

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 01:14 AM EDT

PDB ID	:	6PSO
Title	:	Crystal structure of PsS1_19B C77S in complex with iota-neocarratetraose
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Deposited on	:	2019-07-13
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.35.1
EDS Percentile statistics Ideal geometry (proteins)	: : :	FAILED 20191225.v01 (using entries in the PDB archive December 25th 2019) Engh & Huber (2001) Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7555 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 exo-4S-kappa carrageenan S1 sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Р	447	Total	С	Ν	Ο	S	0	0	0
	D	447	3545	2260	600	676	9	0		
1	Λ	447	Total	С	Ν	0	S	0	0	0
	A	441	3544	2261	599	675	9	0	0	

• Molecule 2 is an oligosaccharide called 3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3) -4-O-sulfo-beta-D-galactopyranose-(1-4)-3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	2 C	1	Total	С	Ο	S	0	0	0	
2		т	59	24	31	4				
0	Л	1	Total	С	Ο	\mathbf{S}	0	0	0	
		4	59	24	31	4	0	U	0	

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Ca 1 1	0	0
3	А	1	Total Ca 1 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Cl 1 1	0	0
4	А	1	Total Cl 1 1	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	140	Total O 140 140	0	0
5	А	204	Total O 204 204	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.26Å 94.00Å 170.55Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.01 - 2.00	Depositor
% Data completeness	98.1 (29.01-2.00)	Depositor
(in resolution range)		-
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$10.73 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.197 , 0.231	Depositor
Wilson B-factor $(Å^2)$	24.3	Xtriage
Anisotropy	0.058	Xtriage
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7555	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

8 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
N101	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	G4S	С	1	2	16,16,16	1.26	2 (12%)	19,24,24	2.24	3 (15%)
2	DGS	С	2	2	15,15,16	1.28	1 (6%)	18,23,25	1.32	3 (16%)
2	G4S	С	3	2	15,15,16	1.36	2 (13%)	17,22,24	1.09	1 (5%)
2	DGS	С	4	2	15,15,16	1.48	2 (13%)	18,23,25	1.43	2 (11%)
2	G4S	D	1	2	16,16,16	1.28	2 (12%)	19,24,24	0.61	0
2	DGS	D	2	2	15,15,16	1.18	1 (6%)	18,23,25	1.72	3 (16%)
2	G4S	D	3	2	15,15,16	1.35	2 (13%)	17,22,24	1.30	2 (11%)
2	DGS	D	4	2	15,15,16	1.22	1 (6%)	18,23,25	1.11	1 (5%)

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	G4S	С	1	2	-	1/7/27/27	0/1/1/1
2	DGS	С	2	2	-	0/5/27/30	0/3/2/2
2	G4S	С	3	2	-	1/7/24/27	0/1/1/1
2	DGS	С	4	2	-	0/5/27/30	0/3/2/2
2	G4S	D	1	2	-	1/7/27/27	0/1/1/1
2	DGS	D	2	2	-	0/5/27/30	0/3/2/2
2	G4S	D	3	2	-	1/7/24/27	0/1/1/1
2	DGS	D	4	2	-	0/5/27/30	0/3/2/2

All	(13)	bond	length	outliers	are	listed	below:	
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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	D	1	G4S	08-S	3.91	1.62	1.45
2	С	1	G4S	O7-S	3.78	1.61	1.45
2	D	3	G4S	O7-S	3.74	1.61	1.45
2	С	3	G4S	08-S	3.74	1.61	1.45
2	С	4	DGS	O9-S	3.72	1.61	1.45
2	С	2	DGS	O2-C2	-3.59	1.41	1.47
2	D	2	DGS	O2-C2	-3.37	1.42	1.47
2	D	4	DGS	O2-C2	-3.09	1.42	1.47
2	С	4	DGS	O2-C2	-2.89	1.42	1.47
2	С	1	G4S	O4-C4	-2.24	1.41	1.46
2	D	3	G4S	O4-C4	-2.16	1.41	1.46
2	D	1	G4S	O4-C4	-2.07	1.42	1.46
2	С	3	G4S	O4-C4	-2.04	1.42	1.46



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1	G4S	08-S-07	-6.35	86.71	112.22
2	С	1	G4S	O9-S-O7	-5.70	88.68	108.49
2	D	2	DGS	O2-C2-C3	5.20	112.41	106.65
2	D	3	G4S	C1-C2-C3	4.02	114.61	109.67
2	С	3	G4S	C1-C2-C3	3.80	114.34	109.67
2	С	4	DGS	C2-O2-S	3.41	122.36	117.91
2	С	1	G4S	O9-S-O8	3.30	119.96	108.49
2	С	2	DGS	O5-C5-C6	-3.23	108.53	113.33
2	С	4	DGS	C2-C3-C4	-3.14	106.21	113.84
2	D	2	DGS	O5-C5-C6	-2.93	108.98	113.33
2	D	4	DGS	C2-C3-C4	-2.82	106.98	113.84
2	С	2	DGS	C2-O2-S	2.74	121.48	117.91
2	С	2	DGS	C2-C3-C4	-2.73	107.21	113.84
2	D	2	DGS	C2-O2-S	2.45	121.11	117.91
2	D	3	G4S	O3-C3-C2	-2.07	106.02	109.99

All (15) bond angle outliers are listed below:

There are no chirality outliers.

All (4) torsion outliers are listed below:

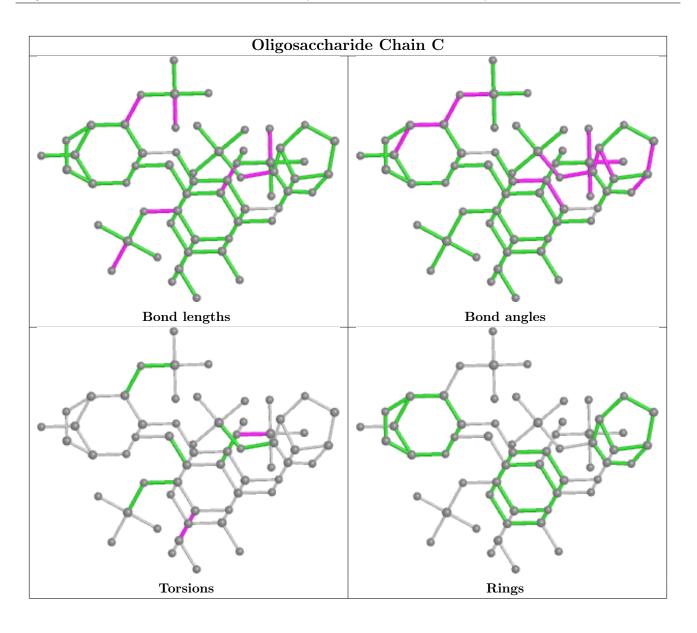
Mol	Chain	Res	Type	Atoms
2	С	1	G4S	C4-O4-S-O8
2	С	3	G4S	O5-C5-C6-O6
2	D	3	G4S	O5-C5-C6-O6
2	D	1	G4S	C4-O4-S-O8

There are no ring outliers.

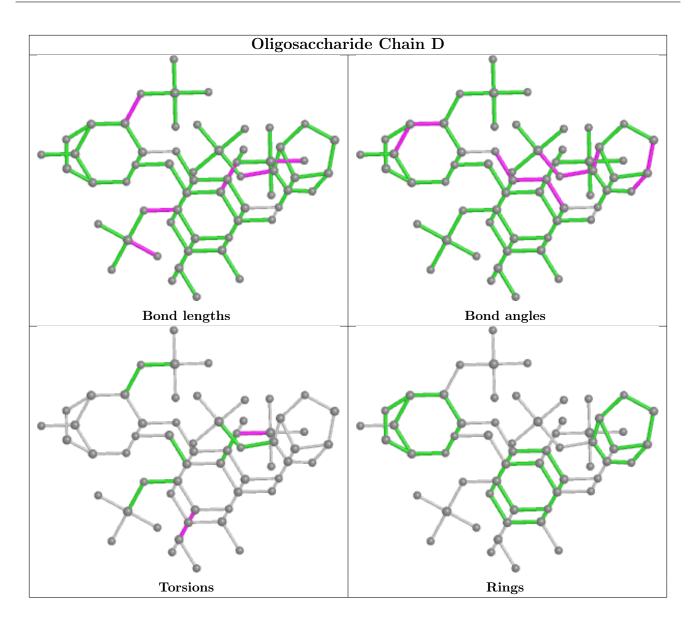
No monomer is involved in short contacts.

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









4.6 Ligand geometry (i)

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.

No monomer is involved in short contacts.



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

