



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:52 AM GMT

PDB ID : 5BCA
Title : BETA-AMYLASE FROM BACILLUS CEREUS VAR. MYCOIDES
Authors : Oyama, T.; Kusunoki, M.; Kishimoto, Y.; Takasaki, Y.; Nitta, Y.
Deposited on : 1999-03-12
Resolution : 2.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

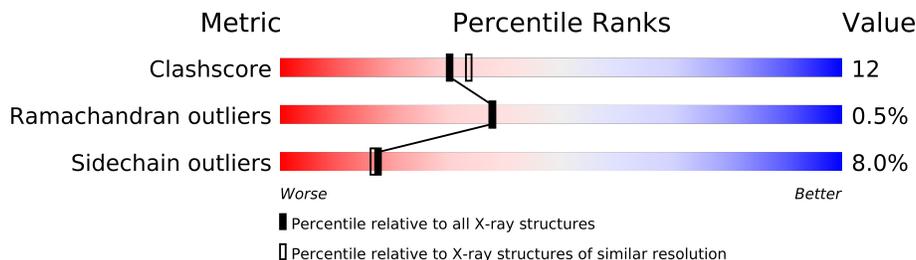
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. 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	516	
1	B	516	
1	C	516	
1	D	516	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17232 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 PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	B	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	C	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	D	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total	O	0	0
			206	206		
3	B	170	Total	O	0	0
			170	170		
3	C	191	Total	O	0	0
			191	191		
3	D	185	Total	O	0	0
			185	185		

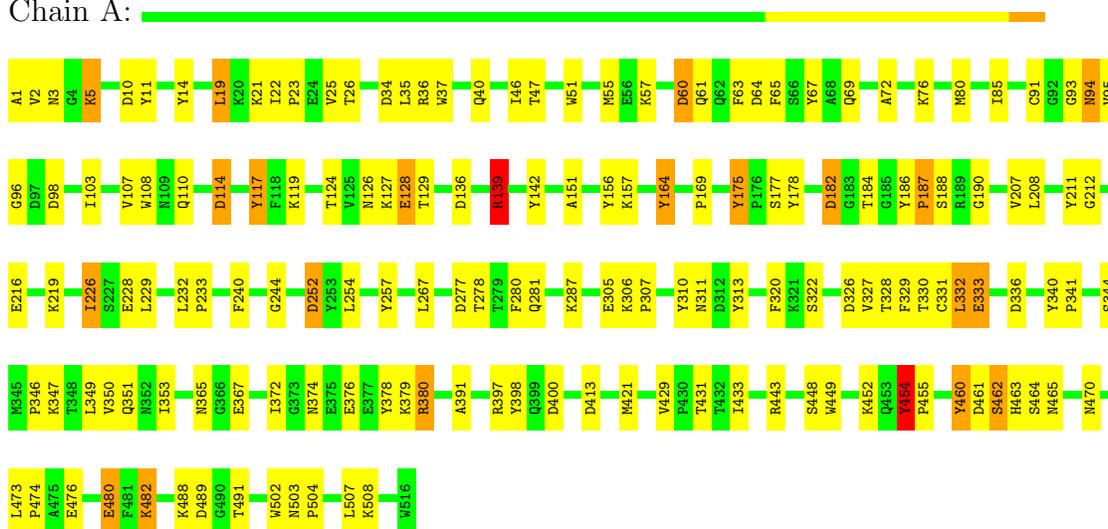
3 Residue-property plots

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.

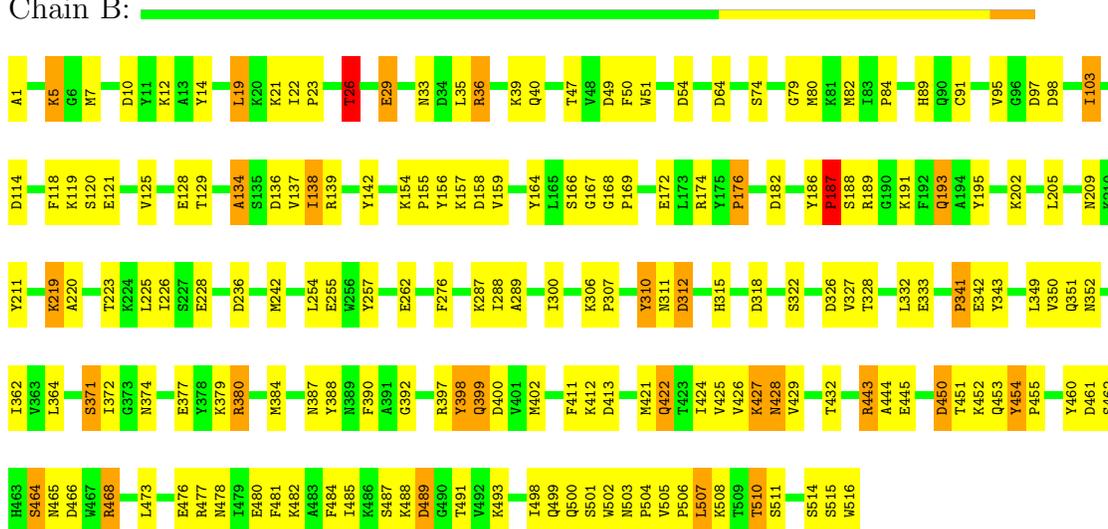
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

Chain A:



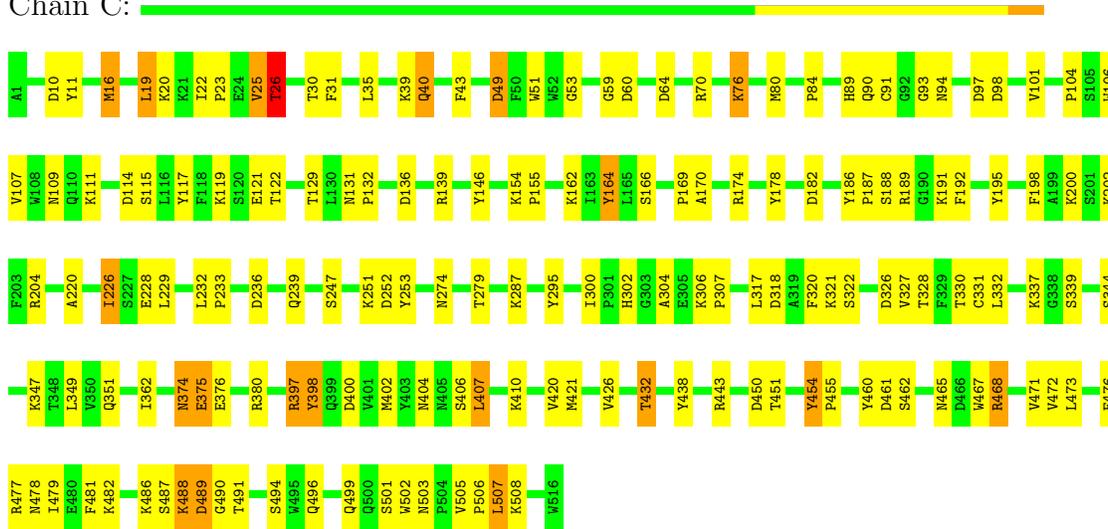
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

Chain B:



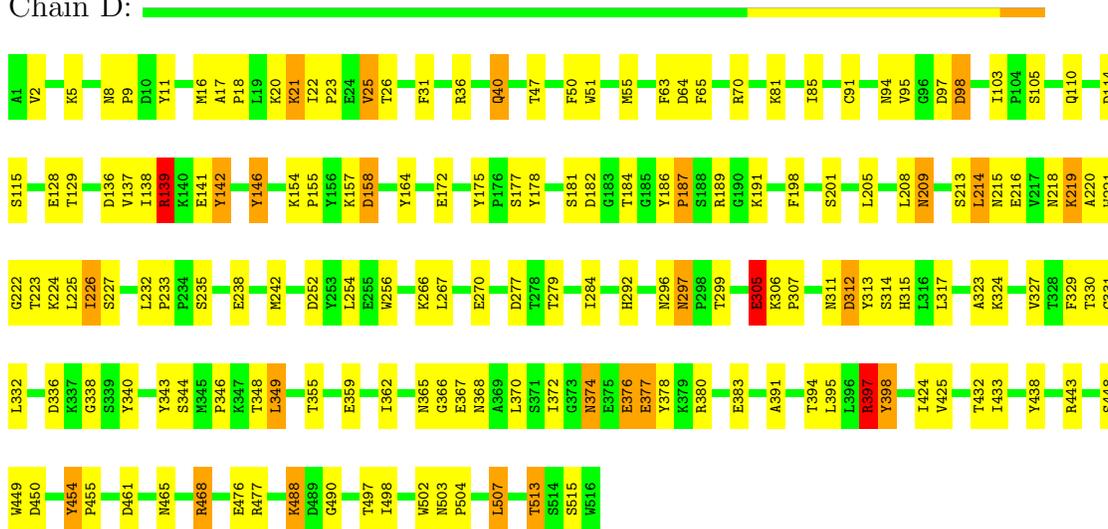
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

Chain C:



- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.90Å 112.90Å 146.20Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	74.0 (8.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17232	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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:
CA

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	0.74	0/4234	1.59	46/5751 (0.8%)
1	B	0.71	0/4234	1.61	52/5751 (0.9%)
1	C	0.74	0/4234	1.66	60/5751 (1.0%)
1	D	0.74	0/4234	1.63	54/5751 (0.9%)
All	All	0.73	0/16936	1.62	212/23004 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ARG	NE-CZ-NH2	-21.41	109.60	120.30
1	D	380	ARG	CD-NE-CZ	17.65	148.31	123.60
1	C	189	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	C	380	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	B	189	ARG	NE-CZ-NH1	13.59	127.10	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ALA	Mainchain
1	B	134	ALA	Mainchain
1	B	276	PHE	Mainchain
1	C	220	ALA	Mainchain
1	D	50	PHE	Mainchain

5.2 Close contacts

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	4119	0	3984	83	0
1	B	4119	0	3984	115	0
1	C	4119	0	3984	92	0
1	D	4119	0	3984	100	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	206	0	0	6	0
3	B	170	0	0	3	0
3	C	191	0	0	6	0
3	D	185	0	0	9	0
All	All	17232	0	15936	389	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 12.

The worst 5 of 389 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:THR:HG21	1:B:169:PRO:HD3	1.36	1.05
1:A:489:ASP:OD1	1:A:491:THR:HG23	1.54	1.05
1:B:422:GLN:NE2	1:B:510:THR:H	1.54	1.04
1:C:164:TYR:HH	1:C:328:THR:HG1	1.04	1.02
1:D:226:ILE:HD12	1:D:227:SER:H	1.24	0.99

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	514/516 (100%)	486 (95%)	26 (5%)	2 (0%)	43	45
1	B	514/516 (100%)	490 (95%)	22 (4%)	2 (0%)	43	45
1	C	514/516 (100%)	486 (95%)	24 (5%)	4 (1%)	27	24
1	D	514/516 (100%)	475 (92%)	37 (7%)	2 (0%)	43	45
All	All	2056/2064 (100%)	1937 (94%)	109 (5%)	10 (0%)	38	38

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TYR
1	B	428	ASN
1	C	489	ASP
1	D	219	LYS
1	C	170	ALA

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	440/440 (100%)	412 (94%)	28 (6%)	25	26
1	B	440/440 (100%)	395 (90%)	45 (10%)	11	9
1	C	440/440 (100%)	409 (93%)	31 (7%)	21	22
1	D	440/440 (100%)	404 (92%)	36 (8%)	17	15
All	All	1760/1760 (100%)	1620 (92%)	140 (8%)	17	16

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	473	LEU
1	C	76	LYS
1	D	344	SER
1	B	489	ASP
1	B	510	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	463	HIS
1	C	351	GLN
1	D	351	GLN
1	B	503	ASN
1	C	352	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.