

wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 03:24 PM EST

PDB ID : 1BYC

Title : CRYSTAL STRUCTURES OF SOYBEAN BETA-AMYLASE REACTED

WITH BETA-MALTOSE AND MALTAL: ACTIVE SITE COMPONENTS

AND THEIR APPARENT ROLE IN CATALYSIS

Authors : Mikami, B.; Degano, M.; Hehre, E.J.; Sacchettini, J.C.

Deposited on : 1994-01-25

Resolution : 2.20 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 (i) 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

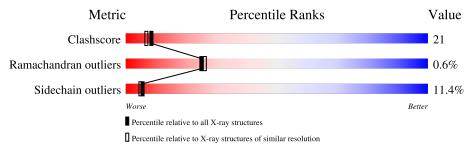
Validation Pipeline (wwPDB-VP) : 2.36

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 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of cha	in	
1	A	495	61%	30%	7% ••
2	В	4	100%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4307 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 BETA-AMYLASE.

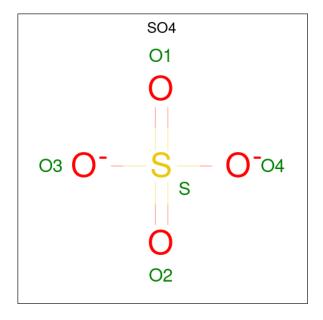
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	491	Total 3925	C 2518	N 662	O 728	S 17	0	0	1

• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	At	oms	1	ZeroOcc	AltConf	Trace
2	В	4	Total 45	C 24	O 21	0	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total () S 4 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	332	Total O 332 332	0	0

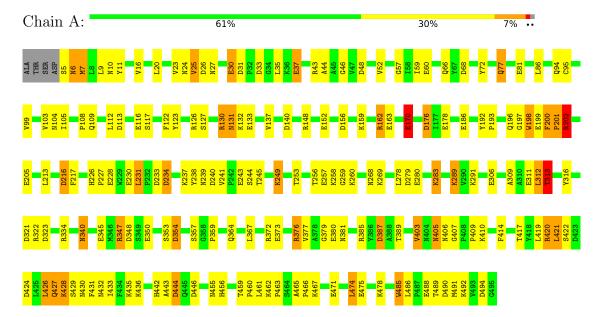


3 Residue-property plots (i)

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. 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. 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: BETA-AMYLASE



 \bullet Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain B: 100%





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	86.20Å 86.20Å 144.20Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	9.00 - 2.20	Depositor	
% Data completeness	(Not available) (9.00-2.20)	Depositor	
(in resolution range)	(110t available) (3.00 2.20)	Беровног	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	TNT, X-PLOR	Depositor	
R, R_{free}	0.149 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4307	wwPDB-VP	
Average B, all atoms (Å ²)	22.0	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: BGC, GLC, SO4

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	Bo	nd lengths	Во	ond angles
MOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	1.21	$26/4032 \ (0.6\%)$	1.34	59/5479 (1.1%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
1	A	306	GLU	CD-OE2	10.70	1.37	1.25
1	A	170	GLU	CD-OE1	9.81	1.36	1.25
1	A	257	GLU	CD-OE2	9.67	1.36	1.25
1	A	37	GLU	CD-OE2	9.53	1.36	1.25
1	A	347	ARG	NE-CZ	8.01	1.43	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	A	313	THR	N-CA-CB	11.92	132.95	110.30
1	A	233	ASP	CB-CG-OD2	-10.45	108.89	118.30
1	A	240	ASP	CB-CG-OD2	10.06	127.36	118.30
1	A	240	ASP	CB-CG-OD1	-9.45	109.79	118.30
1	A	279	ASP	CB-CG-OD1	-9.18	110.04	118.30

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	6	ASN	CA
1	A	256	THR	СВ

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	TYR	Sidechain

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	3925	0	3824	160	0
2	В	45	0	39	3	0
3	A	5	0	0	0	0
4	A	332	0	0	22	0
All	All	4307	0	3863	163	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 21.

The worst 5 of 163 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:202:ARG:HG3	1:A:239:ASN:CA	1.54	1.37
1:A:202:ARG:HG3	1:A:239:ASN:C	1.46	1.32
1:A:200:PHE:CB	1:A:201:PRO:HD3	1.69	1.22
1:A:200:PHE:HB3	1:A:201:PRO:CD	1.68	1.17
1:A:421:LEU:C	1:A:421:LEU:HD22	1.67	1.13

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	489/495 (99%)	466 (95%)	20 (4%)	3 (1%)	25 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	PHE
1	A	313	THR
1	A	198	TRP

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	Analysed Rotameric		Percentiles	
1	A	422/425~(99%)	374 (89%)	48 (11%)	5 5	

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	SER
1	A	426	LEU
1	A	403	VAL
1	A	409	PRO
1	A	428	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:



Mol	Chain	Res	Type
1	A	307	ASN
1	A	340	ASN
1	A	455	ASN
1	A	405	ASN
1	A	131	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)

4 monosaccharides 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 Cl		Chain	Chain Res		Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	В	1	2	12,12,12	0.69	0	17,17,17	1.86	4 (23%)
2	GLC	В	2	2	11,11,12	2.08	3 (27%)	15,15,17	1.63	3 (20%)
2	GLC	В	3	2	11,11,12	0.99	0	15,15,17	1.62	3 (20%)
2	GLC	В	4	2	11,11,12	0.90	1 (9%)	15,15,17	1.49	2 (13%)

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	BGC	В	1	2	-	2/2/22/22	0/1/1/1
2	GLC	В	2	2	-	0/2/19/22	0/1/1/1

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	В	3	2	-	0/2/19/22	0/1/1/1
2	GLC	В	4	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	В	2	GLC	C2-C3	4.93	1.59	1.52
2	В	2	GLC	C4-C3	3.15	1.60	1.52
2	В	2	GLC	O4-C4	2.76	1.49	1.43
2	В	4	GLC	C2-C3	-2.09	1.49	1.52

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

Mol	Chain	Res	Type	Atoms	Atoms Z		$\mathbf{Ideal}(^{o})$
2	В	1	BGC	C6-C5-C4	-4.15	103.27	113.00
2	В	3	GLC	O5-C1-C2	-3.69	105.08	110.77
2	В	2	GLC	O4-C4-C3	3.60	118.67	110.35
2	В	4	GLC	O2-C2-C1	3.24	115.77	109.15
2	В	1	BGC	C3-C4-C5	2.95	115.50	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1	BGC	C4-C5-C6-O6
2	В	1	BGC	O5-C5-C6-O6

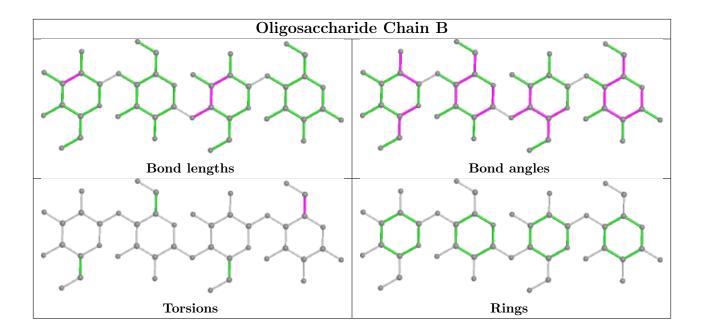
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Res Type Clashes		Symm-Clashes		
2	В	1	BGC	1	0		
2	В	3	GLC	1	0		
2	В	2	GLC	2	0		
2	В	4	GLC	1	0		

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry (i)

1 ligand is 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		
IVIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	860	-	4,4,4	0.38	0	6,6,6	0.47	0

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.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

