



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID : 1SMA / pdb_00001sma
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

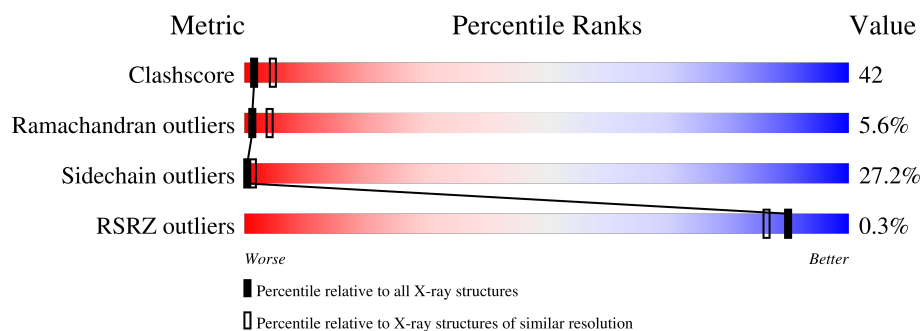
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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			

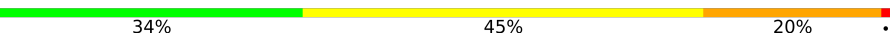
- Molecule 2 is water.

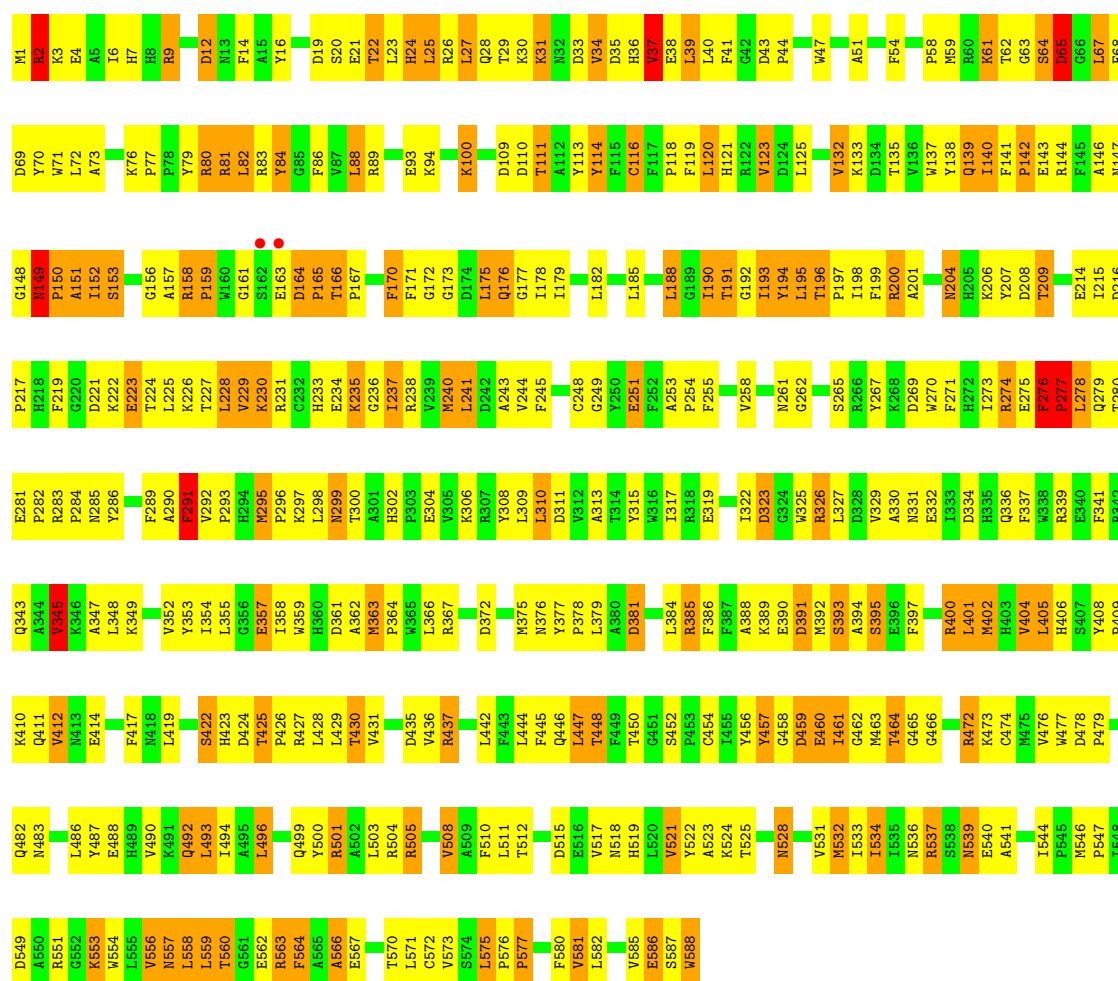
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		
2	B	98	Total	O	0	0
			98	98		

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.

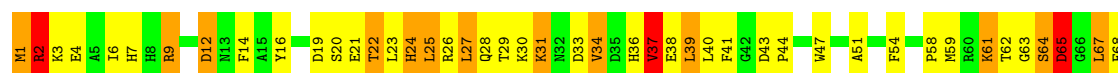
• Molecule 1: MALTOGENIC AMYLASE

Chain A: 



• Molecule 1: MALTOGENIC AMYLASE

Chain B: 



D69	G148	P217	R283	V345	V412	E486	R551
Y70	R149	R218	P284	R346	R413	L486	G552
W71	P150	F219	N286	A347	E414	Y487	R553
L72	A151		Y286	L348		E488	W554
A73	I152	K222	K349	K349	F417	H439	L555
	S153	K223	F289			V490	Y556
K76		T224	A290	V352	S422	K491	N557
P77	G156	L225	F291	Y353	H423	Q492	L558
P78	A157	K226	V292	I354	D424	L493	L559
Y79	R158	T227	P293	L355	T425	I494	T560
R80	P159	L228	H294	G356	P426	A495	G561
R81	W160	V229	M295	E357	R427	L496	E562
L82	G161	K230	P296	I358	L428		R563
R83	S182	R231	K297	W359	L429	Q499	R564
Y84	E163	C232	L298	H360	T430	Y500	A565
G85	D164	H233	N299	D361	V431	R501	A566
F86	P165	E234	T300	A362		L502	E567
V87	T166	K235	R301	N363	D435	L503	
L88	P167	G236	H302	P364	V436	R504	T570
R89		I237	P383	V365	R437	R505	L571
	F170	R238	E304	L366			C572
E93	F171	V239	V305	R367	L441	V508	V573
K94	G172	M240	K306		L442	A509	G574
	G173	L241	R307		F443	F510	L575
K100	D174	D242	Y308	D372	I444	L511	P576
	L175	A243	L309		F445	T512	P577
D109	Q176	F244	L310	R376	Q446		
D110	G177	F245	D311	Y377	L447	D515	F580
T111	I178		V312	P378	T448	E516	V581
A112	I179	C248	A313	L379	F449	V517	L582
Y113		G249	T314	A380	T450	N518	
Y114	L182	Y250	Y315	D381	G451	H519	V585
F115		E251	R316		S452	L520	E586
C116	L185	F252	I317	L384	P453	V521	S587
F117		A253	R318	R385	C454	Y522	
P118	L188	P254	E319	F386	L455	A523	
F119	G189			F387	Y456	K524	
L120	I190	V258	I322	A388	Y457	T525	
H121	T191		D323	K389	G458		
R122	G192	N261	G324	E390	D459	N528	
V123	I193	G262	W325	D391	E460	V531	
D124	Y194		R326	N392	I461	M532	
L125	L195	S265	L327	S393	G462	I533	
	T196	R266	D328	A394	M463	L534	
V132	P197	Y267	V329	S395	T464	I536	
K133	I198	R268	A330	E396	G465	N537	
D134	F199	D269	N331	F397	G466		
T135	R200	W270	E332			R537	
W136	A201	F271	I333	R400	R472	S538	
Y137		H272	D334	L401	K473	N539	
Y138	N204	I273	R335	M402	C474	E540	
Q139	R205	R274	Q336	H403	R475	A541	
I140	K206	E275	F337	V404	V476		
F141	Y207	P276	W338	L405	W477	I544	
D142	D208	P277	R339	H406	D478	P545	
E143	E143	T209	F340	S407	P479	N546	
R144			F341	Y408		P547	
F145		E214	R342	P409	Q482	L548	
A146		T215	Q343	K410	N483	D549	
N147	D216	P282	A344	Q411	F484	A550	

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	118.37Å 118.37Å 266.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (8.00-2.80) 94.1 (8.00-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	44.9	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.37	0/4895	0.89	16/6661 (0.2%)
1	B	0.37	0/4895	0.88	14/6661 (0.2%)
All	All	0.37	0/9790	0.88	30/13322 (0.2%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ALA	N-CA-C	-7.69	100.30	111.30
1	B	151	ALA	N-CA-C	-7.64	100.37	111.30
1	A	291	PHE	N-CA-C	-7.55	102.63	113.21
1	B	277	PRO	N-CA-CB	7.09	110.70	103.25
1	A	277	PRO	N-CA-CB	7.07	110.67	103.25

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	392	0
1	B	4746	0	4458	395	0
2	A	93	0	0	2	0
2	B	98	0	0	1	0
All	All	9683	0	8916	775	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 42.

The worst 5 of 775 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%)	1	4
1	B	586/588 (100%)	460 (78%)	93 (16%)	33 (6%)	1	4
All	All	1172/1176 (100%)	921 (79%)	185 (16%)	66 (6%)	1	4

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%)	351 (73%)	131 (27%)	0	1
1	B	482/505 (95%)	351 (73%)	131 (27%)	0	1
All	All	964/1010 (95%)	702 (73%)	262 (27%)	0	1

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	472	ARG
1	B	508	VAL
1	B	587	SER
1	A	460	GLU
1	A	437	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	528	ASN
1	B	370	GLN
1	B	499	GLN
1	B	557	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 oligosaccharides 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, 95th 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	588/588 (100%)	-1.41	2 (0%) 90 86	13, 39, 84, 100	0
1	B	588/588 (100%)	-1.44	2 (0%) 90 86	12, 39, 85, 100	0
All	All	1176/1176 (100%)	-1.42	4 (0%) 90 86	12, 39, 85, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	3.2
1	B	163	GLU	2.8
1	A	162	SER	2.3
1	B	162	SER	2.2

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 oligosaccharides 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.