



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:35 AM GMT

PDB ID : 1M7X  
Title : The X-ray Crystallographic Structure of Branching Enzyme  
Authors : Abad, M.C.; Binderup, K.; Rios-Steiner, J.; Arni, R.K.; Preiss, J.; Geiger, J.H.  
Deposited on : 2002-07-23  
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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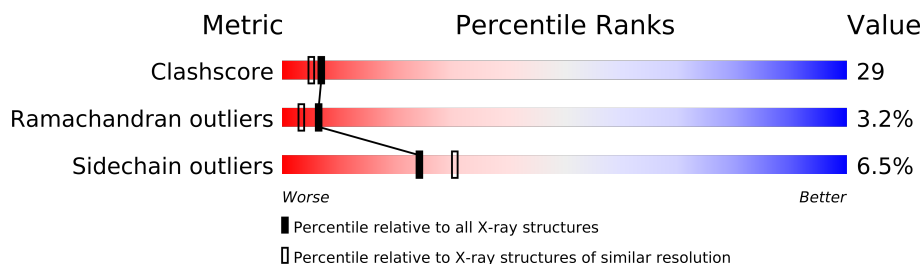
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
1	D	617	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20372 atoms, of which 0 are hydrogen and 0 are deuterium.

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 1,4-alpha-glucan Branching Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4823	3083	857	867	16			
1	B	591	Total	C	N	O	S	0	0	0
			4852	3102	859	876	15			
1	C	578	Total	C	N	O	S	0	0	0
			4750	3041	840	854	15			
1	D	585	Total	C	N	O	S	0	0	0
			4805	3072	853	864	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	MET	-	INITIATING MET	UNP P07762
B	112	MET	-	INITIATING MET	UNP P07762
C	112	MET	-	INITIATING MET	UNP P07762
D	112	MET	-	INITIATING MET	UNP P07762

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	301	Total	O	0	0
			301	301		
2	B	425	Total	O	0	0
			425	425		
2	C	108	Total	O	0	0
			108	108		
2	D	308	Total	O	0	0
			308	308		

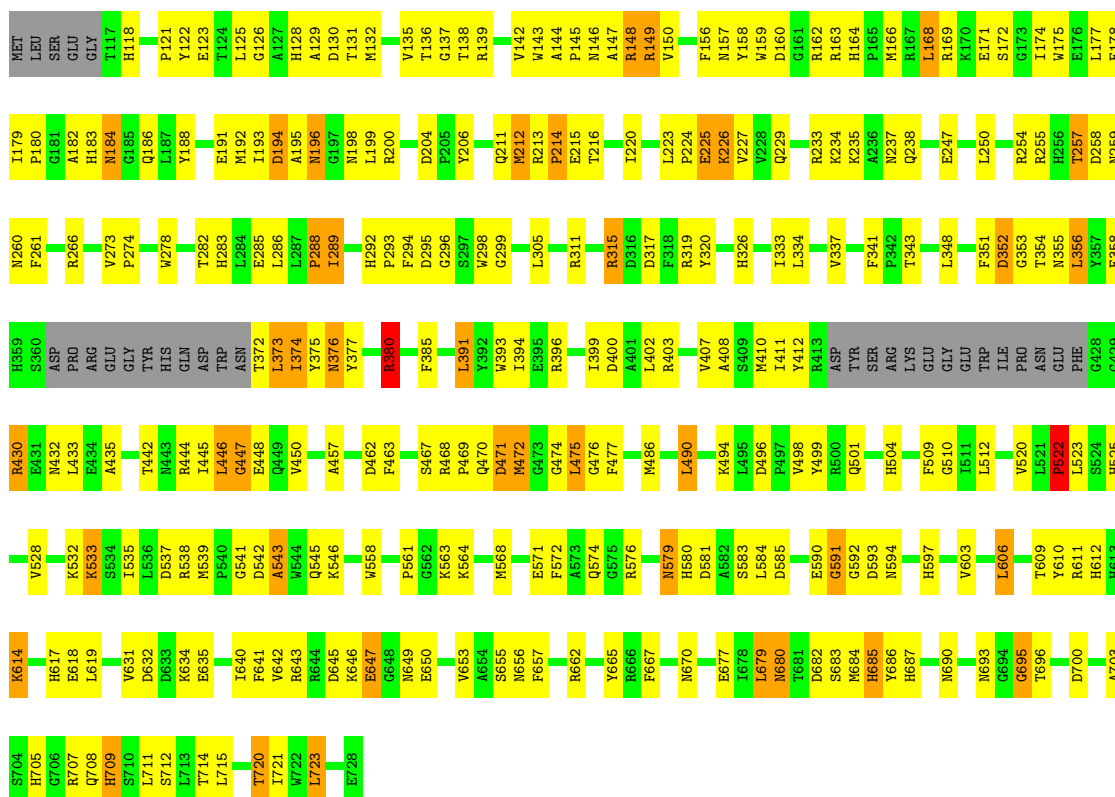
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

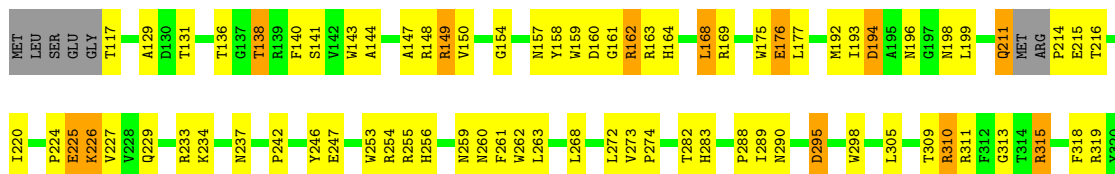
#### • Molecule 1: 1,4-alpha-glucan Branching Enzyme

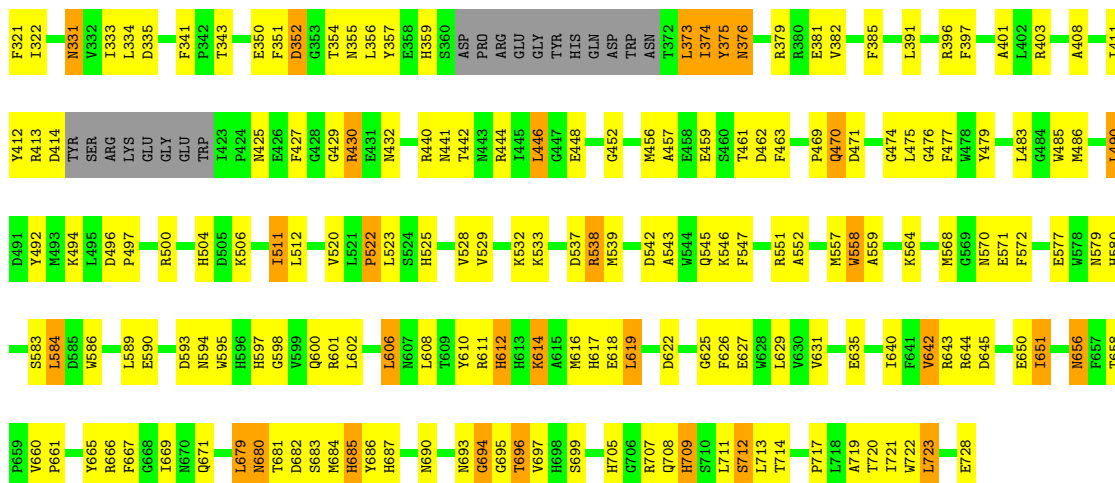
Chain A:



#### • Molecule 1: 1,4-alpha-glucan Branching Enzyme

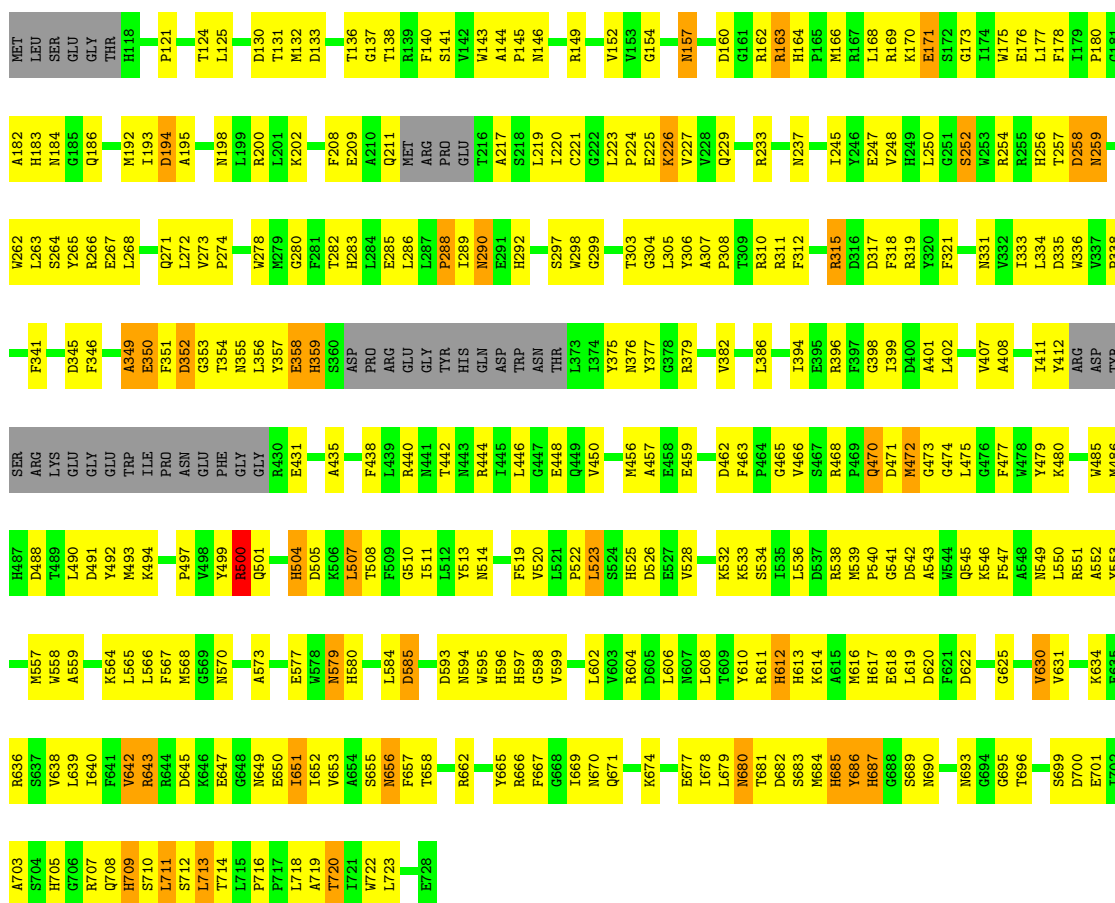
Chain B:





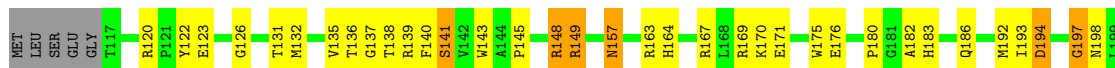
• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain C:



• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain D:



T714	L619	K546	M456	R379	P288	R200
L715	V631	F547	E459	V382	I289	
P717	D632	R551	V466	F385	N290	D204
L718	K634	A552	P469	R389	E291	P205
A719	R635	G555	Q470	Y392	H292	Q211
T720	R636	W558	M472	K393	P293	W212
T721	L639	P561	G473	I394	ARG	PRD
W722	V642	K564	G474	E395	GLU	T216
L723	R643	L565	L475	R396		
W724	R644	L566	G476	T399	L219	
R725	D645	L567	P477		R310	T220
E726	K646	F567	W478	R403	R311	
	E647	M568	Y479	V404	L223	P224
	I651	G569	T489	D405	D317	V227
		N570	L490		R316	
	N656	A573	D491	I411	D315	E232
	P659	Q574	M492	Y412	R318	
		E577	K494	R413	N331	N237
	R662	N578	L495	D414	V332	P242
	Y665	N579	D496	TYR	I333	
	R666	H580	P497	SER	L334	
	F667		V498	ARG		Y246
	G668	S583	Y499	LYS	V337	E247
		L584	R500	GLY	H340	L250
	K674	D585	H504	GLY	F341	
		E590	L507	TRP		R254
	L679	G591	N514	ILE	F346	
	N680	D592		PRD	A347	T257
	T681	N593		ASN	D258	D259
	D682	N594		GLU	L348	
	S683	N595		PHE	F351	
	M684	H596	E517	GLY	D352	V262
	H685	H597	N518	G429		L263
	Y686	G598	P519	R430	L356	S264
	H687		V520	E431	Y357	Y265
			L521	N432	E358	R266
			P522		H359	E267
	N690	L602	L523	A435	S350	L268
		V603	S524	I436	ASP	A269
	N693	R604	H525	E437	PRD	D270
	G694	D605	D526		ARG	Q271
	G695	L606	E527	R440	GLU	L272
	T696	N607	W528		GLY	V273
		L608	V529	N443	TYR	P274
	D700	T609	H530	R443	HIS	
	H705	Y610	G531	R444	GLN	W278
		R611	I535	I445	ASP	N279
		H612		L446	TRP	G280
	Q708	H613		G447	N371	F281
	H709	K614	R538	E448	T372	T282
	S710	K615	D542	Q449	L373	H283
	L711	H616		V450		
	S712	H617	Q545	S451		L284
	L713	E618		T455	N376	E285

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.47Å 102.62Å 185.06Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	0.40	0/4976	0.68	1/6756 (0.0%)
1	B	0.42	0/5006	0.70	2/6797 (0.0%)
1	C	0.39	0/4900	0.61	0/6653
1	D	0.42	0/4956	0.69	1/6728 (0.0%)
All	All	0.41	0/19838	0.67	4/26934 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	TYR	N-CA-C	6.06	127.35	111.00
1	A	685	HIS	N-CA-C	-5.83	95.25	111.00
1	B	685	HIS	N-CA-C	-5.75	95.46	111.00
1	D	685	HIS	N-CA-C	-5.36	96.53	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4823	0	4559	263	0
1	B	4852	0	4571	255	0
1	C	4750	0	4485	325	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4805	0	4537	240	0
2	A	301	0	0	19	0
2	B	425	0	0	33	0
2	C	108	0	0	21	0
2	D	308	0	0	20	0
All	All	20372	0	18152	1077	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

The worst 5 of 1077 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:643:ARG:HB3	1:C:643:ARG:HH11	1.12	1.08
1:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	1.02
1:A:430:ARG:HH21	1:A:430:ARG:HB3	1.22	1.02
1:A:224:PRO:HG2	1:A:396:ARG:HB3	1.38	1.01
1:B:430:ARG:H	1:B:430:ARG:HD2	1.22	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	581/617 (94%)	502 (86%)	52 (9%)	27 (5%)	4	1
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	10	7
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	6	3
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	8	5
All	All	2311/2468 (94%)	2040 (88%)	197 (8%)	74 (3%)	6	3

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	212	MET
1	A	215	GLU
1	A	225	GLU
1	A	257	THR

### 5.3.2 Protein sidechains ⓘ

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	498/525 (95%)	466 (94%)	32 (6%)	25	31
1	B	501/525 (95%)	464 (93%)	37 (7%)	20	24
1	C	490/525 (93%)	460 (94%)	30 (6%)	26	34
1	D	496/525 (94%)	466 (94%)	30 (6%)	27	35
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	24	30

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	558	TRP
1	C	163	ARG
1	D	579	ASN
1	B	606	LEU
1	B	656	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	ASN
1	C	256	HIS
1	D	617	HIS
1	B	687	HIS
1	C	146	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.