

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 07:49 PM EDT

PDB ID : 6PT6

Title: Crystal structure of PsS1 NC C84S in complex with i-neocarratetraose

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Deposited on : 2019-07-15

Resolution : 2.25 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 : 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) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.25 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 4 unique types of molecules in this entry. The entry contains 7887 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-2S-iota carrageenan S1 sulfatase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	В	472	Total 3751	C 2382	N 643	O 707	S 19	0	0	0
1	A	473	Total 3762	C 2384	N 647	O 712	S 19	0	0	1

• Molecule 2 is an oligosaccharide called 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	С	9	Total	С	О	S	0	0	0
2		2	30	12	16	2	0	U	
2	D	9	Total	С	О	S	0	0	0
2	D	2	30	12	16	2	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	A	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	154	Total O 154 154	0	0
4	A	158	Total O 158 158	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	57.73Å 102.21Å 170.75Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.78 - 2.25	Depositor
% Data completeness	98.6 (31.78-2.25)	Depositor
(in resolution range)	` ,	_
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.16 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.200 , 0.252	Depositor
Wilson B-factor (A^2)	33.5	Xtriage
Anisotropy	0.016	Xtriage
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ 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)

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	Trunc	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	G4S	С	1	2	16,16,16	1.28	1 (6%)	19,24,24	0.81	1 (5%)
2	DGS	С	2	3,2	15,15,16	1.45	2 (13%)	18,23,25	1.84	3 (16%)
2	G4S	D	1	2	16,16,16	1.32	1 (6%)	19,24,24	0.78	0
2	DGS	D	2	3,2	15,15,16	1.48	2 (13%)	18,23,25	1.31	3 (16%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\mathring{A}})$	Ideal(A)
2	D	1	G4S	O8-S	4.23	1.63	1.45
2	D	2	DGS	O8-S	4.21	1.63	1.45
2	С	1	G4S	O7-S	4.19	1.63	1.45
2	С	2	DGS	O9-S	4.14	1.62	1.45
2	D	2	DGS	O2-C2	-2.68	1.43	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	С	2	DGS	C2-O2-S	5.48	125.05	117.91
2	С	2	DGS	O5-C5-C6	-3.53	108.08	113.33
2	D	2	DGS	O5-C5-C6	-3.09	108.75	113.33
2	С	2	DGS	C2-C3-C4	-2.71	107.26	113.84
2	D	2	DGS	C2-C3-C4	-2.52	107.72	113.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

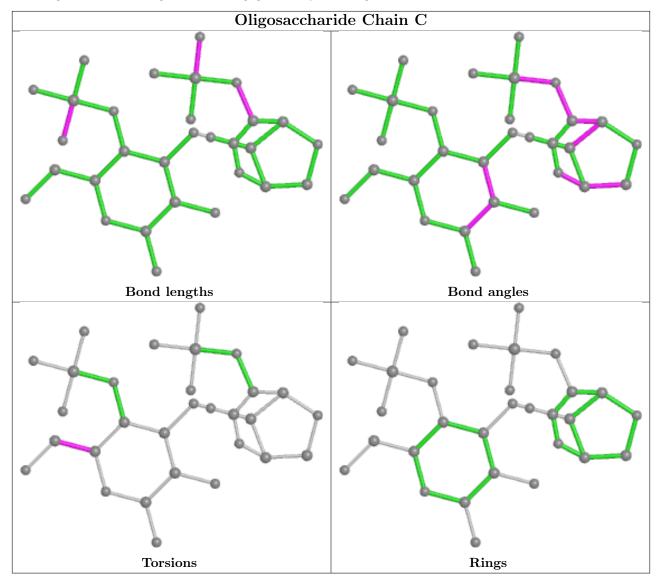
Mol	Chain	Res	Type	Atoms
2	С	1	G4S	O5-C5-C6-O6
2	С	1	G4S	C4-C5-C6-O6



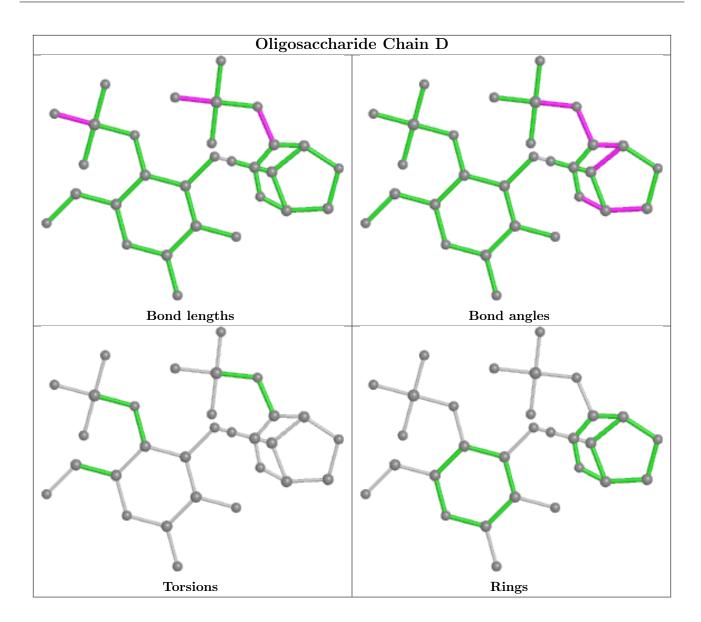
There are no ring outliers.

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 2 ligands modelled in this entry, 2 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.

