	UNP A0A139KTC9
A	11	MET	-	expression tag	UNP A0A139KTC9
A	12	LEU	-	expression tag	UNP A0A139KTC9
A	13	LEU	-	expression tag	UNP A0A139KTC9
A	14	PHE	-	expression tag	UNP A0A139KTC9
A	15	ILE	-	expression tag	UNP A0A139KTC9
A	16	LEU	-	expression tag	UNP A0A139KTC9
A	17	PHE	-	expression tag	UNP A0A139KTC9
A	18	VAL	-	expression tag	UNP A0A139KTC9
A	19	GLY	-	expression tag	UNP A0A139KTC9
A	20	ASN	-	expression tag	UNP A0A139KTC9
A	21	ALA	-	expression tag	UNP A0A139KTC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	VAL	-	expression tag	UNP A0A139KTC9
A	23	ALA	-	expression tag	UNP A0A139KTC9
A	24	GLN	-	expression tag	UNP A0A139KTC9
A	25	GLN	-	expression tag	UNP A0A139KTC9
A	26	ASN	-	expression tag	UNP A0A139KTC9
A	568	TRP	-	expression tag	UNP A0A139KTC9
A	569	ASN	-	expression tag	UNP A0A139KTC9
A	570	ARG	-	expression tag	UNP A0A139KTC9
A	571	LYS	-	expression tag	UNP A0A139KTC9
A	572	GLY	-	expression tag	UNP A0A139KTC9
A	573	LEU	-	expression tag	UNP A0A139KTC9
A	574	VAL	-	expression tag	UNP A0A139KTC9
A	575	SER	-	expression tag	UNP A0A139KTC9
A	576	ASP	-	expression tag	UNP A0A139KTC9
A	577	GLN	-	expression tag	UNP A0A139KTC9
A	578	GLY	-	expression tag	UNP A0A139KTC9
A	579	ILE	-	expression tag	UNP A0A139KTC9
A	580	ARG	-	expression tag	UNP A0A139KTC9
A	581	LYS	-	expression tag	UNP A0A139KTC9
A	582	LYS	-	expression tag	UNP A0A139KTC9
A	583	ALA	-	expression tag	UNP A0A139KTC9
A	584	TRP	-	expression tag	UNP A0A139KTC9
A	585	TYR	-	expression tag	UNP A0A139KTC9
A	586	LEU	-	expression tag	UNP A0A139KTC9
A	587	MET	-	expression tag	UNP A0A139KTC9
A	588	ARG	-	expression tag	UNP A0A139KTC9
A	589	GLU	-	expression tag	UNP A0A139KTC9
A	590	TYR	-	expression tag	UNP A0A139KTC9
A	591	TYR	-	expression tag	UNP A0A139KTC9
A	592	LYS	-	expression tag	UNP A0A139KTC9
A	593	THR	-	expression tag	UNP A0A139KTC9
A	594	LYS	-	expression tag	UNP A0A139KTC9
A	595	PHE	-	expression tag	UNP A0A139KTC9
A	596	GLY	-	expression tag	UNP A0A139KTC9
A	597	GLU	-	expression tag	UNP A0A139KTC9
B	1	MET	-	initiating methionine	UNP A0A139KTC9
B	2	GLN	-	expression tag	UNP A0A139KTC9
B	3	ILE	-	expression tag	UNP A0A139KTC9
B	4	ARG	-	expression tag	UNP A0A139KTC9
B	5	LYS	-	expression tag	UNP A0A139KTC9
B	6	LYS	-	expression tag	UNP A0A139KTC9
B	7	THR	-	expression tag	UNP A0A139KTC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ILE	-	expression tag	UNP A0A139KTC9
B	9	VAL	-	expression tag	UNP A0A139KTC9
B	10	CYS	-	expression tag	UNP A0A139KTC9
B	11	MET	-	expression tag	UNP A0A139KTC9
B	12	LEU	-	expression tag	UNP A0A139KTC9
B	13	LEU	-	expression tag	UNP A0A139KTC9
B	14	PHE	-	expression tag	UNP A0A139KTC9
B	15	ILE	-	expression tag	UNP A0A139KTC9
B	16	LEU	-	expression tag	UNP A0A139KTC9
B	17	PHE	-	expression tag	UNP A0A139KTC9
B	18	VAL	-	expression tag	UNP A0A139KTC9
B	19	GLY	-	expression tag	UNP A0A139KTC9
B	20	ASN	-	expression tag	UNP A0A139KTC9
B	21	ALA	-	expression tag	UNP A0A139KTC9
B	22	VAL	-	expression tag	UNP A0A139KTC9
B	23	ALA	-	expression tag	UNP A0A139KTC9
B	24	GLN	-	expression tag	UNP A0A139KTC9
B	25	GLN	-	expression tag	UNP A0A139KTC9
B	26	ASN	-	expression tag	UNP A0A139KTC9
B	568	TRP	-	expression tag	UNP A0A139KTC9
B	569	ASN	-	expression tag	UNP A0A139KTC9
B	570	ARG	-	expression tag	UNP A0A139KTC9
B	571	LYS	-	expression tag	UNP A0A139KTC9
B	572	GLY	-	expression tag	UNP A0A139KTC9
B	573	LEU	-	expression tag	UNP A0A139KTC9
B	574	VAL	-	expression tag	UNP A0A139KTC9
B	575	SER	-	expression tag	UNP A0A139KTC9
B	576	ASP	-	expression tag	UNP A0A139KTC9
B	577	GLN	-	expression tag	UNP A0A139KTC9
B	578	GLY	-	expression tag	UNP A0A139KTC9
B	579	ILE	-	expression tag	UNP A0A139KTC9
B	580	ARG	-	expression tag	UNP A0A139KTC9
B	581	LYS	-	expression tag	UNP A0A139KTC9
B	582	LYS	-	expression tag	UNP A0A139KTC9
B	583	ALA	-	expression tag	UNP A0A139KTC9
B	584	TRP	-	expression tag	UNP A0A139KTC9
B	585	TYR	-	expression tag	UNP A0A139KTC9
B	586	LEU	-	expression tag	UNP A0A139KTC9
B	587	MET	-	expression tag	UNP A0A139KTC9
B	588	ARG	-	expression tag	UNP A0A139KTC9
B	589	GLU	-	expression tag	UNP A0A139KTC9
B	590	TYR	-	expression tag	UNP A0A139KTC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	591	TYR	-	expression tag	UNP A0A139KTC9
B	592	LYS	-	expression tag	UNP A0A139KTC9
B	593	THR	-	expression tag	UNP A0A139KTC9
B	594	LYS	-	expression tag	UNP A0A139KTC9
B	595	PHE	-	expression tag	UNP A0A139KTC9
B	596	GLY	-	expression tag	UNP A0A139KTC9
B	597	GLU	-	expression tag	UNP A0A139KTC9
C	1	MET	-	initiating methionine	UNP A0A139KTC9
C	2	GLN	-	expression tag	UNP A0A139KTC9
C	3	ILE	-	expression tag	UNP A0A139KTC9
C	4	ARG	-	expression tag	UNP A0A139KTC9
C	5	LYS	-	expression tag	UNP A0A139KTC9
C	6	LYS	-	expression tag	UNP A0A139KTC9
C	7	THR	-	expression tag	UNP A0A139KTC9
C	8	ILE	-	expression tag	UNP A0A139KTC9
C	9	VAL	-	expression tag	UNP A0A139KTC9
C	10	CYS	-	expression tag	UNP A0A139KTC9
C	11	MET	-	expression tag	UNP A0A139KTC9
C	12	LEU	-	expression tag	UNP A0A139KTC9
C	13	LEU	-	expression tag	UNP A0A139KTC9
C	14	PHE	-	expression tag	UNP A0A139KTC9
C	15	ILE	-	expression tag	UNP A0A139KTC9
C	16	LEU	-	expression tag	UNP A0A139KTC9
C	17	PHE	-	expression tag	UNP A0A139KTC9
C	18	VAL	-	expression tag	UNP A0A139KTC9
C	19	GLY	-	expression tag	UNP A0A139KTC9
C	20	ASN	-	expression tag	UNP A0A139KTC9
C	21	ALA	-	expression tag	UNP A0A139KTC9
C	22	VAL	-	expression tag	UNP A0A139KTC9
C	23	ALA	-	expression tag	UNP A0A139KTC9
C	24	GLN	-	expression tag	UNP A0A139KTC9
C	25	GLN	-	expression tag	UNP A0A139KTC9
C	26	ASN	-	expression tag	UNP A0A139KTC9
C	568	TRP	-	expression tag	UNP A0A139KTC9
C	569	ASN	-	expression tag	UNP A0A139KTC9
C	570	ARG	-	expression tag	UNP A0A139KTC9
C	571	LYS	-	expression tag	UNP A0A139KTC9
C	572	GLY	-	expression tag	UNP A0A139KTC9
C	573	LEU	-	expression tag	UNP A0A139KTC9
C	574	VAL	-	expression tag	UNP A0A139KTC9
C	575	SER	-	expression tag	UNP A0A139KTC9
C	576	ASP	-	expression tag	UNP A0A139KTC9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	577	GLN	-	expression tag	UNP A0A139KTC9
C	578	GLY	-	expression tag	UNP A0A139KTC9
C	579	ILE	-	expression tag	UNP A0A139KTC9
C	580	ARG	-	expression tag	UNP A0A139KTC9
C	581	LYS	-	expression tag	UNP A0A139KTC9
C	582	LYS	-	expression tag	UNP A0A139KTC9
C	583	ALA	-	expression tag	UNP A0A139KTC9
C	584	TRP	-	expression tag	UNP A0A139KTC9
C	585	TYR	-	expression tag	UNP A0A139KTC9
C	586	LEU	-	expression tag	UNP A0A139KTC9
C	587	MET	-	expression tag	UNP A0A139KTC9
C	588	ARG	-	expression tag	UNP A0A139KTC9
C	589	GLU	-	expression tag	UNP A0A139KTC9
C	590	TYR	-	expression tag	UNP A0A139KTC9
C	591	TYR	-	expression tag	UNP A0A139KTC9
C	592	LYS	-	expression tag	UNP A0A139KTC9
C	593	THR	-	expression tag	UNP A0A139KTC9
C	594	LYS	-	expression tag	UNP A0A139KTC9
C	595	PHE	-	expression tag	UNP A0A139KTC9
C	596	GLY	-	expression tag	UNP A0A139KTC9
C	597	GLU	-	expression tag	UNP A0A139KTC9
D	1	MET	-	initiating methionine	UNP A0A139KTC9
D	2	GLN	-	expression tag	UNP A0A139KTC9
D	3	ILE	-	expression tag	UNP A0A139KTC9
D	4	ARG	-	expression tag	UNP A0A139KTC9
D	5	LYS	-	expression tag	UNP A0A139KTC9
D	6	LYS	-	expression tag	UNP A0A139KTC9
D	7	THR	-	expression tag	UNP A0A139KTC9
D	8	ILE	-	expression tag	UNP A0A139KTC9
D	9	VAL	-	expression tag	UNP A0A139KTC9
D	10	CYS	-	expression tag	UNP A0A139KTC9
D	11	MET	-	expression tag	UNP A0A139KTC9
D	12	LEU	-	expression tag	UNP A0A139KTC9
D	13	LEU	-	expression tag	UNP A0A139KTC9
D	14	PHE	-	expression tag	UNP A0A139KTC9
D	15	ILE	-	expression tag	UNP A0A139KTC9
D	16	LEU	-	expression tag	UNP A0A139KTC9
D	17	PHE	-	expression tag	UNP A0A139KTC9
D	18	VAL	-	expression tag	UNP A0A139KTC9
D	19	GLY	-	expression tag	UNP A0A139KTC9
D	20	ASN	-	expression tag	UNP A0A139KTC9
D	21	ALA	-	expression tag	UNP A0A139KTC9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	VAL	-	expression tag	UNP A0A139KTC9
D	23	ALA	-	expression tag	UNP A0A139KTC9
D	24	GLN	-	expression tag	UNP A0A139KTC9
D	25	GLN	-	expression tag	UNP A0A139KTC9
D	26	ASN	-	expression tag	UNP A0A139KTC9
D	568	TRP	-	expression tag	UNP A0A139KTC9
D	569	ASN	-	expression tag	UNP A0A139KTC9
D	570	ARG	-	expression tag	UNP A0A139KTC9
D	571	LYS	-	expression tag	UNP A0A139KTC9
D	572	GLY	-	expression tag	UNP A0A139KTC9
D	573	LEU	-	expression tag	UNP A0A139KTC9
D	574	VAL	-	expression tag	UNP A0A139KTC9
D	575	SER	-	expression tag	UNP A0A139KTC9
D	576	ASP	-	expression tag	UNP A0A139KTC9
D	577	GLN	-	expression tag	UNP A0A139KTC9
D	578	GLY	-	expression tag	UNP A0A139KTC9
D	579	ILE	-	expression tag	UNP A0A139KTC9
D	580	ARG	-	expression tag	UNP A0A139KTC9
D	581	LYS	-	expression tag	UNP A0A139KTC9
D	582	LYS	-	expression tag	UNP A0A139KTC9
D	583	ALA	-	expression tag	UNP A0A139KTC9
D	584	TRP	-	expression tag	UNP A0A139KTC9
D	585	TYR	-	expression tag	UNP A0A139KTC9
D	586	LEU	-	expression tag	UNP A0A139KTC9
D	587	MET	-	expression tag	UNP A0A139KTC9
D	588	ARG	-	expression tag	UNP A0A139KTC9
D	589	GLU	-	expression tag	UNP A0A139KTC9
D	590	TYR	-	expression tag	UNP A0A139KTC9
D	591	TYR	-	expression tag	UNP A0A139KTC9
D	592	LYS	-	expression tag	UNP A0A139KTC9
D	593	THR	-	expression tag	UNP A0A139KTC9
D	594	LYS	-	expression tag	UNP A0A139KTC9
D	595	PHE	-	expression tag	UNP A0A139KTC9
D	596	GLY	-	expression tag	UNP A0A139KTC9
D	597	GLU	-	expression tag	UNP A0A139KTC9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	39	Total O 39 39	0	0

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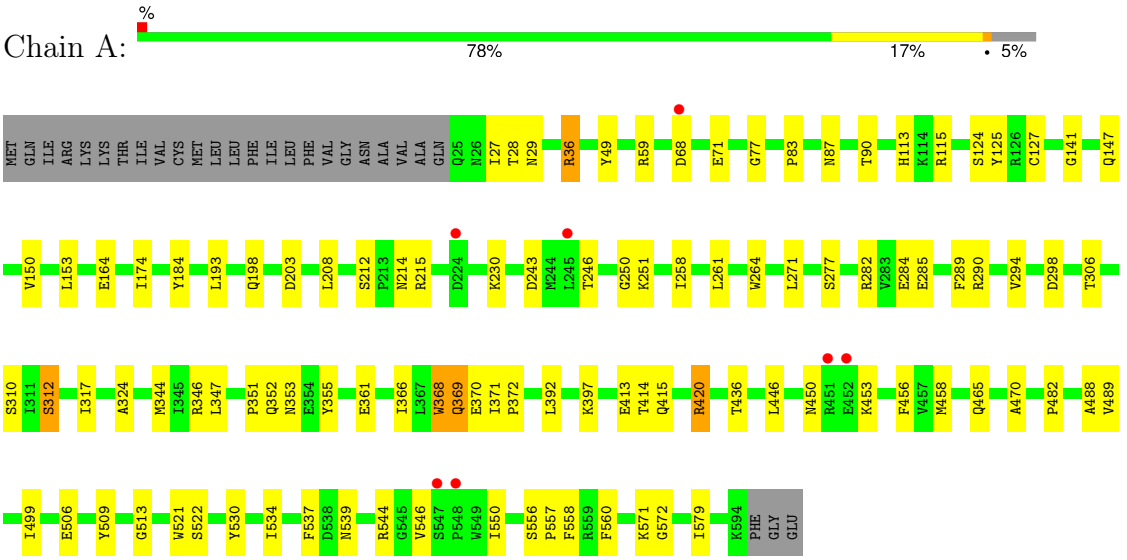
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	23	Total O 23 23	0	0
2	D	14	Total O 14 14	0	0

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.

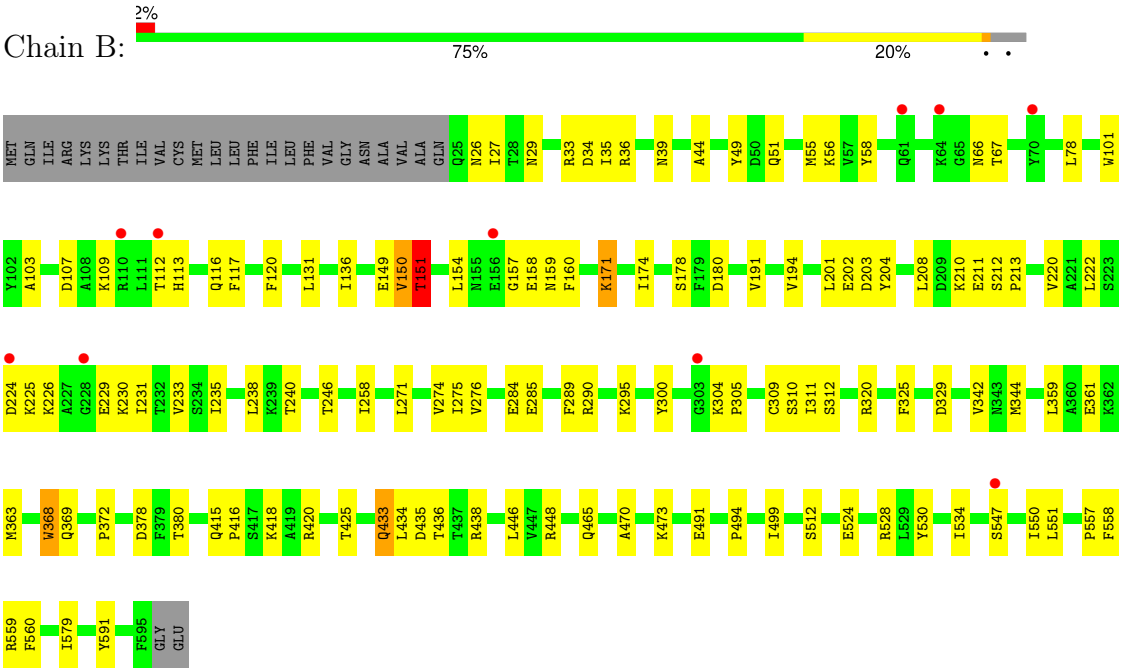
• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain A:



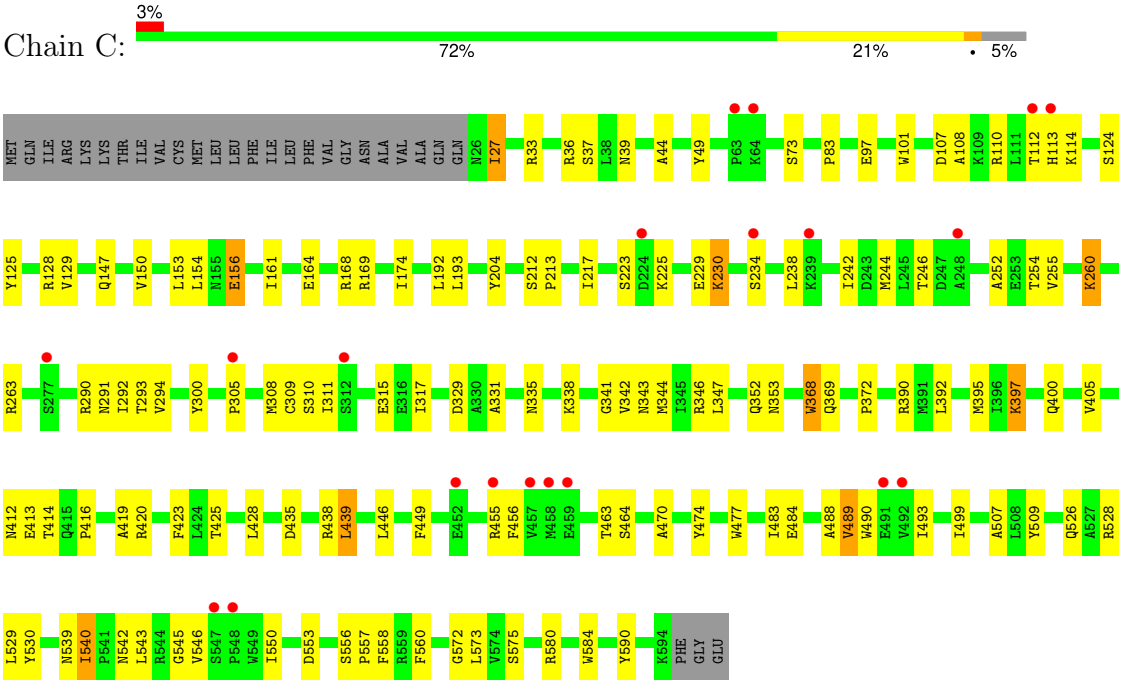
• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain B:



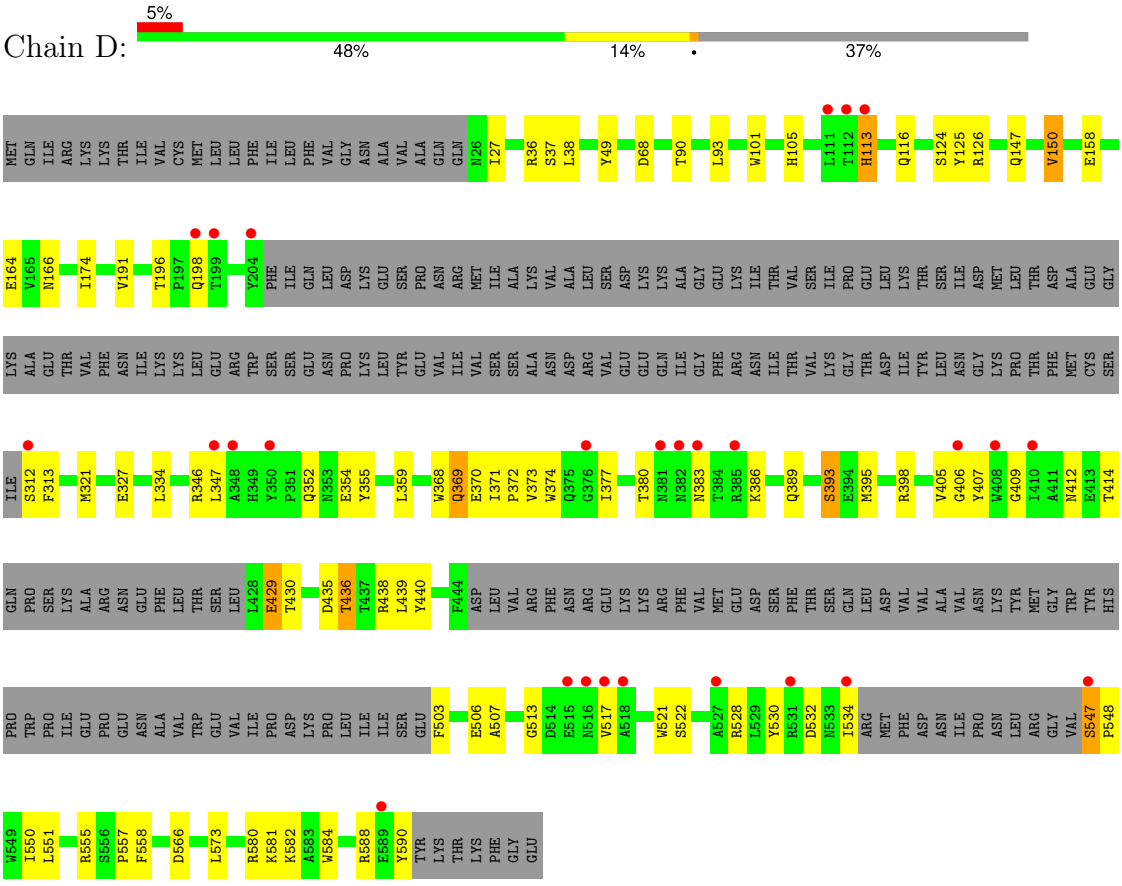
• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain C:



• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	213.46Å 213.46Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 2.65 29.43 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.43-2.65) 99.8 (29.43-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.64Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.207 , 0.283 0.210 , 0.282	Depositor DCC
R_{free} test set	2002 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17233	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

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	0.46	0/4793	0.62	0/6485
1	B	0.46	0/4805	0.62	0/6501
1	C	0.41	0/4784	0.61	0/6473
1	D	0.44	0/3172	0.59	0/4287
All	All	0.44	0/17554	0.61	0/23746

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ASP	Peptide
1	D	68	ASP	Peptide

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	4676	0	4557	53	0
1	B	4687	0	4566	68	0
1	C	4667	0	4549	96	0
1	D	3093	0	2949	57	0
2	A	34	0	0	3	0
2	B	39	0	0	0	0
2	C	23	0	0	1	0
2	D	14	0	0	0	0
All	All	17233	0	16621	265	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 8.

The worst 5 of 265 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:D:312:SER:HB3	1:D:346:ARG:HB3	1.61	0.82
1:D:105:HIS:ND1	1:D:158:GLU:OE2	2.12	0.80
1:A:294:VAL:O	2:A:601:HOH:O	2.00	0.79
1:D:352:GLN:O	1:D:398:ARG:NH2	2.17	0.78
1:C:540:ILE:HD12	1:C:543:LEU:HD11	1.68	0.74

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	568/597 (95%)	530 (93%)	37 (6%)	1 (0%)	47 64
1	B	569/597 (95%)	539 (95%)	27 (5%)	3 (0%)	29 43
1	C	567/597 (95%)	517 (91%)	50 (9%)	0	100 100
1	D	365/597 (61%)	337 (92%)	28 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2069/2388 (87%)	1923 (93%)	142 (7%)	4 (0%)	47 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	THR
1	B	66	ASN
1	B	325	PHE
1	A	482	PRO

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	498/521 (96%)	480 (96%)	18 (4%)	35 51
1	B	499/521 (96%)	479 (96%)	20 (4%)	31 47
1	C	497/521 (95%)	479 (96%)	18 (4%)	35 51
1	D	319/521 (61%)	304 (95%)	15 (5%)	26 40
All	All	1813/2084 (87%)	1742 (96%)	71 (4%)	32 48

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	150	VAL
1	D	198	GLN
1	D	436	THR
1	B	150	VAL
1	B	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	400	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	570/597 (95%)	-0.16	7 (1%)	79	77	34, 55, 81, 102	0
1	B	571/597 (95%)	-0.04	10 (1%)	68	65	37, 59, 89, 101	0
1	C	569/597 (95%)	0.05	20 (3%)	44	40	39, 67, 96, 116	0
1	D	375/597 (62%)	0.19	27 (7%)	15	12	37, 68, 95, 102	0
All	All	2085/2388 (87%)	-0.01	64 (3%)	49	45	34, 61, 93, 116	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	517	VAL	5.0
1	C	64	LYS	4.4
1	D	312	SER	4.2
1	C	452	GLU	3.9
1	C	305	PRO	3.5

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.