



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:48 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 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  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

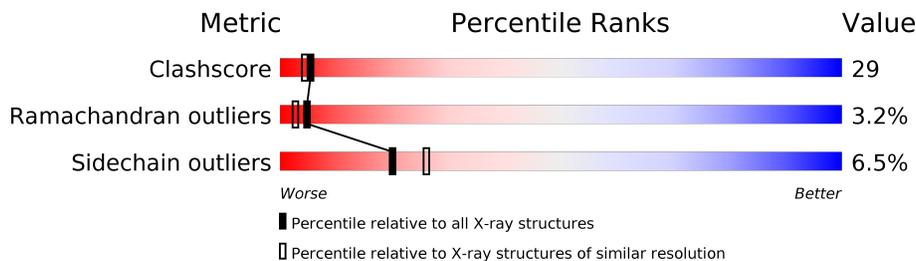
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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. 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.

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 [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20372 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 1,4-alpha-glucan Branching Enzyme.

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

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.

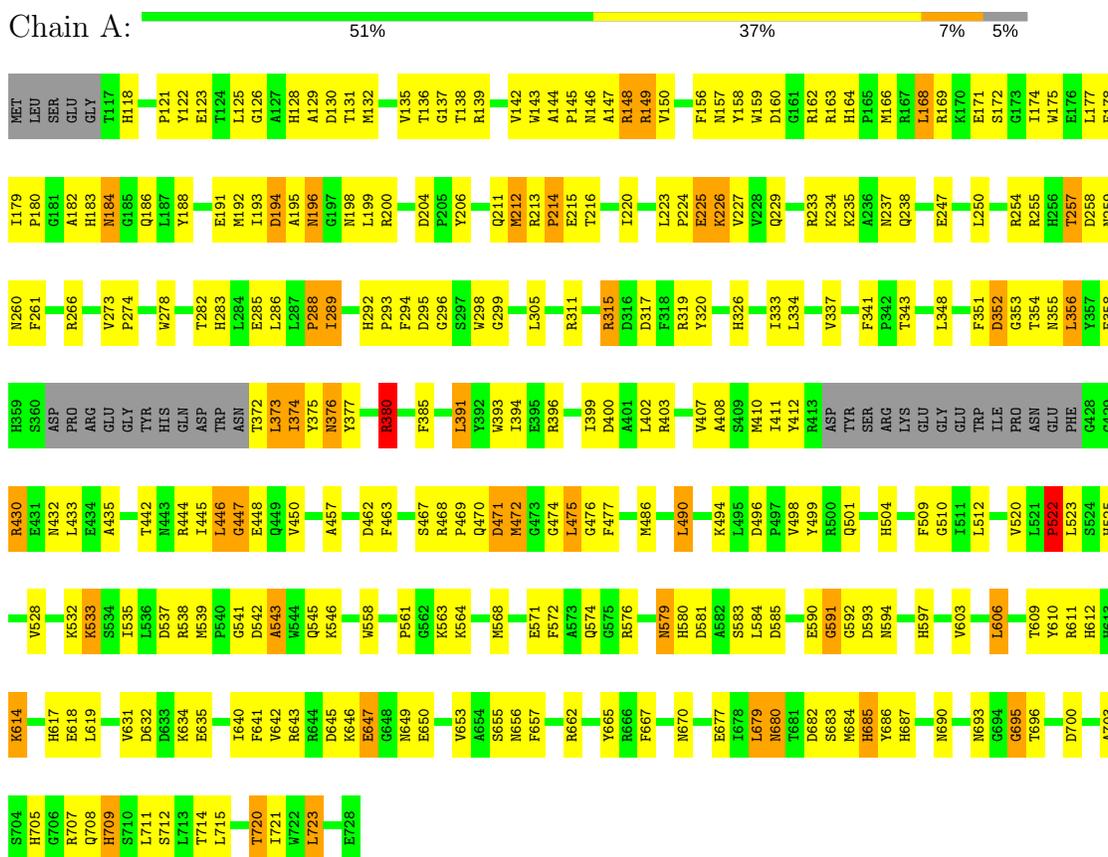
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	301	Total 301	O 301	0	0
2	B	425	Total 425	O 425	0	0
2	C	108	Total 108	O 108	0	0
2	D	308	Total 308	O 308	0	0

### 3 Residue-property plots

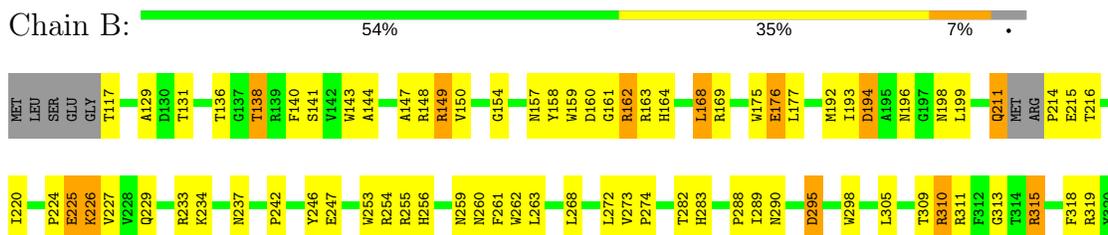
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

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



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





MET	R200	P288	R379	M456	K546	L619	T714
LEU	R201	I289	V382	E459	F547	V631	L715
SER	D204	M290	F385	V466	R551	D632	P716
GLU	P205	E291	H292	P469	A552	K634	P717
GLY	Q211	P293	N389	Q470	G555	E635	L718
T117	W212	W298	Y392	D471	W558	R636	A719
R120	ARG	G299	W393	M472	P561	L639	T720
P121	PRD	T303	I394	G473	K564	V642	I721
Y122	GLU	R310	E395	G474	L565	R643	W722
E123	T216	R311	R396	L475	L566	R644	L723
G126	L219	R315	I399	G476	M568	D645	V724
T131	I220	R317	Y478	F477	G569	E647	R725
M132	L223	R318	Y479	Y479	N570	I651	E728
V135	P224	R319	T489	L490	A573	N656	
T136	V227	F318	L491	Y492	Q574	P659	
G137	E232	N331	M493	K494	E577	R662	
T138	N237	I332	L495	D496	M579	Y665	
R139	F140	L334	P497	Y498	H580	R666	
F140	F141	Y337	Y499	R500	S583	F667	
S141	V142	H340	GLY	H504	L584	G668	
W143	W144	F341	TRP	L507	D585	K674	
A144	P145	F346	ILE	G591	E590	L679	
P145	R148	L348	PRD	N514	G592	N680	
R149	R163	L348	ASN	N517	D593	T681	
M157	H164	F351	GLU	E517	N594	D682	
R167	R167	D352	PHE	N518	W595	S683	
L168	L168	L356	GLY	F519	H596	M684	
R169	R169	Y357	G429	W520	H597	H685	
K170	K170	E431	R430	L521	G598	Y686	
E171	E171	N432	N432	P522	R601	H687	
E175	E267	H359	A435	L523	L602	N690	
E176	L268	S360	I436	S524	V603	M693	
P180	D270	ASP	E437	H525	R604	N693	
G181	Q271	ARG	R440	D526	D605	G694	
A182	L272	GLU	R443	E527	L606	G695	
H183	V273	GLY	N443	N528	N607	T696	
Q186	P274	TYR	R444	H529	I608	D700	
M192	W278	HIS	L444	H530	T609	H705	
I193	M279	GLN	L445	G531	Y610	R708	
D194	G280	ASP	L446	I535	R611	W709	
G197	F281	TRP	G447	R538	H612	S710	
N198	T282	N371	E448	D542	H613	L711	
L199	H283	L372	G449	E545	K614	S712	
	E284	L373	V450		A615	L713	
	L285	N376	S451		M616		
	E285		T455		H617		

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
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 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	4823	0	4559	263	0
1	B	4852	0	4571	255	0
1	C	4750	0	4485	325	0
1	D	4805	0	4537	240	0
2	A	301	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 29.

The worst 5 of 1077 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:C:643:ARG:HH11	1:C:643:ARG:HB3	1.12	1.08
1:A:430:ARG:HH21	1:A:430:ARG:HB3	1.22	1.02
1:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	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 [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	581/617 (94%)	502 (86%)	52 (9%)	27 (5%)	<b>3</b> <b>1</b>
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	<b>8</b> <b>6</b>
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	<b>4</b> <b>2</b>
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	<b>6</b> <b>4</b>
All	All	2311/2468 (94%)	2040 (88%)	197 (8%)	74 (3%)	<b>5</b> <b>3</b>

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 [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	498/525 (95%)	466 (94%)	32 (6%)	20	27
1	B	501/525 (95%)	464 (93%)	37 (7%)	16	20
1	C	490/525 (93%)	460 (94%)	30 (6%)	22	29
1	D	496/525 (94%)	466 (94%)	30 (6%)	22	30
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	20	26

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 [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 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.