



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:19 PM GMT

PDB ID : 3WQ8  
Title : Monomer structure of hyperthermophilic beta-glucosidase mutant forming a dodecameric structure in the crystal form  
Authors : Nakabayashi, M.; Kataoka, M.; Watanabe, M.; Ishikawa, K.  
Deposited on : 2014-01-23  
Resolution : 2.81 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

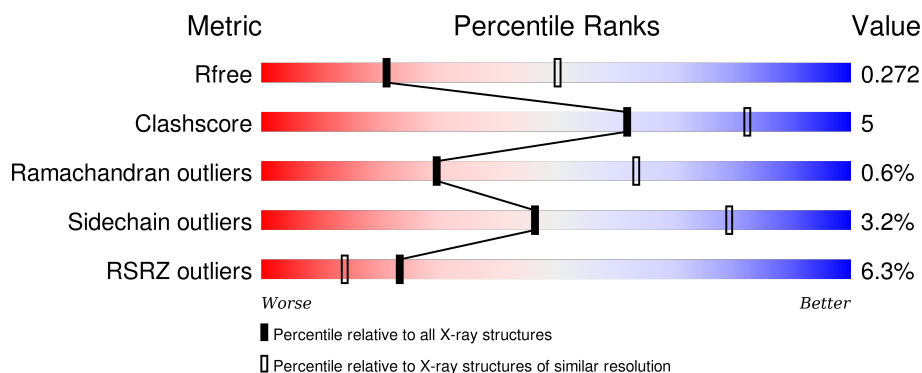
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	450	<div> <div></div> <div>86%12% .</div> </div>
1	B	450	<div> <div>4%</div> <div>86%11% ..</div> </div>
1	C	450	<div> <div>%</div> <div>85%13% ..</div> </div>
1	D	450	<div> <div>3%</div> <div>85%12% ..</div> </div>
1	E	450	<div> <div>%</div> <div>84%14% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	450	<div><div></div><div>30%84%13%..</div></div>
1	G	450	<div><div></div><div>88%11%.</div></div>
1	H	450	<div><div></div><div>3%84%14%.</div></div>
1	I	450	<div><div></div><div>%85%13%..</div></div>
1	J	450	<div><div></div><div>28%82%14%..</div></div>
1	K	450	<div><div></div><div>%83%15%..</div></div>
1	L	450	<div><div></div><div>2%87%12%.</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43762 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 Beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	B	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	C	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	D	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	E	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	F	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	G	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	H	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	I	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	J	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	K	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	L	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q51723
A	1	ALA	-	EXPRESSION TAG	UNP Q51723
A	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
A	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
A	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
A	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
A	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
A	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
B	0	MET	-	EXPRESSION TAG	UNP Q51723
B	1	ALA	-	EXPRESSION TAG	UNP Q51723
B	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
B	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
B	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
B	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
B	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
B	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
C	0	MET	-	EXPRESSION TAG	UNP Q51723
C	1	ALA	-	EXPRESSION TAG	UNP Q51723
C	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
C	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
C	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
C	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
C	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
C	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
D	0	MET	-	EXPRESSION TAG	UNP Q51723
D	1	ALA	-	EXPRESSION TAG	UNP Q51723
D	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
D	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
D	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
D	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
D	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
D	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
E	0	MET	-	EXPRESSION TAG	UNP Q51723
E	1	ALA	-	EXPRESSION TAG	UNP Q51723
E	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
E	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
E	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
E	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
E	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
E	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
F	0	MET	-	EXPRESSION TAG	UNP Q51723
F	1	ALA	-	EXPRESSION TAG	UNP Q51723
F	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
F	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
F	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
F	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
F	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
F	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
G	0	MET	-	EXPRESSION TAG	UNP Q51723
G	1	ALA	-	EXPRESSION TAG	UNP Q51723
G	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
G	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
G	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
G	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
G	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
G	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
H	0	MET	-	EXPRESSION TAG	UNP Q51723
H	1	ALA	-	EXPRESSION TAG	UNP Q51723
H	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
H	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
H	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
H	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
H	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
H	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
I	0	MET	-	EXPRESSION TAG	UNP Q51723
I	1	ALA	-	EXPRESSION TAG	UNP Q51723
I	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
I	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
I	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
I	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
I	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
I	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
J	0	MET	-	EXPRESSION TAG	UNP Q51723
J	1	ALA	-	EXPRESSION TAG	UNP Q51723
J	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
J	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
J	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
J	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
J	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
J	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
K	0	MET	-	EXPRESSION TAG	UNP Q51723
K	1	ALA	-	EXPRESSION TAG	UNP Q51723
K	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
K	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
K	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
K	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
K	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
K	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
L	0	MET	-	EXPRESSION TAG	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ALA	-	EXPRESSION TAG	UNP Q51723
L	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
L	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
L	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
L	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
L	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
L	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723

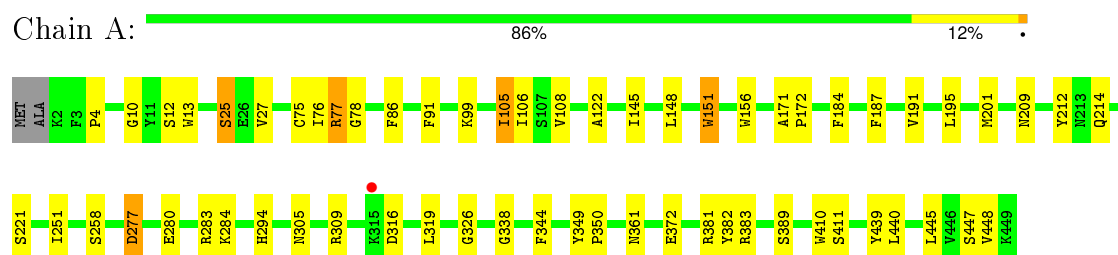
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	10	Total O 10 10	0	0
2	C	16	Total O 16 16	0	0
2	D	11	Total O 11 11	0	0
2	E	20	Total O 20 20	0	0
2	F	3	Total O 3 3	0	0
2	G	11	Total O 11 11	0	0
2	H	5	Total O 5 5	0	0
2	I	16	Total O 16 16	0	0
2	J	2	Total O 2 2	0	0
2	K	9	Total O 9 9	0	0
2	L	9	Total O 9 9	0	0

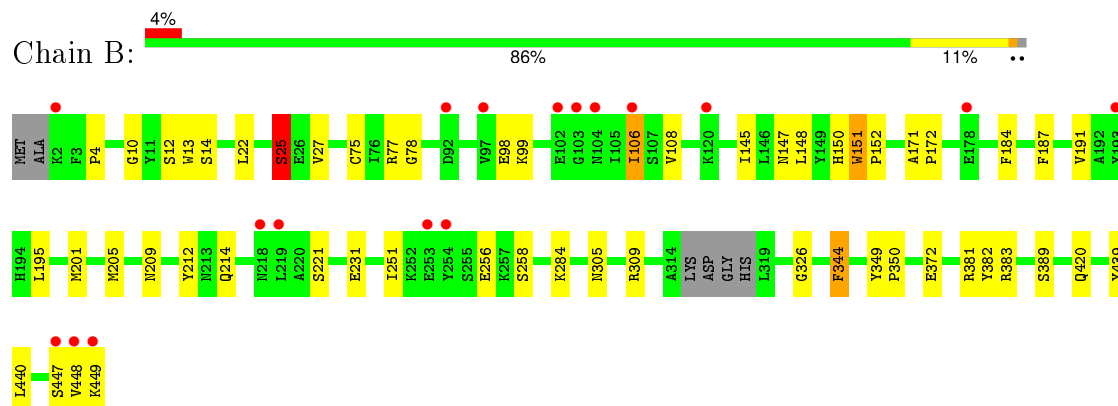
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

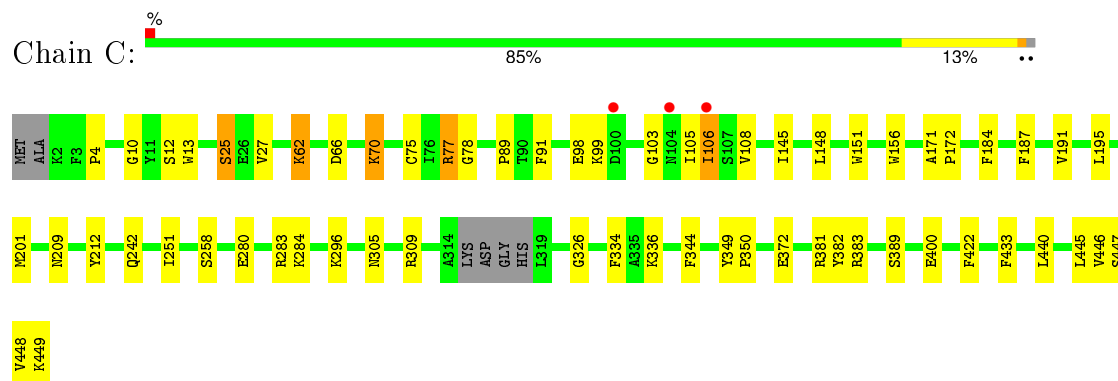
#### • Molecule 1: Beta-glucosidase



#### • Molecule 1: Beta-glucosidase

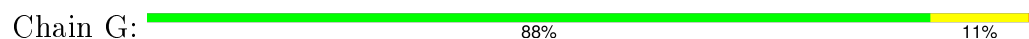
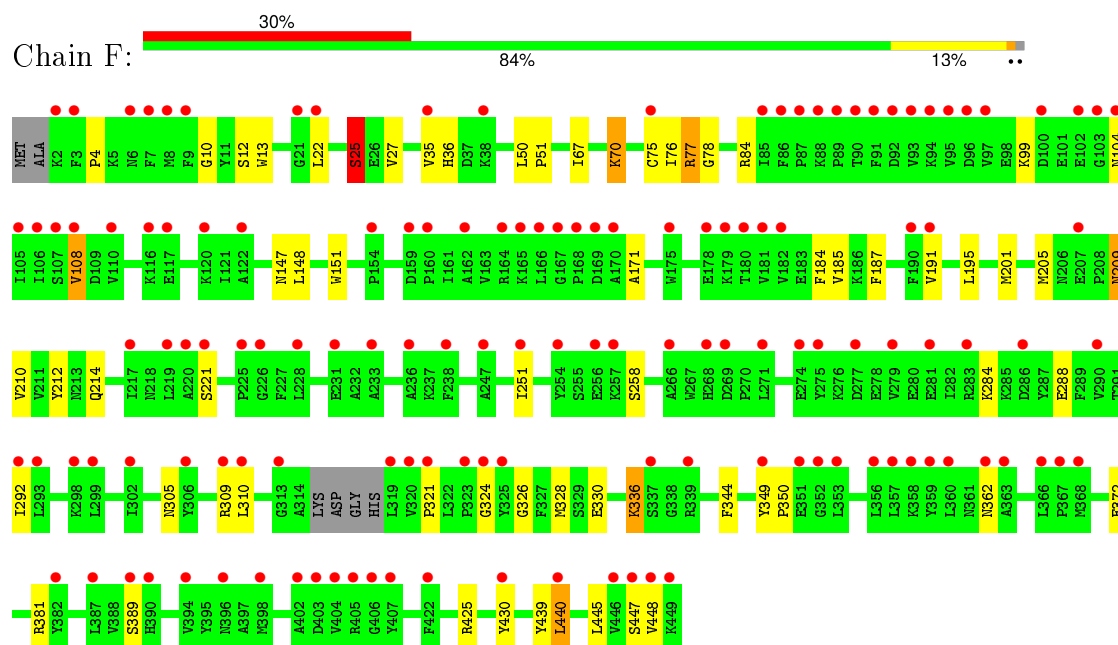
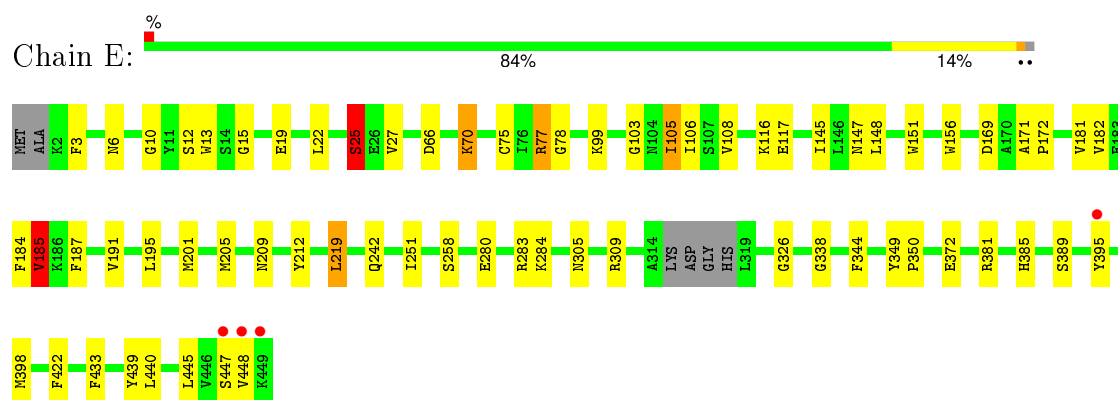
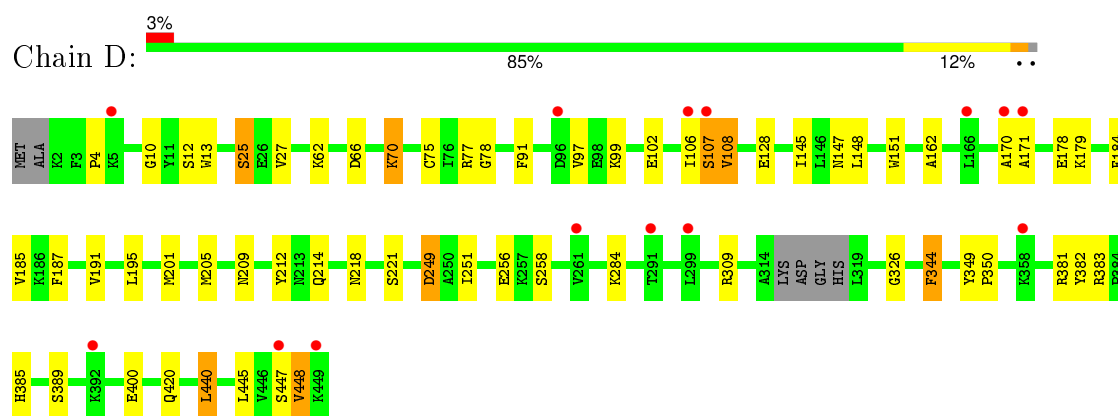


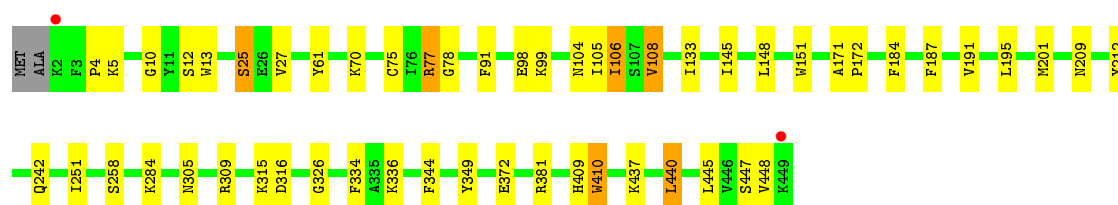
#### • Molecule 1: Beta-glucosidase



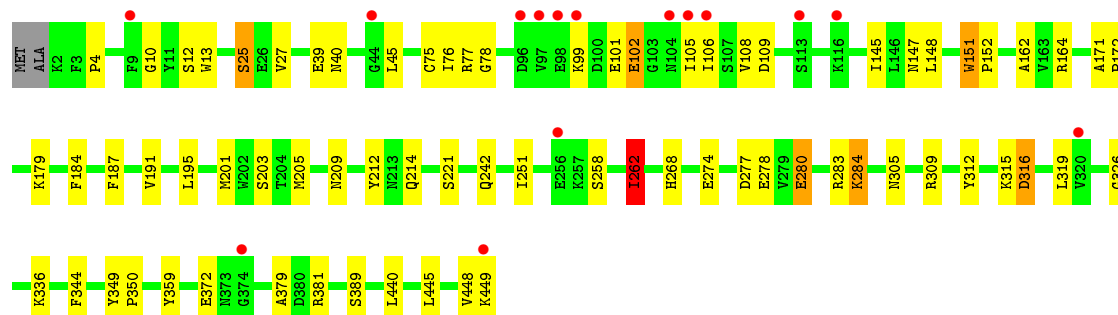
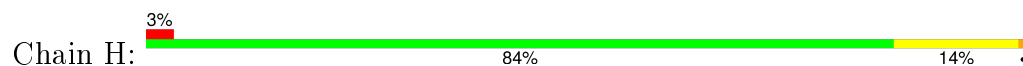
#### • Molecule 1: Beta-glucosidase



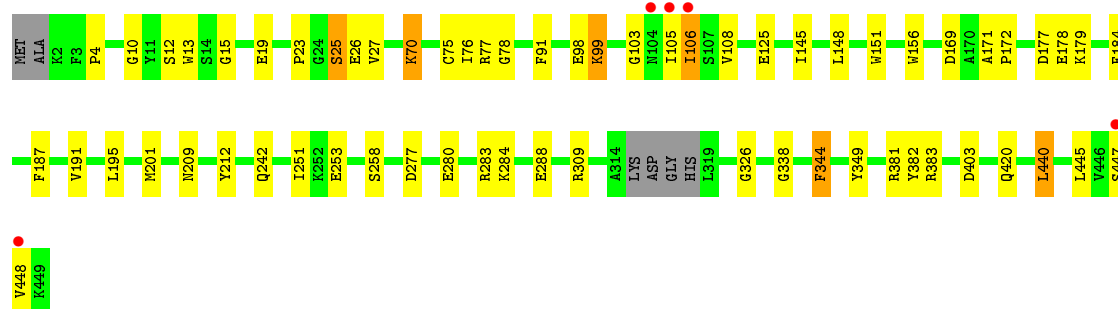
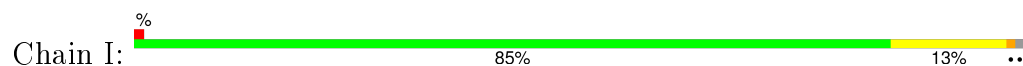




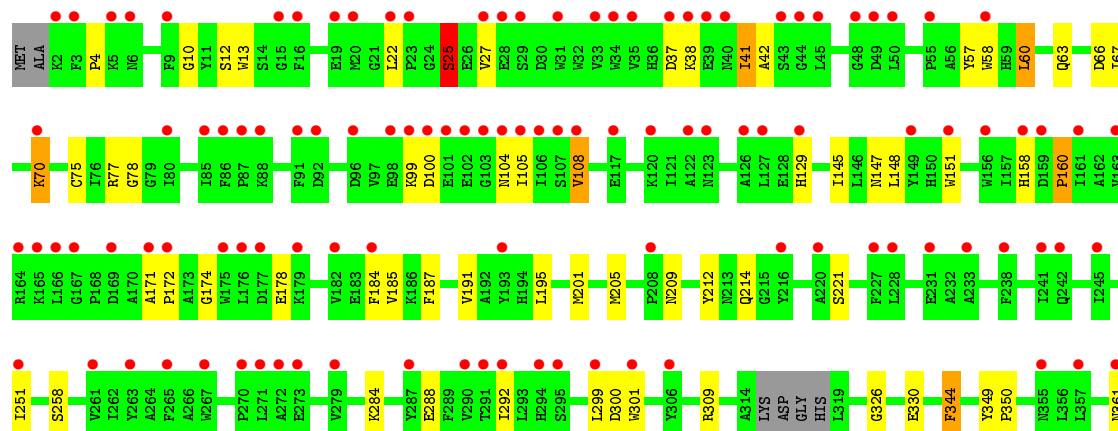
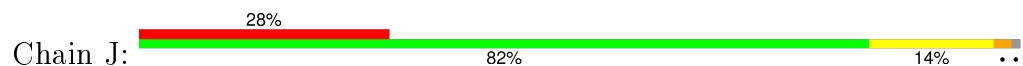
• Molecule 1: Beta-glucosidase

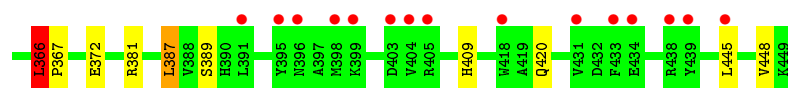


• Molecule 1: Beta-glucosidase

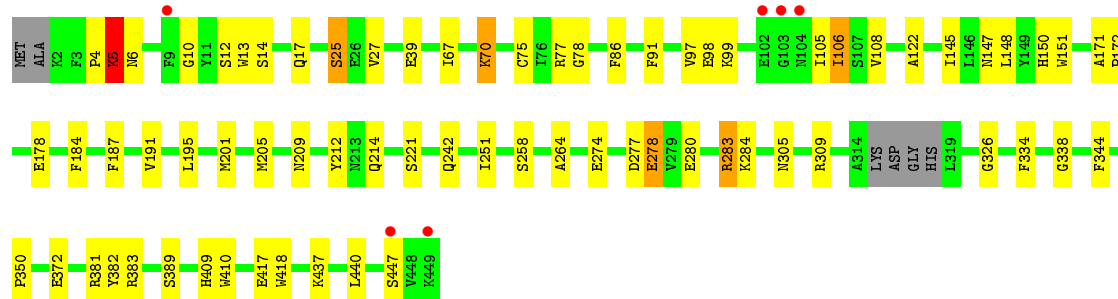
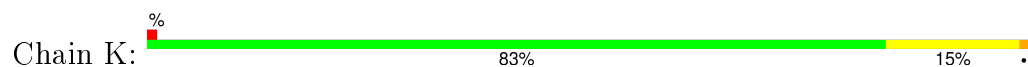


• Molecule 1: Beta-glucosidase

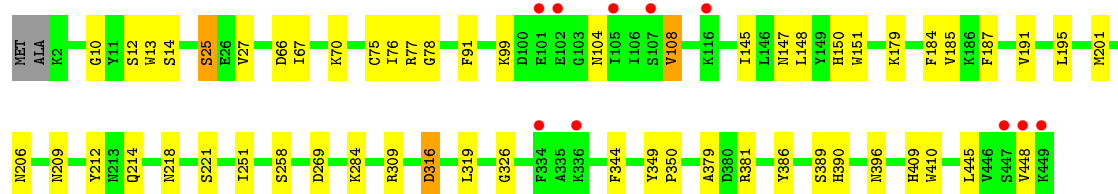
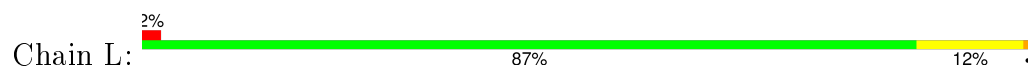




- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.36Å 148.87Å 148.56Å 120.08° 94.00° 99.70°	Depositor
Resolution (Å)	48.28 – 2.81 48.28 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.28-2.81) 78.5 (48.28-2.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.243 , 0.275 0.241 , 0.272	Depositor DCC
$R_{free}$ test set	8286 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 165239 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	43762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.77	0/3776	0.80	4/5124 (0.1%)
1	B	0.60	0/3743	0.71	0/5079
1	C	0.75	0/3743	0.77	2/5079 (0.0%)
1	D	0.63	2/3743 (0.1%)	0.75	2/5079 (0.0%)
1	E	0.72	0/3743	0.77	3/5079 (0.1%)
1	F	0.55	1/3743 (0.0%)	0.74	7/5079 (0.1%)
1	G	0.73	1/3776 (0.0%)	0.76	1/5124 (0.0%)
1	H	0.62	1/3776 (0.0%)	0.76	6/5124 (0.1%)
1	I	0.72	0/3743	0.77	5/5079 (0.1%)
1	J	0.54	0/3743	0.75	6/5079 (0.1%)
1	K	0.71	1/3743 (0.0%)	0.77	3/5079 (0.1%)
1	L	0.61	1/3776 (0.0%)	0.74	2/5124 (0.0%)
All	All	0.67	7/45048 (0.0%)	0.76	41/61128 (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	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	14

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	39	GLU	CD-OE2	-6.01	1.19	1.25
1	K	39	GLU	CD-OE2	-5.65	1.19	1.25
1	D	128	GLU	CB-CG	5.43	1.62	1.52
1	L	316	ASP	CB-CG	5.39	1.63	1.51
1	D	128	GLU	CD-OE2	5.33	1.31	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	219	LEU	CA-CB-CG	11.57	141.91	115.30
1	H	277	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	277	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	G	5	LYS	CD-CE-NZ	9.35	133.21	111.70
1	I	277	ASP	CB-CG-OD2	-8.94	110.25	118.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	SER	Peptide
1	A	448	VAL	Peptide
1	B	25	SER	Peptide
1	C	25	SER	Peptide
1	D	25	SER	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	3657	0	3505	34	1
1	B	3626	0	3477	31	1
1	C	3626	0	3477	39	0
1	D	3626	0	3477	32	0
1	E	3626	0	3477	58	0
1	F	3626	0	3477	48	0
1	G	3657	0	3505	38	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3657	0	3505	50	1
1	I	3626	0	3477	55	0
1	J	3626	0	3477	74	0
1	K	3626	0	3477	52	2
1	L	3657	0	3505	43	2
2	A	14	0	0	0	0
2	B	10	0	0	0	0
2	C	16	0	0	0	0
2	D	11	0	0	1	0
2	E	20	0	0	2	0
2	F	3	0	0	0	0
2	G	11	0	0	0	0
2	H	5	0	0	0	1
2	I	16	0	0	1	0
2	J	2	0	0	1	0
2	K	9	0	0	2	0
2	L	9	0	0	1	0
All	All	43762	0	41836	464	5

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 5.

The worst 5 of 464 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:I:440:LEU:CD1	1:J:445:LEU:HD11	1.59	1.31
1:I:440:LEU:HD11	1:J:445:LEU:CD1	1.79	1.11
1:J:60:LEU:HB3	1:J:63:GLN:OE1	1.51	1.11
1:E:182:VAL:O	1:E:185:VAL:HG23	1.50	1.11
1:J:366:LEU:HD23	1:J:367:PRO:HD2	1.19	1.10

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:274:GLU:O	1:L:316:ASP:OD2[1_655]	1.81	0.39
1:G:316:ASP:OD2	1:H:274:GLU:O[1_655]	1.92	0.28
1:G:316:ASP:OD2	2:H:504:HOH:O[1_655]	2.03	0.17
1:K:277:ASP:OD2	1:L:316:ASP:N[1_655]	2.09	0.11
1:A:277:ASP:OD2	1:B:231:GLU:OE1[1_655]	2.18	0.02

## 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	446/450 (99%)	430 (96%)	13 (3%)	3 (1%)	26	60
1	B	440/450 (98%)	424 (96%)	13 (3%)	3 (1%)	26	60
1	C	440/450 (98%)	422 (96%)	15 (3%)	3 (1%)	26	60
1	D	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	E	440/450 (98%)	422 (96%)	16 (4%)	2 (0%)	34	68
1	F	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	G	446/450 (99%)	427 (96%)	16 (4%)	3 (1%)	26	60
1	H	446/450 (99%)	428 (96%)	14 (3%)	4 (1%)	21	53
1	I	440/450 (98%)	423 (96%)	14 (3%)	3 (1%)	26	60
1	J	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	K	440/450 (98%)	426 (97%)	11 (2%)	3 (1%)	26	60
1	L	446/450 (99%)	428 (96%)	16 (4%)	2 (0%)	39	73
All	All	5304/5400 (98%)	5099 (96%)	173 (3%)	32 (1%)	30	63

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	B	151	TRP
1	C	151	TRP
1	D	151	TRP
1	E	151	TRP

### 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	378/379 (100%)	365 (97%)	13 (3%)	44	77
1	B	375/379 (99%)	365 (97%)	10 (3%)	52	84
1	C	375/379 (99%)	363 (97%)	12 (3%)	46	79
1	D	375/379 (99%)	358 (96%)	17 (4%)	34	67
1	E	375/379 (99%)	360 (96%)	15 (4%)	38	72
1	F	375/379 (99%)	363 (97%)	12 (3%)	46	79
1	G	378/379 (100%)	367 (97%)	11 (3%)	50	82
1	H	378/379 (100%)	366 (97%)	12 (3%)	46	79
1	I	375/379 (99%)	362 (96%)	13 (4%)	43	76
1	J	375/379 (99%)	365 (97%)	10 (3%)	52	84
1	K	375/379 (99%)	362 (96%)	13 (4%)	43	76
1	L	378/379 (100%)	370 (98%)	8 (2%)	61	89
All	All	4512/4548 (99%)	4366 (97%)	146 (3%)	46	79

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	447	SER
1	G	77	ARG
1	K	284	LYS
1	F	25	SER
1	F	344	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	213	ASN
1	H	40	ASN
1	L	150	HIS
1	G	218	ASN
1	G	355	ASN

### 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	448/450 (99%)	-0.35	1 (0%) 95 94	12, 38, 79, 120	0
1	B	444/450 (98%)	0.09	17 (3%) 44 32	33, 61, 106, 149	0
1	C	444/450 (98%)	-0.34	3 (0%) 89 84	16, 40, 72, 160	0
1	D	444/450 (98%)	-0.02	14 (3%) 51 39	26, 59, 95, 139	0
1	E	444/450 (98%)	-0.23	4 (0%) 85 79	19, 42, 78, 159	0
1	F	444/450 (98%)	1.56	136 (30%) 1 0	43, 99, 143, 186	0
1	G	448/450 (99%)	-0.34	2 (0%) 93 90	22, 41, 74, 134	0
1	H	448/450 (99%)	-0.06	15 (3%) 50 38	31, 57, 97, 168	0
1	I	444/450 (98%)	-0.30	5 (1%) 82 75	14, 42, 76, 146	0
1	J	444/450 (98%)	1.37	126 (28%) 1 0	54, 109, 165, 225	0
1	K	444/450 (98%)	-0.22	6 (1%) 78 69	19, 45, 75, 147	0
1	L	448/450 (99%)	-0.01	10 (2%) 65 54	24, 58, 98, 149	0
All	All	5344/5400 (98%)	0.10	339 (6%) 23 14	12, 52, 126, 225	0

The worst 5 of 339 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	366	LEU	10.6
1	E	449	LYS	10.6
1	F	367	PRO	10.2
1	J	28	GLU	9.4
1	J	122	ALA	9.3

### 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.