wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 01:00 PM JST

PDB ID	:	8J53
Title	:	Crystal structure of Bacteroides salyersiae GH31 alpha-galactosidase
Authors	:	Ikegaya, M.; Miyazaki, T.
Deposited on	:	2023-04-21
Resolution	:	3.50 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:

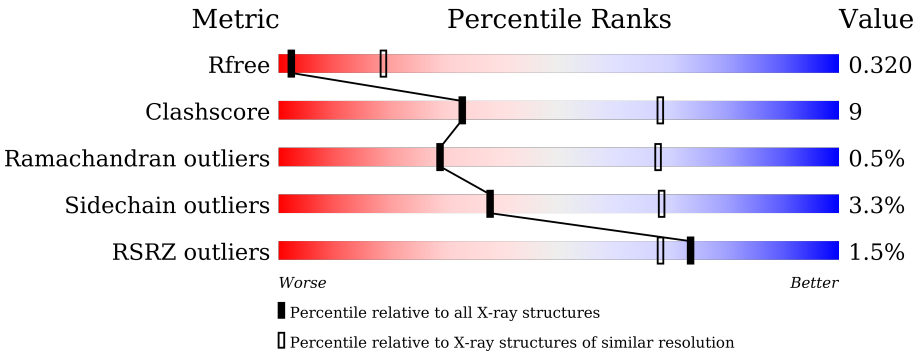
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	532	72% 22% • 5%
1	B	532	% 76% 18% • 5%
1	C	532	% 74% 20% • 5%
1	D	532	3% 74% 20% •• •
1	E	532	% 76% 18% • •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 40710 atoms, of which 20099 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 GH31 alpha-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	507	Total	C	H	N	O	S	96	0	0
			8136	2654	4019	686	748	29			
1	B	503	Total	C	H	N	O	S	96	0	0
			8064	2632	3980	681	742	29			
1	C	508	Total	C	H	N	O	S	96	0	0
			8150	2658	4025	688	750	29			
1	D	510	Total	C	H	N	O	S	97	0	0
			8178	2666	4038	691	754	29			
1	E	511	Total	C	H	N	O	S	100	0	0
			8182	2668	4037	692	755	30			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7J4XIY8
A	2	GLY	-	expression tag	UNP A0A7J4XIY8
A	3	SER	-	expression tag	UNP A0A7J4XIY8
A	4	SER	-	expression tag	UNP A0A7J4XIY8
A	5	HIS	-	expression tag	UNP A0A7J4XIY8
A	6	HIS	-	expression tag	UNP A0A7J4XIY8
A	7	HIS	-	expression tag	UNP A0A7J4XIY8
A	8	HIS	-	expression tag	UNP A0A7J4XIY8
A	9	HIS	-	expression tag	UNP A0A7J4XIY8
A	10	HIS	-	expression tag	UNP A0A7J4XIY8
A	11	SER	-	expression tag	UNP A0A7J4XIY8
A	12	SER	-	expression tag	UNP A0A7J4XIY8
A	13	GLY	-	expression tag	UNP A0A7J4XIY8
A	14	LEU	-	expression tag	UNP A0A7J4XIY8
A	15	VAL	-	expression tag	UNP A0A7J4XIY8
A	16	PRO	-	expression tag	UNP A0A7J4XIY8
A	17	ARG	-	expression tag	UNP A0A7J4XIY8
A	18	GLY	-	expression tag	UNP A0A7J4XIY8
A	19	SER	-	expression tag	UNP A0A7J4XIY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	HIS	-	expression tag	UNP A0A7J4XIY8
A	21	MET	-	expression tag	UNP A0A7J4XIY8
A	22	ALA	-	expression tag	UNP A0A7J4XIY8
A	23	SER	-	expression tag	UNP A0A7J4XIY8
A	24	GLN	-	expression tag	UNP A0A7J4XIY8
A	25	ASN	-	expression tag	UNP A0A7J4XIY8
A	26	VAL	-	expression tag	UNP A0A7J4XIY8
A	27	PHE	-	expression tag	UNP A0A7J4XIY8
A	28	THR	-	expression tag	UNP A0A7J4XIY8
B	1	MET	-	initiating methionine	UNP A0A7J4XIY8
B	2	GLY	-	expression tag	UNP A0A7J4XIY8
B	3	SER	-	expression tag	UNP A0A7J4XIY8
B	4	SER	-	expression tag	UNP A0A7J4XIY8
B	5	HIS	-	expression tag	UNP A0A7J4XIY8
B	6	HIS	-	expression tag	UNP A0A7J4XIY8
B	7	HIS	-	expression tag	UNP A0A7J4XIY8
B	8	HIS	-	expression tag	UNP A0A7J4XIY8
B	9	HIS	-	expression tag	UNP A0A7J4XIY8
B	10	HIS	-	expression tag	UNP A0A7J4XIY8
B	11	SER	-	expression tag	UNP A0A7J4XIY8
B	12	SER	-	expression tag	UNP A0A7J4XIY8
B	13	GLY	-	expression tag	UNP A0A7J4XIY8
B	14	LEU	-	expression tag	UNP A0A7J4XIY8
B	15	VAL	-	expression tag	UNP A0A7J4XIY8
B	16	PRO	-	expression tag	UNP A0A7J4XIY8
B	17	ARG	-	expression tag	UNP A0A7J4XIY8
B	18	GLY	-	expression tag	UNP A0A7J4XIY8
B	19	SER	-	expression tag	UNP A0A7J4XIY8
B	20	HIS	-	expression tag	UNP A0A7J4XIY8
B	21	MET	-	expression tag	UNP A0A7J4XIY8
B	22	ALA	-	expression tag	UNP A0A7J4XIY8
B	23	SER	-	expression tag	UNP A0A7J4XIY8
B	24	GLN	-	expression tag	UNP A0A7J4XIY8
B	25	ASN	-	expression tag	UNP A0A7J4XIY8
B	26	VAL	-	expression tag	UNP A0A7J4XIY8
B	27	PHE	-	expression tag	UNP A0A7J4XIY8
B	28	THR	-	expression tag	UNP A0A7J4XIY8
C	1	MET	-	initiating methionine	UNP A0A7J4XIY8
C	2	GLY	-	expression tag	UNP A0A7J4XIY8
C	3	SER	-	expression tag	UNP A0A7J4XIY8
C	4	SER	-	expression tag	UNP A0A7J4XIY8
C	5	HIS	-	expression tag	UNP A0A7J4XIY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP A0A7J4XIY8
C	7	HIS	-	expression tag	UNP A0A7J4XIY8
C	8	HIS	-	expression tag	UNP A0A7J4XIY8
C	9	HIS	-	expression tag	UNP A0A7J4XIY8
C	10	HIS	-	expression tag	UNP A0A7J4XIY8
C	11	SER	-	expression tag	UNP A0A7J4XIY8
C	12	SER	-	expression tag	UNP A0A7J4XIY8
C	13	GLY	-	expression tag	UNP A0A7J4XIY8
C	14	LEU	-	expression tag	UNP A0A7J4XIY8
C	15	VAL	-	expression tag	UNP A0A7J4XIY8
C	16	PRO	-	expression tag	UNP A0A7J4XIY8
C	17	ARG	-	expression tag	UNP A0A7J4XIY8
C	18	GLY	-	expression tag	UNP A0A7J4XIY8
C	19	SER	-	expression tag	UNP A0A7J4XIY8
C	20	HIS	-	expression tag	UNP A0A7J4XIY8
C	21	MET	-	expression tag	UNP A0A7J4XIY8
C	22	ALA	-	expression tag	UNP A0A7J4XIY8
C	23	SER	-	expression tag	UNP A0A7J4XIY8
C	24	GLN	-	expression tag	UNP A0A7J4XIY8
C	25	ASN	-	expression tag	UNP A0A7J4XIY8
C	26	VAL	-	expression tag	UNP A0A7J4XIY8
C	27	PHE	-	expression tag	UNP A0A7J4XIY8
C	28	THR	-	expression tag	UNP A0A7J4XIY8
D	1	MET	-	initiating methionine	UNP A0A7J4XIY8
D	2	GLY	-	expression tag	UNP A0A7J4XIY8
D	3	SER	-	expression tag	UNP A0A7J4XIY8
D	4	SER	-	expression tag	UNP A0A7J4XIY8
D	5	HIS	-	expression tag	UNP A0A7J4XIY8
D	6	HIS	-	expression tag	UNP A0A7J4XIY8
D	7	HIS	-	expression tag	UNP A0A7J4XIY8
D	8	HIS	-	expression tag	UNP A0A7J4XIY8
D	9	HIS	-	expression tag	UNP A0A7J4XIY8
D	10	HIS	-	expression tag	UNP A0A7J4XIY8
D	11	SER	-	expression tag	UNP A0A7J4XIY8
D	12	SER	-	expression tag	UNP A0A7J4XIY8
D	13	GLY	-	expression tag	UNP A0A7J4XIY8
D	14	LEU	-	expression tag	UNP A0A7J4XIY8
D	15	VAL	-	expression tag	UNP A0A7J4XIY8
D	16	PRO	-	expression tag	UNP A0A7J4XIY8
D	17	ARG	-	expression tag	UNP A0A7J4XIY8
D	18	GLY	-	expression tag	UNP A0A7J4XIY8
D	19	SER	-	expression tag	UNP A0A7J4XIY8

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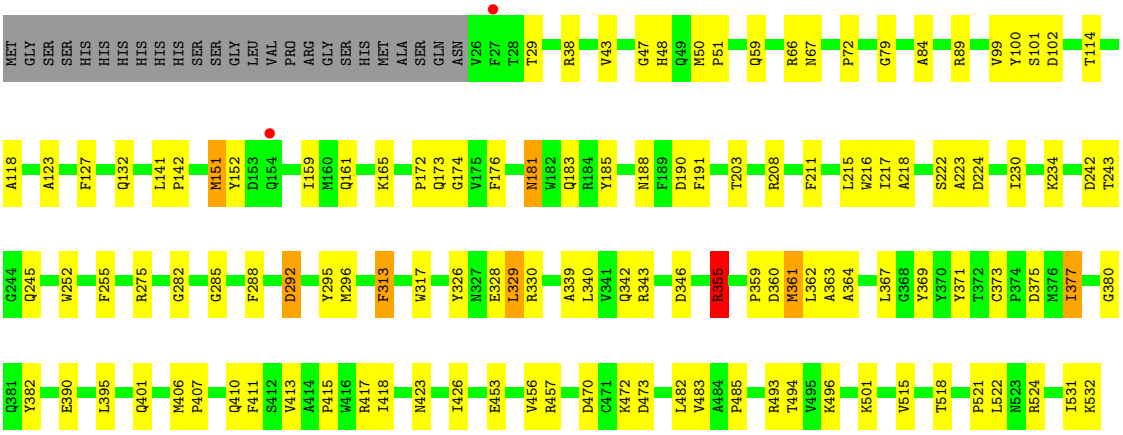
Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP A0A7J4XIY8
D	21	MET	-	expression tag	UNP A0A7J4XIY8
D	22	ALA	-	expression tag	UNP A0A7J4XIY8
D	23	SER	-	expression tag	UNP A0A7J4XIY8
D	24	GLN	-	expression tag	UNP A0A7J4XIY8
D	25	ASN	-	expression tag	UNP A0A7J4XIY8
D	26	VAL	-	expression tag	UNP A0A7J4XIY8
D	27	PHE	-	expression tag	UNP A0A7J4XIY8
D	28	THR	-	expression tag	UNP A0A7J4XIY8
E	1	MET	-	initiating methionine	UNP A0A7J4XIY8
E	2	GLY	-	expression tag	UNP A0A7J4XIY8
E	3	SER	-	expression tag	UNP A0A7J4XIY8
E	4	SER	-	expression tag	UNP A0A7J4XIY8
E	5	HIS	-	expression tag	UNP A0A7J4XIY8
E	6	HIS	-	expression tag	UNP A0A7J4XIY8
E	7	HIS	-	expression tag	UNP A0A7J4XIY8
E	8	HIS	-	expression tag	UNP A0A7J4XIY8
E	9	HIS	-	expression tag	UNP A0A7J4XIY8
E	10	HIS	-	expression tag	UNP A0A7J4XIY8
E	11	SER	-	expression tag	UNP A0A7J4XIY8
E	12	SER	-	expression tag	UNP A0A7J4XIY8
E	13	GLY	-	expression tag	UNP A0A7J4XIY8
E	14	LEU	-	expression tag	UNP A0A7J4XIY8
E	15	VAL	-	expression tag	UNP A0A7J4XIY8
E	16	PRO	-	expression tag	UNP A0A7J4XIY8
E	17	ARG	-	expression tag	UNP A0A7J4XIY8
E	18	GLY	-	expression tag	UNP A0A7J4XIY8
E	19	SER	-	expression tag	UNP A0A7J4XIY8
E	20	HIS	-	expression tag	UNP A0A7J4XIY8
E	21	MET	-	expression tag	UNP A0A7J4XIY8
E	22	ALA	-	expression tag	UNP A0A7J4XIY8
E	23	SER	-	expression tag	UNP A0A7J4XIY8
E	24	GLN	-	expression tag	UNP A0A7J4XIY8
E	25	ASN	-	expression tag	UNP A0A7J4XIY8
E	26	VAL	-	expression tag	UNP A0A7J4XIY8
E	27	PHE	-	expression tag	UNP A0A7J4XIY8
E	28	THR	-	expression tag	UNP A0A7J4XIY8

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.

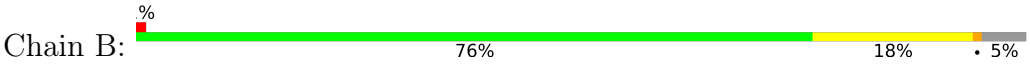
• Molecule 1: GH31 alpha-galactosidase

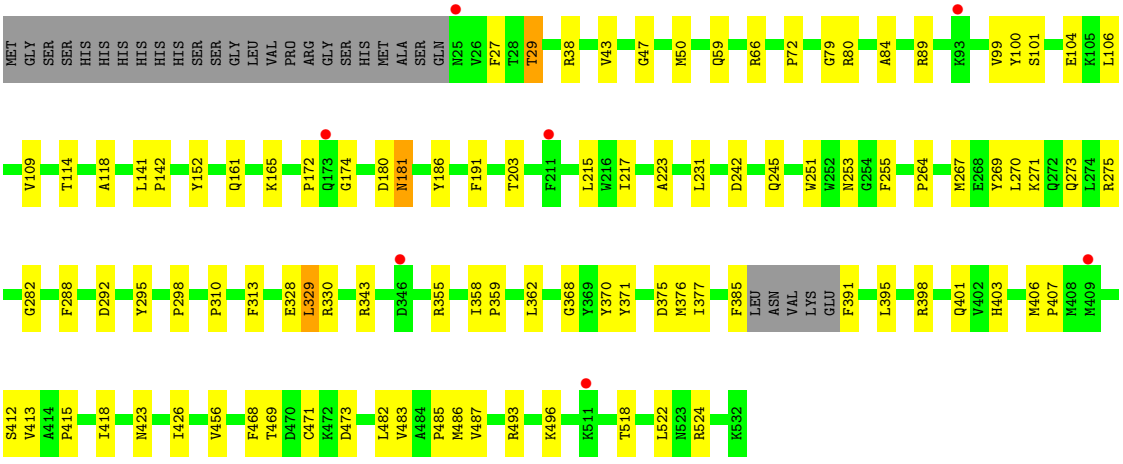
Chain A:



• Molecule 1: GH31 alpha-galactosidase

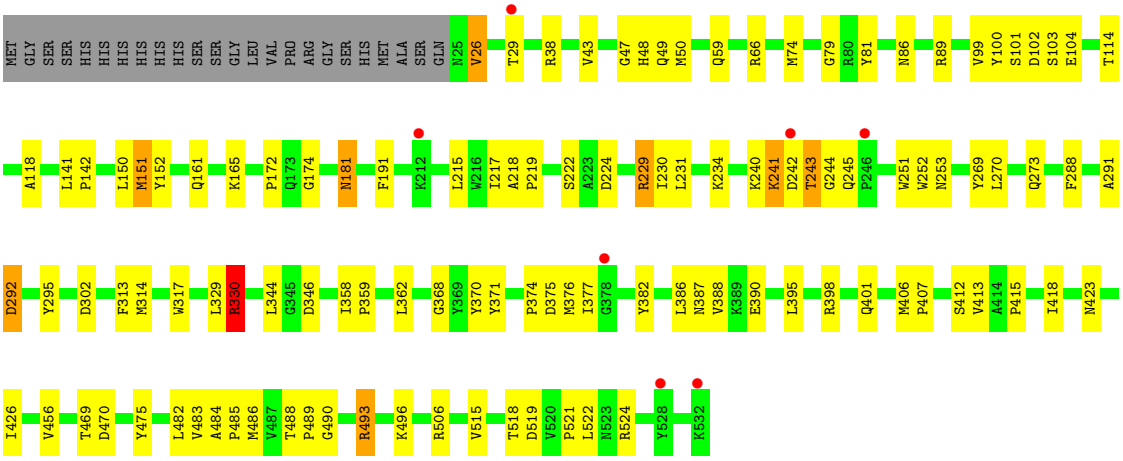
Chain B:





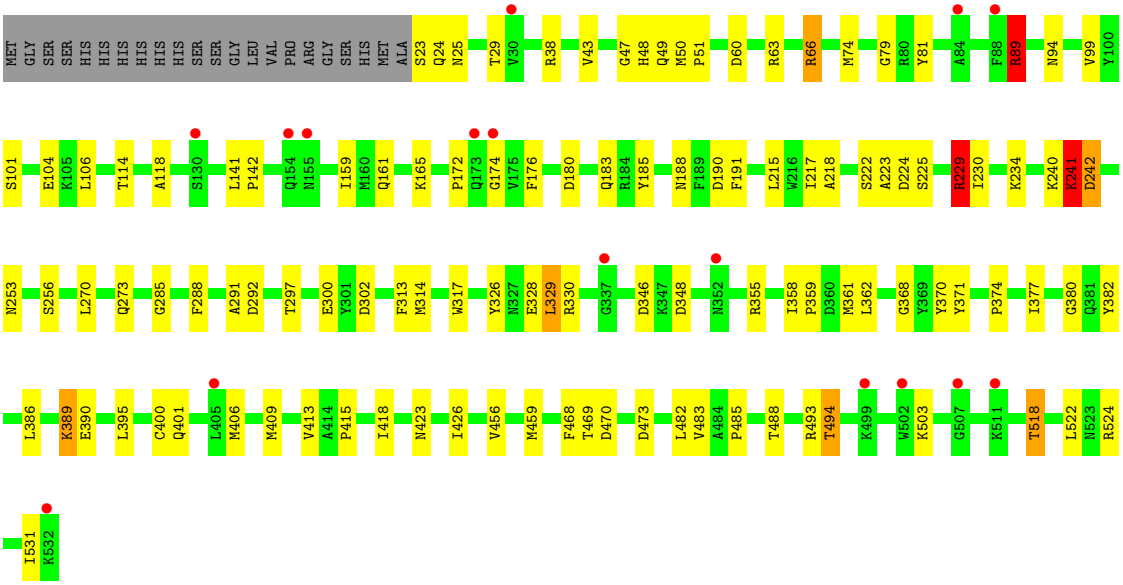
• Molecule 1: GH31 alpha-galactosidase

Chain C:



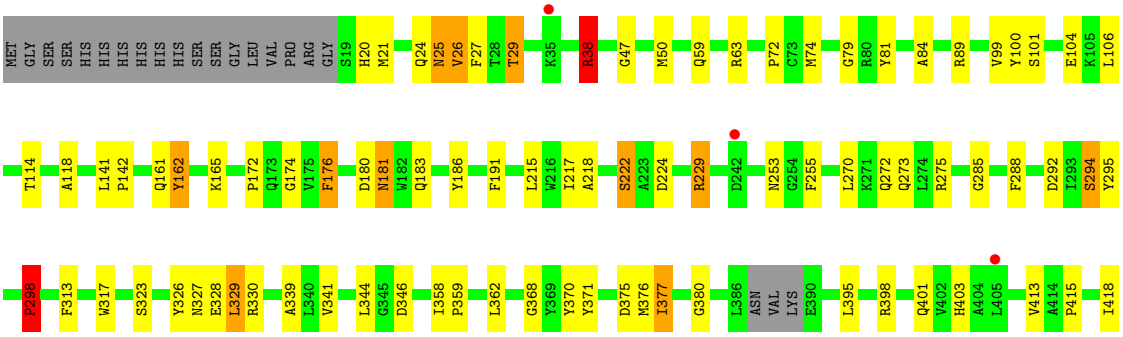
• Molecule 1: GH31 alpha-galactosidase

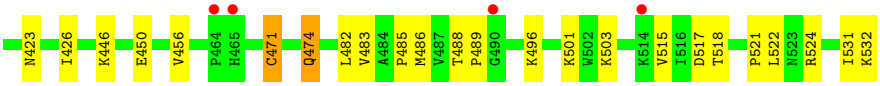
Chain D:



• Molecule 1: GH31 alpha-galactosidase

Chain E:




N423
I426
K446
E450
V456
P464
H465
C471
Q474
L482
V483
A484
P485
M486
V487
T488
P489
G490
K496
K501
W502
K503
K514
V515
I516
D517
T518
P521
L522
N523
R524
I531
K532

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.52Å 157.53Å 131.41Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	48.63 – 3.50 48.59 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-3.50) 100.0 (48.59-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.257 , 0.313 0.270 , 0.320	Depositor DCC
R_{free} test set	2223 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	40710	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.48	0/4237	0.86	1/5733 (0.0%)
1	B	0.46	0/4203	0.82	1/5686 (0.0%)
1	C	0.47	0/4245	0.82	0/5744
1	D	0.46	0/4260	0.81	2/5764 (0.0%)
1	E	0.48	0/4265	0.84	3/5769 (0.1%)
All	All	0.47	0/21210	0.83	7/28696 (0.0%)

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	4
1	C	0	2
1	D	0	3
1	E	0	2
All	All	0	11

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	298	PRO	N-CA-CB	-7.44	94.37	103.30
1	B	343	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	D	89	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	D	229	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	355	ARG	NE-CZ-NH1	-5.88	117.36	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	417	ARG	Sidechain
1	C	229	ARG	Sidechain

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	4117	4019	4008	82	0
1	B	4084	3980	3968	68	0
1	C	4125	4025	4014	68	0
1	D	4140	4038	4027	82	0
1	E	4145	4037	4024	72	0
All	All	20611	20099	20041	355	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 9.

The worst 5 of 355 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:B:355:ARG:HG2	1:B:487:VAL:CG1	2.13	0.78
1:A:493:ARG:NH1	1:A:494:THR:O	2.18	0.77
1:D:29:THR:CG2	1:D:99:VAL:HB	2.14	0.77
1:D:473:ASP:O	1:D:493:ARG:NH2	2.19	0.75
1:A:355:ARG:HH21	1:A:355:ARG:HB2	1.52	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	505/532 (95%)	469 (93%)	34 (7%)	2 (0%)	34	72
1	B	499/532 (94%)	466 (93%)	32 (6%)	1 (0%)	47	81
1	C	506/532 (95%)	468 (92%)	34 (7%)	4 (1%)	19	58
1	D	508/532 (96%)	478 (94%)	29 (6%)	1 (0%)	47	81
1	E	507/532 (95%)	469 (92%)	34 (7%)	4 (1%)	19	58
All	All	2525/2660 (95%)	2350 (93%)	163 (6%)	12 (0%)	29	68

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	26	VAL
1	E	181	ASN
1	A	181	ASN
1	C	26	VAL
1	C	330	ARG

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	435/456 (95%)	424 (98%)	11 (2%)	47	75
1	B	431/456 (94%)	424 (98%)	7 (2%)	62	83
1	C	436/456 (96%)	419 (96%)	17 (4%)	32	64
1	D	438/456 (96%)	423 (97%)	15 (3%)	37	68
1	E	438/456 (96%)	417 (95%)	21 (5%)	25	60
All	All	2178/2280 (96%)	2107 (97%)	71 (3%)	38	68

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

Mol	Chain	Res	Type
1	E	162	TYR
1	E	183	GLN
1	E	329	LEU
1	C	241	LYS
1	C	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	HIS
1	D	64	ASN
1	C	273	GLN
1	D	86	ASN
1	B	132	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)

There are no ligands in this entry.

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	507/532 (95%)	-0.01	2 (0%)	92	90	26, 91, 125, 178	0
1	B	503/532 (94%)	0.13	7 (1%)	75	69	54, 103, 144, 170	0
1	C	508/532 (95%)	0.07	7 (1%)	75	69	37, 100, 137, 186	0
1	D	510/532 (95%)	0.20	16 (3%)	49	43	44, 111, 158, 212	0
1	E	511/532 (96%)	0.19	7 (1%)	75	69	48, 105, 138, 207	0
All	All	2539/2660 (95%)	0.12	39 (1%)	73	68	26, 102, 145, 212	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	TRP	4.1
1	B	173	GLN	3.7
1	D	337	GLY	3.5
1	D	154	GLN	3.2
1	D	405	LEU	3.1

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.