

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 08:05 AM EST

PDB ID : 1FQA

Title : STRUCTURE OF MALTOTETRAITOL BOUND TO OPEN-FORM MAL-

TODEXTRIN BINDING PROTEIN IN P2(1)CRYSTAL FORM

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Deposited on : 2000-09-04

Resolution : 1.90 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)

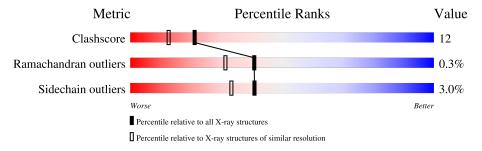
Validation Pipeline (wwPDB-VP) : 2.36

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 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 chain					
1	A	370		82%		17%	-		
2	В	4	25%	50%	25	%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3442 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.

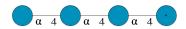
• Molecule 1 is a protein called MALTODEXTRIN-BINDING PROTEIN.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	A	370	Total 2874	C 1850	N 468	O 550	S 6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	LYS	cloning artifact	UNP P02928

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



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

• Molecule 3 is water.

Mo	l Cha	ain	Residues	Ato	$\mathbf{m}\mathbf{s}$	ZeroOcc	AltConf
3	A	L	523	Total 523	O 523	0	0

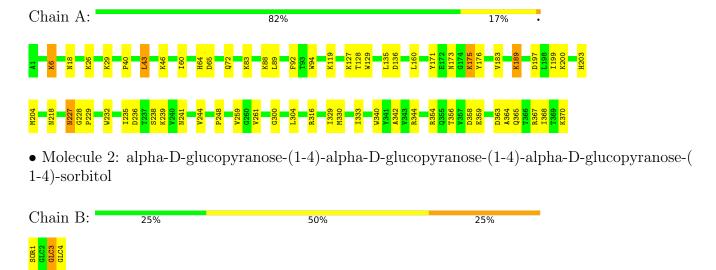


3 Residue-property plots (i)

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: MALTODEXTRIN-BINDING PROTEIN





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	43.90Å 65.80Å 57.80Å	Depositor	
a, b, c, α , β , γ	90.00° 101.20° 90.00°	Depositor	
Resolution (Å)	30.00 - 1.90	Depositor	
% Data completeness	(Not available) (30.00-1.90)	Depositor	
(in resolution range)	(1101 available) (90.00 1.90)	Беровног	
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.176 , 0.215	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3442	wwPDB-VP	
Average B, all atoms (Å ²)	14.0	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: SOR, GLC

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).

Mal	Chain	Bond	lengths	Bond	angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.31	0/2943	0.54	0/3994

There are no bond length outliers.

There are no bond angle outliers.

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	2874	0	2851	69	0
2	В	45	0	41	3	0
3	A	523	0	0	17	0
All	All	3442	0	2892	70	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 12.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:342:ALA:HA	1:A:367:ARG:NH2	1.21	1.50

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:342:ALA:CA	1:A:367:ARG:HH21	1.47	1.26
1:A:342:ALA:CA	1:A:367:ARG:NH2	2.01	1.20
1:A:342:ALA:CB	1:A:367:ARG:HH21	1.61	1.13
1:A:342:ALA:HA	1:A:367:ARG:HH22	1.20	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	Perce	ntiles
1	A	368/370 (100%)	355 (96%)	12 (3%)	1 (0%)	41	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN

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.

Mo	l Chain	Analysed	Analysed Rotameric Outliers		Percentiles	
1	A	296/296 (100%)	287 (97%)	9 (3%)	41 33	

5 of 9 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	189	LYS
1	A	227	ASN
1	A	65	ASP
1	A	83	LYS
1	A	160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	227	ASN
1	A	325	GLN
1	A	72	GLN
1	A	86	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)

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	Chain	Res	Link	Bo	nd leng	$ ag{ths}$	В	ond ang	les
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SOR	В	1	2	11,11,11	0.27	0	14,14,14	0.40	0
2	GLC	В	2	2	11,11,12	0.46	0	15,15,17	0.51	0
2	GLC	В	3	2	11,11,12	0.43	0	15,15,17	0.66	1 (6%)
2	GLC	В	4	2	11,11,12	0.50	0	15,15,17	0.51	0



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	SOR	В	1	2	-	2/16/16/16	-
2	GLC	В	2	2	-	1/2/19/22	0/1/1/1
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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	3	GLC	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

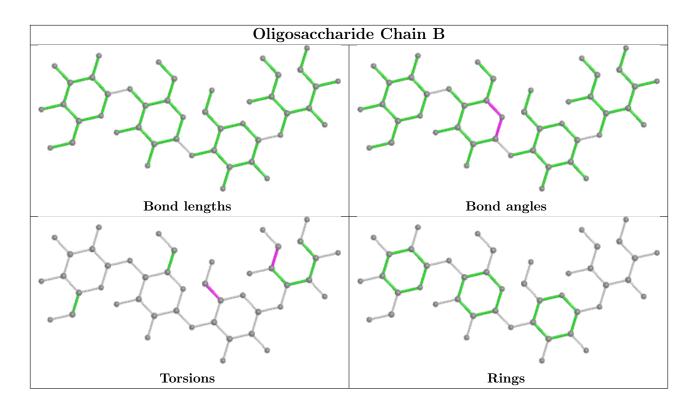
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	3	GLC	1	0
2	В	1	SOR	1	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)

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)

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.

