



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1SMA  
Title : CRYSTAL STRUCTURE OF A MALTOGENIC AMYLASE  
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Deposited on : 1999-04-21  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2



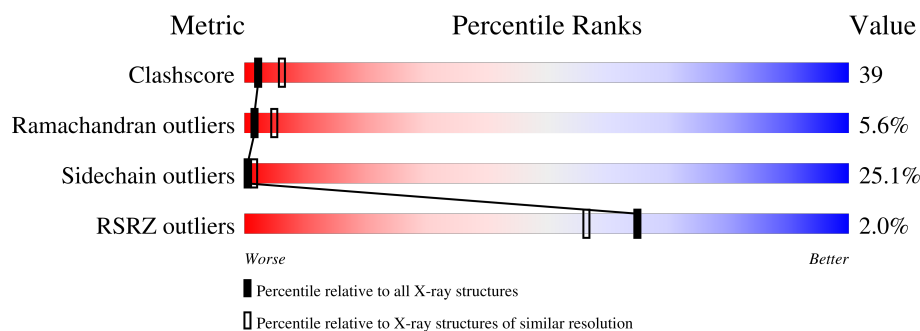
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	588	
1	B	588	



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9683 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 MALTOGENIC AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4746	3062	804	859	21			
1	B	588	Total	C	N	O	S	0	0	0
			4746	3062	804	859	21			

- Molecule 2 is water.

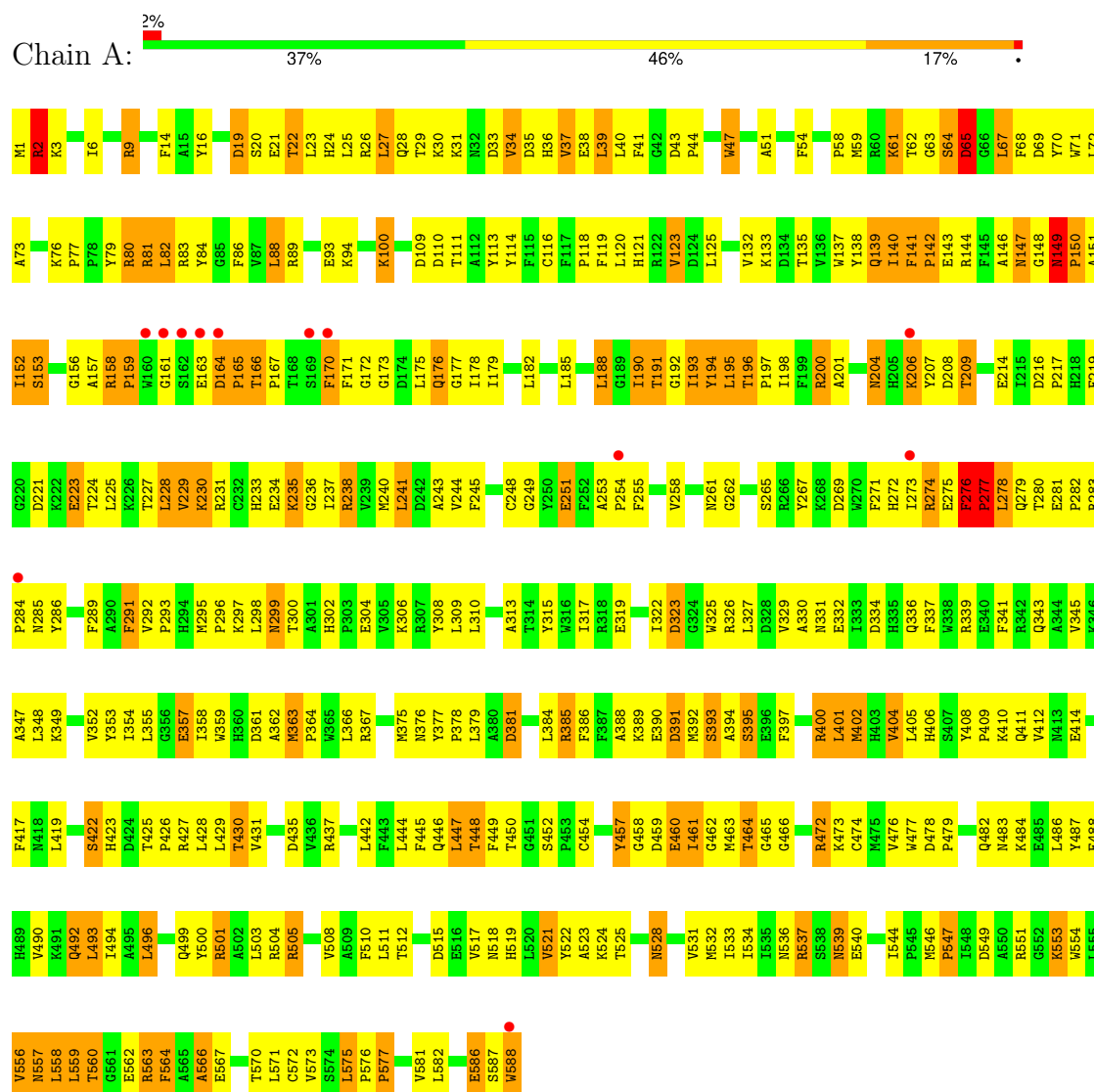
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		
2	B	98	Total	O	0	0
			98	98		



### 3 Residue-property plots

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: MALTOGENIC AMYLASE



#### • Molecule 1: MALTOGENIC AMYLASE





G561	A494	V352	F289	E223	T152	A73	M1
E562	A495	Y353	A290	T224	S153		R2
R563	L496	P426	F291	T225		K76	K3
F564		R427	V292	K226	G156	P77	I6
A565	Q499	L428	P293	T227	A157	P78	
A566	Y500	T430	H294	L228	R158	Y79	R9
E567	R501	V431	M295	V229	P159	R80	
	A502	D435	P296	K230	W160	R81	
T570	L503	V436	H297	R231	G161	L82	F14
L571	R504	R437	D361	L298	C232	R83	A15
C572	R505		A362	H233	S162	Y84	Y16
V573			M363	E234	E163	G85	
S574	V508	L441	T300	K235	D164		D19
L575	A509	L442	A301	E236	P165	P86	S20
P576	F510	F443	H302	G236	T166	V87	E21
P577	L511	G230	P303	I237	P167	L88	T22
	T512	L444	E304	R238	R89		L23
		F445	V805	W239	F170		L23
		Q446	K306	M240	F171	E93	H24
	D515	L447	R307	L241	G172	K94	
E516		T448	Y308	D242	G173		L25
V517	F449	F450	L309	A243	D174	K100	R26
N518	T450	T451	L310	V244	L175		L27
H519	G451	A380		F245	Q176	D109	Q28
L520	S452	D381	A313		G177	D110	T29
V521	P453		T314	C248	I178	T111	K30
Y522	C454	R384	Y315	I179		K31	K31
A523	L455	L385	W316	Y250	A112	Y113	N32
K524	Y456	F386	I317	E251	F386	Y114	D33
T525	Y457	F387	R318	P252	L182	F115	V34
		A388	E319	A253	L185	C116	D35
	D459	K389		P254		F117	H36
N528	E460	E390	I322	V258	L188	P118	V37
V531	I461	D391	D823		G189	E38	E38
M532	G462	M392	G324		I190	F119	L39
I533	M463	S393	K325	N261	T191	L120	L40
I534	T464	A394	R326	G262	G192	H121	F41
I535	G465	S395	L327		R122	G42	G42
N536	G466	E396	D328	S265	I193	D43	D43
R537		F397	V329	R266	D124	P44	P44
	R472	S538	A330	Y267	L195	L125	
N539	K473	E460	N331	K268	T196		W47
E540	C474	L401	E332	D269	P197	V132	
	M475	M402	I333	W270	I198	K133	A51
I544	P476	V476	D334	F271	F199	D134	
P545	W477	H403	F271	H272	R200	T135	F54
M546	D478	L405	Q336	I273	A201	V136	
P547	P479	H406	F337	K274	W137	Y138	P58
L548	S407	Y407	W338	E275	N204	X138	M59
D549	Q482	Y408	R339	F276	H205	Q139	K60
A550	N483	P409	E340	P277	K206	I140	K61
R551	K484	M410	F341	L278	Y207	F141	T62
G552	E485	Q411	R342	Q279	D208	P142	G63
K553	L486	V412	Q343	E143	T209	S64	
W554	Y487	M413	A344	E281	R144	R144	D65
L555	E488	E414	V345	P282	F145	G66	G66
V556	H489	F417	K346	R283	L215	L67	L67
N557	V490		X346	P217	D146	F68	
L558	K491		L348	N285	G148	D69	D69
L559	Q492		S422	Y286	N149	Y70	Y70
T560	L492		H423		F219	P150	W71
					A151	L72	L72



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.37Å 118.37Å 266.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 29.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (8.00-2.80) 93.8 (29.59-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.209 , 0.267 0.237 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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	0.32	0/4895	0.56	2/6661 (0.0%)
1	B	0.31	0/4895	0.56	2/6661 (0.0%)
All	All	0.32	0/9790	0.56	4/13322 (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	277	PRO	N-CA-CB	6.16	110.70	103.30
1	A	277	PRO	N-CA-CB	6.14	110.67	103.30
1	B	282	PRO	N-CA-CB	5.63	110.06	103.30
1	A	282	PRO	N-CA-CB	5.60	110.02	103.30

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	4746	0	4458	362	0
1	B	4746	0	4458	367	0
2	A	93	0	0	2	0
2	B	98	0	0	1	0
All	All	9683	0	8916	717	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 39.

The worst 5 of 717 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:158:ARG:HD3	1:B:159:PRO:HD2	1.35	1.04
1:A:158:ARG:HD3	1:A:159:PRO:HD2	1.35	1.04
1:B:27:LEU:HD12	1:B:37:VAL:HG21	1.49	0.95
1:A:27:LEU:HD12	1:A:37:VAL:HG21	1.49	0.92
1:B:201:ALA:HB3	1:B:206:LYS:HG3	1.52	0.90

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	586/588 (100%)	461 (79%)	92 (16%)	33 (6%)	2	5
1	B	586/588 (100%)	460 (78%)	93 (16%)	33 (6%)	2	5
All	All	1172/1176 (100%)	921 (79%)	185 (16%)	66 (6%)	2	5

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	37	VAL
1	A	64	SER
1	A	156	GLY
1	A	159	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	482/505 (95%)	361 (75%)	121 (25%)	0	1
1	B	482/505 (95%)	361 (75%)	121 (25%)	0	1
All	All	964/1010 (95%)	722 (75%)	242 (25%)	0	1

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	571	LEU
1	B	515	ASP
1	B	111	THR
1	B	501	ARG
1	B	571	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	499	GLN
1	B	518	ASN
1	B	539	ASN
1	A	518	ASN
1	A	499	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	588/588 (100%)	0.19	12 (2%) 65 56	13, 39, 84, 100	0
1	B	588/588 (100%)	0.18	11 (1%) 66 59	12, 39, 85, 100	0
All	All	1176/1176 (100%)	0.18	23 (1%) 65 56	12, 39, 85, 100	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	GLY	14.4
1	A	162	SER	8.5
1	B	161	GLY	8.1
1	B	162	SER	6.3
1	B	160	TRP	4.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.