



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:42 PM GMT

PDB ID : 1GVI
Title : THERMUS MALTOGENIC AMYLASE IN COMPLEX WITH BETA-CD
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Deposited on : 2002-02-14
Resolution : 3.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

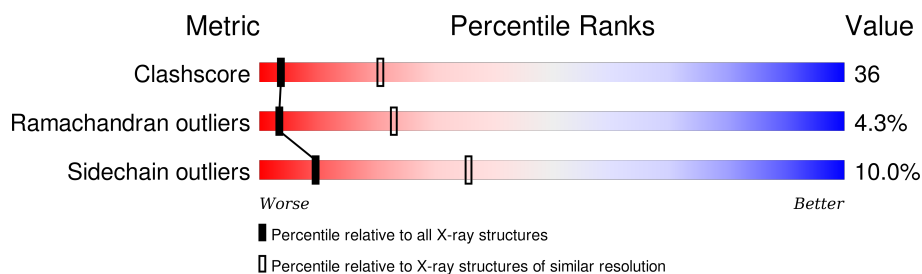
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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 ≥ 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	588	 43% 48% 9%
1	B	588	 41% 49% 9%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9810 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.

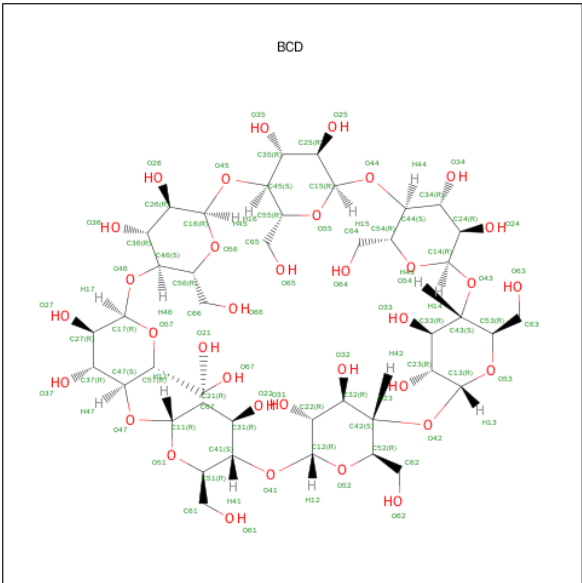
- Molecule 1 is a protein called MALTOGENIC AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4828	3119	819	869	21			
1	B	588	Total	C	N	O	S	0	0	0
			4828	3119	819	869	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	LEU	GLU	CONFLICT	UNP O69007
B	357	LEU	GLU	CONFLICT	UNP O69007

- Molecule 2 is SUGAR (BETA-CYCLODEXTRIN) (three-letter code: BCD) (formula: C₄₂H₇₀O₃₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			77	42	35		

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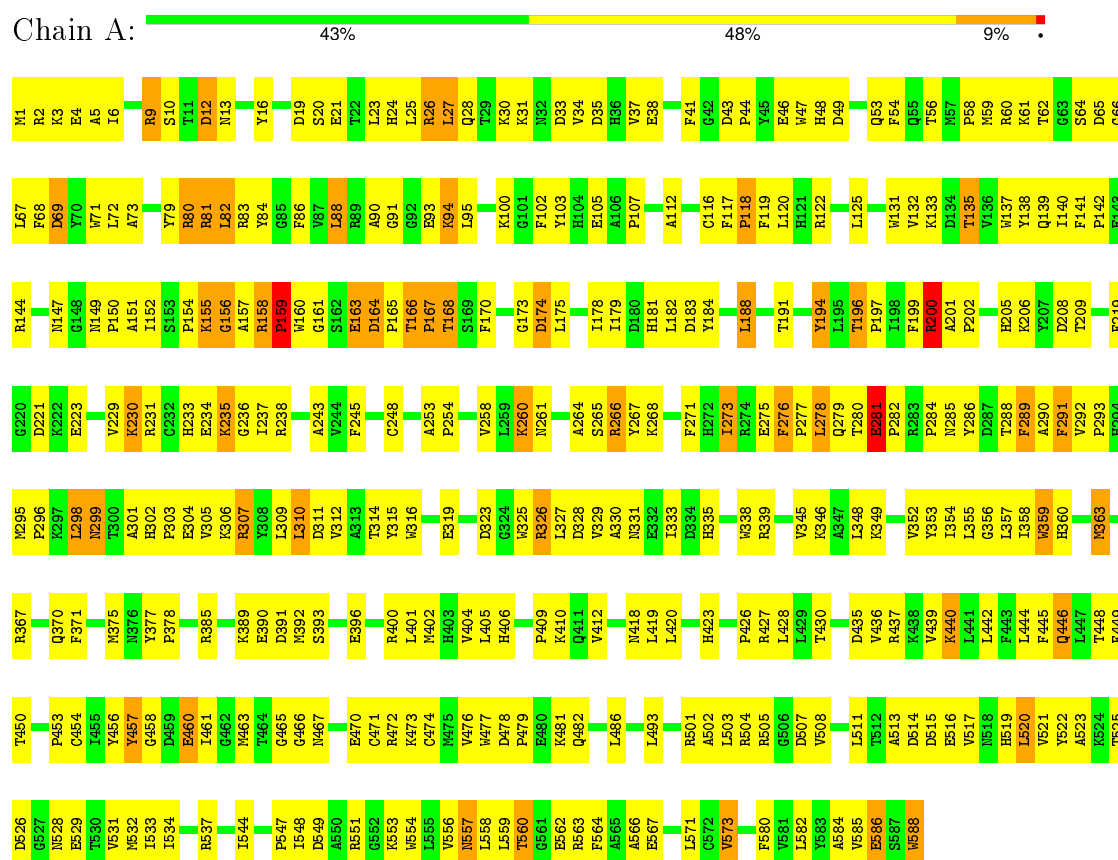
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			77	42	35		

3 Residue-property plots

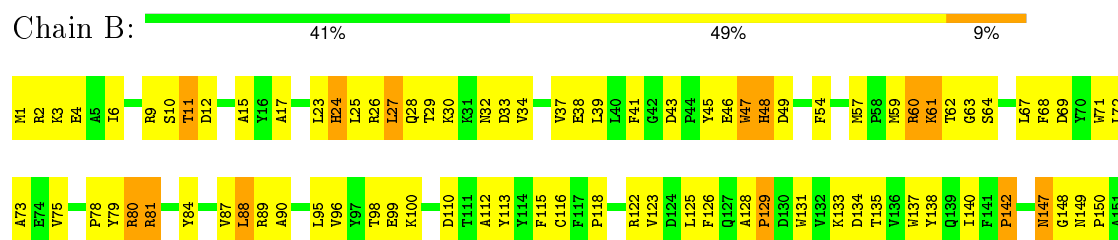
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MALTOGENIC AMYLASE



• Molecule 1: MALTOGENIC AMYLASE



L520	V521	T525	M528	E529	T530	V531	M532	I533	I534	R537	E540	A541	I544	P545	M546	P547	I548	R551	G552	A553	W554	L555	V556	N557	L558	L559	T560	G561	E562	R563	P564	A565	A566	E567	A568	E569	T570	L571	S574	L575	P576	P577	Y578	V581	L582	Y583	A584	V585	E586	S587	W588							
L442	F443	L444	F445	T448	F449	T450	P453	C454	I455	Y456	Y457	G458	D459	E460	I461	G462	M463	T464	G465	G466	P469	E470	C471	R472	K473	C474	N475	W476	W477	D478	P479	Q482	M483	K484	E485	L486	B489	L493	L496	L497	K498	Q499	Y500	L503	R504	R505	F510	L511	H519	L520								
A362	M363	P364	W365	L366	G368	D369	Q370	F371	V374	M375	M376	Y377	P378	L379	R385	F386	F387	E390	D391	M392	E396	D399	R400	L401	M402	H403	V404	H405	H406	S407	Y408	P409	V412	M418	L419	H423	R427	L428	L429	T430	V431	D435	V436	R437	K438	V439	K440	L441										
V292	P293	H294	M295	P296	K297	L298	M299	T300	A301	H302	P303	E304	V305	K306	P307	Y308	L309	L310	T314	Y315	K316	F320	D323	G324	W325	R326	L327	R328	V329	A330	N331	E332	L333	D334	H335	W338	F341	V345	K346	L347	R348	K349	P350	D351	V352	Y353	L354	L357	L358	W359	R360	D361						
K226	T227	L228	W229	K230	R231	C232	H233	E234	K235	G236	L237	M240	A243	V244	T245	W246	H247	C248	G249	Y250	A253	P254	F255	Q256	D257	V258	L259	K260	N261	A264	S265	K268	F271	H272	I273	R274	E275	F276	P277	L278	Q279	T280	E281	P282	R283	P284	N285	Y286	D287	T288	F289	A290	F291					
I152	S153	P154	K155	G156	A157	R158	P159	W160	G161	S162	E163	D164	P165	T166	P167	T168	S169	F170	F171	G172	G173	D174	L175	O176	G177	I178	L179			L182	L188	G189	I190	Y194	L195	T196	P197	I198	F199	R200	A201	H205	K206	Y207	D208	T209			F213	E214	L215	D216	P217	D218	F219		T224	L225

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	119.09 Å 119.09 Å 270.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	89.3 (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCD

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	0.41	0/4982	0.67	0/6770
1	B	0.42	0/4982	0.68	1/6770 (0.0%)
All	All	0.41	0/9964	0.68	1/13540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	PHE	N-CA-C	6.04	127.32	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	4828	0	4629	347	0
1	B	4828	0	4629	349	0
2	A	77	0	70	2	0
2	B	77	0	70	3	0
All	All	9810	0	9398	683	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 36.

The worst 5 of 683 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:A:281:GLU:HB2	1:A:282:PRO:HD3	1.33	1.08
1:B:281:GLU:HB2	1:B:282:PRO:CD	1.93	0.99
1:B:275:GLU:HG3	1:B:277:PRO:HD2	1.46	0.97
1:B:155:LYS:HG3	1:B:170:PHE:HB2	1.47	0.96
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.44	0.95

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%)	486 (83%)	76 (13%)	24 (4%)	3	24
1	B	586/588 (100%)	467 (80%)	93 (16%)	26 (4%)	3	22
All	All	1172/1176 (100%)	953 (81%)	169 (14%)	50 (4%)	3	23

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	118	PRO
1	A	156	GLY
1	A	158	ARG
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	505/505 (100%)	452 (90%)	53 (10%)	8	33
1	B	505/505 (100%)	457 (90%)	48 (10%)	11	38
All	All	1010/1010 (100%)	909 (90%)	101 (10%)	9	36

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	LEU
1	B	47	TRP
1	B	525	THR
1	A	556	VAL
1	A	586	GLU

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	A	499	GLN
1	B	7	HIS
1	B	482	GLN
1	A	518	ASN
1	A	528	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BCD	A	1589	-	84,84,84	1.88	6 (7%)	126,126,126	1.71	15 (11%)
2	BCD	B	1589	-	84,84,84	1.90	6 (7%)	126,126,126	1.69	15 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCD	A	1589	-	-	0/42/182/182	0/0/8/8
2	BCD	B	1589	-	-	0/42/182/182	0/0/8/8

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1589	BCD	O47-C11	-12.98	1.06	1.41
2	A	1589	BCD	O47-C11	-12.94	1.06	1.41
2	B	1589	BCD	O44-C15	-4.13	1.30	1.41
2	A	1589	BCD	O44-C15	-4.01	1.30	1.41
2	B	1589	BCD	O52-C12	2.02	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1589	BCD	O41-C12-C22	-6.56	92.15	108.10
2	B	1589	BCD	O41-C12-C22	-5.90	93.74	108.10
2	A	1589	BCD	O44-C15-O55	-5.46	96.85	110.68
2	B	1589	BCD	O44-C15-O55	-5.22	97.48	110.68
2	B	1589	BCD	C14-O43-C43	-4.64	105.87	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1589	BCD	2	0
2	B	1589	BCD	3	0

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 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.