



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 02:09 PM JST

PDB ID : 7VEW  
Title : Crystal structure of bacterial chemotaxis-dependent pectin-binding protein SPH1118 in complex with unsaturated trigalacturonic acid  
Authors : Anamizu, K.; Takase, R.; Hio, M.; Watanebe, D.; Mikami, B.; Hashimoto, W.  
Deposited on : 2021-09-10  
Resolution : 1.92 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

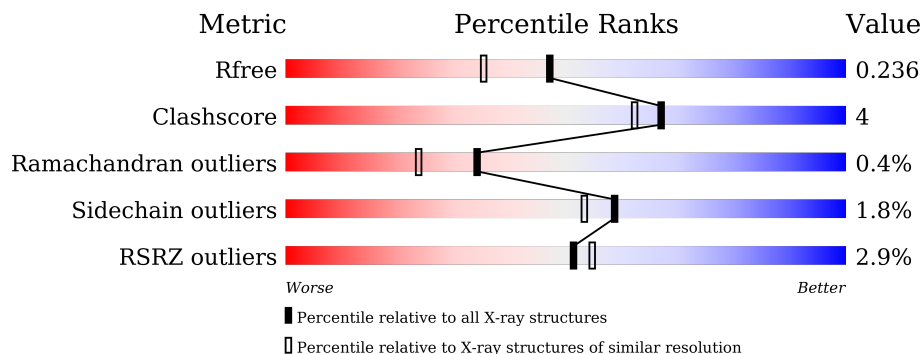
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	619	 3% 88% 9% ..
1	B	619	 3% 89% 9% .
2	C	3	 67% 33%
2	D	3	 67% 33%

## 2 Entry composition [i](#)

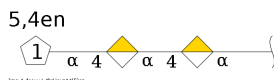
There are 6 unique types of molecules in this entry. The entry contains 10339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SPH1118.

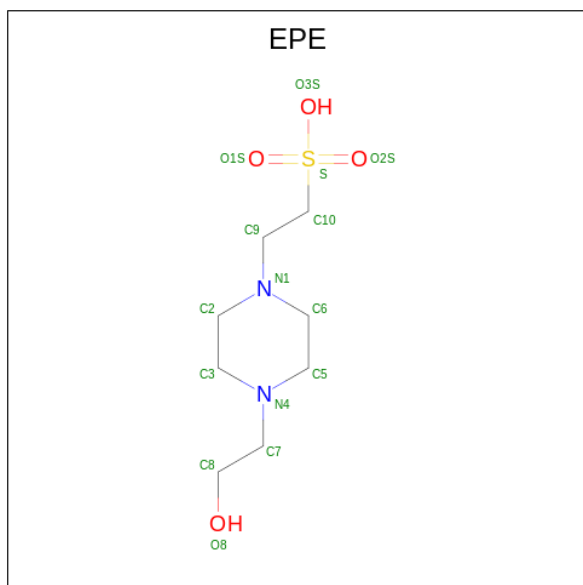
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	609	4854	3099	832	904	19	0	1	0
1	B	609	4854	3100	832	902	20	0	1	0

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	3	36	18	18	0	0	0
2	D	3	36	18	18	0	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	A	1	Total	15	8	2	4	1	0	0
3	B	1	Total	15	8	2	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



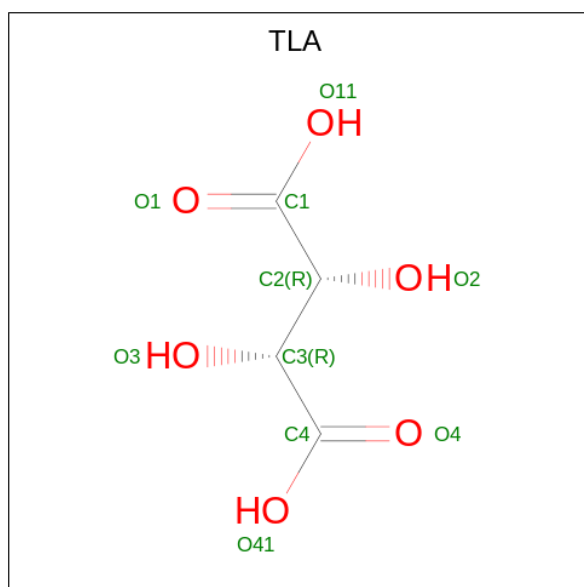
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			
4	A	1	Total	6	3	3	0	0
4	B	1	Total	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		
5	B	1	Total	C	O	0	0
			10	4	6		

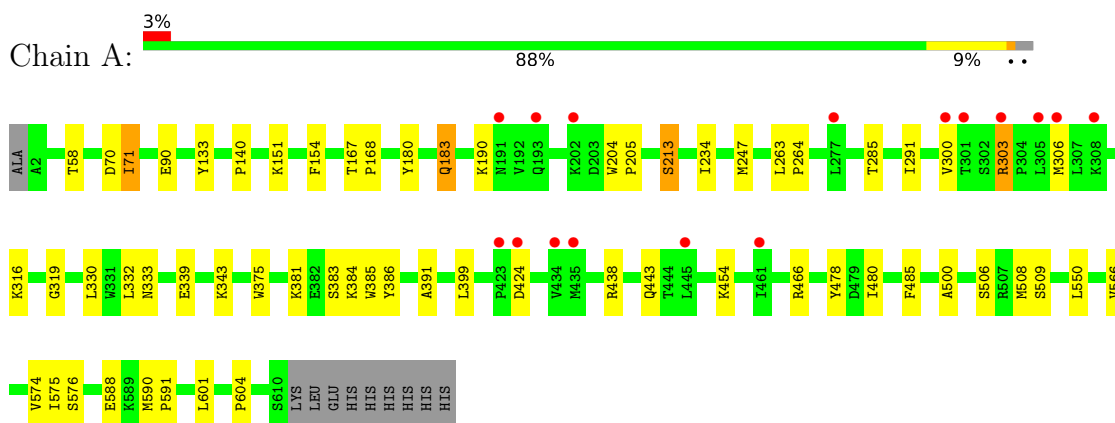
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	252	Total	O	0	0
			252	252		
6	B	227	Total	O	0	0
			227	227		

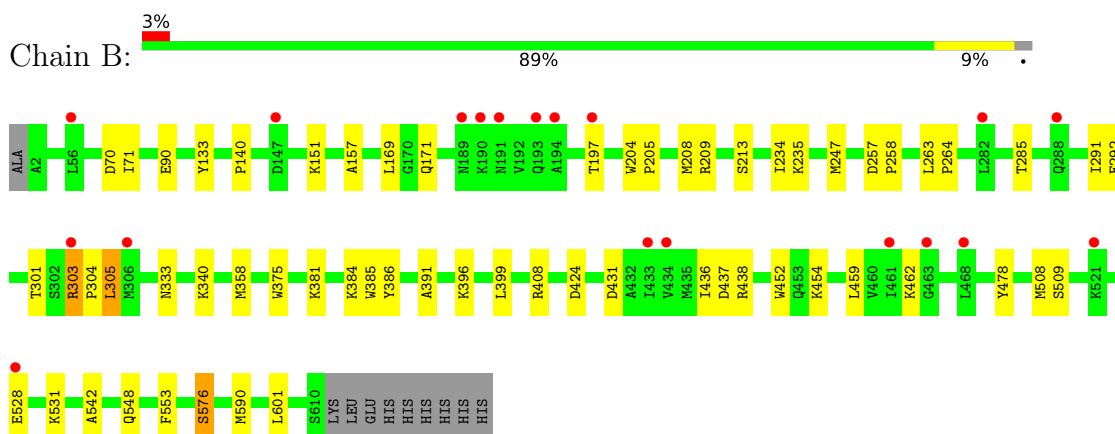
### 3 Residue-property plots [i](#)

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 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.

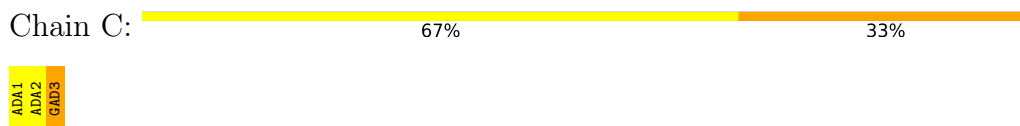
- Molecule 1: SPH1118



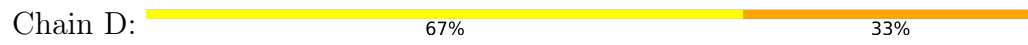
- Molecule 1: SPH1118



- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid



- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid



ADA1  
ADA2  
GAD3

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.69Å 83.66Å 148.52Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	48.59 – 1.92 48.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.59-1.92) 99.6 (48.59-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.210 , 0.232 0.212 , 0.236	Depositor DCC
$R_{free}$ test set	5421 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.684	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.



## 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: EPE, ADA, TLA, GOL, GAD

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	0.37	0/4976	0.53	0/6760
1	B	0.37	0/4976	0.52	0/6759
All	All	0.37	0/9952	0.53	0/13519

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	4854	0	4819	37	0
1	B	4854	0	4824	37	0
2	C	36	0	20	2	0
2	D	36	0	20	2	0
3	A	15	0	17	3	0
3	B	15	0	17	1	0
4	A	6	0	8	1	0
4	B	24	0	32	4	0
5	A	10	0	4	1	0
5	B	10	0	4	0	0
6	A	252	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	227	0	0	1	0
All	All	10339	0	9765	76	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 4.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HH11	1:B:576:SER:HB2	1.42	0.82
1:A:90:GLU:OE2	1:A:151:LYS:HD2	1.84	0.76
1:B:303:ARG:NH1	1:B:576:SER:HB2	2.04	0.73
1:A:180:TYR:O	1:A:183:GLN:HG3	1.90	0.72
1:B:303:ARG:HD2	1:B:576:SER:CB	2.21	0.70

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	608/619 (98%)	583 (96%)	22 (4%)	3 (0%)	29 18
1	B	608/619 (98%)	580 (95%)	26 (4%)	2 (0%)	41 31
All	All	1216/1238 (98%)	1163 (96%)	48 (4%)	5 (0%)	34 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	B	213	SER
1	A	213	SER

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Mol	Chain	Res	Type
1	B	509	SER
1	A	71	ILE

### 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	Rotameric	Outliers	Percentiles	
1	A	522/530 (98%)	514 (98%)	8 (2%)	65	61
1	B	522/530 (98%)	511 (98%)	11 (2%)	53	46
All	All	1044/1060 (98%)	1025 (98%)	19 (2%)	59	53

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	LEU
1	B	548	GLN
1	B	576	SER
1	B	508	MET
1	B	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADA	C	1	2	13,13,13	1.08	1 (7%)	18,19,19	0.93	0
2	ADA	C	2	2	12,12,13	1.09	1 (8%)	14,17,19	0.75	0
2	GAD	C	3	2	10,11,11	3.12	4 (40%)	13,15,15	1.36	3 (23%)
2	ADA	D	1	2	13,13,13	1.18	2 (15%)	18,19,19	0.98	1 (5%)
2	ADA	D	2	2	12,12,13	1.20	1 (8%)	14,17,19	0.72	0
2	GAD	D	3	2	10,11,11	3.27	3 (30%)	13,15,15	1.35	2 (15%)

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	ADA	C	1	2	-	0/4/24/24	0/1/1/1
2	ADA	C	2	2	-	0/4/21/24	0/1/1/1
2	GAD	C	3	2	-	0/4/17/17	0/1/1/1
2	ADA	D	1	2	-	0/4/24/24	0/1/1/1
2	ADA	D	2	2	-	1/4/21/24	0/1/1/1
2	GAD	D	3	2	-	0/4/17/17	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	GAD	C3-C4	-8.53	1.39	1.50
2	C	3	GAD	C3-C4	-7.97	1.40	1.50
2	D	3	GAD	C4-C5	4.05	1.39	1.33
2	C	3	GAD	C4-C5	3.81	1.39	1.33
2	D	3	GAD	C5-C6	-3.69	1.39	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GAD	O6B-C6-C5	2.79	121.17	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GAD	O5-C5-C6	2.59	115.41	111.52
2	C	3	GAD	C2-C3-C4	-2.30	109.18	112.32
2	C	3	GAD	O5-C5-C6	2.23	114.86	111.52
2	C	3	GAD	O6B-C6-C5	2.18	119.63	114.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

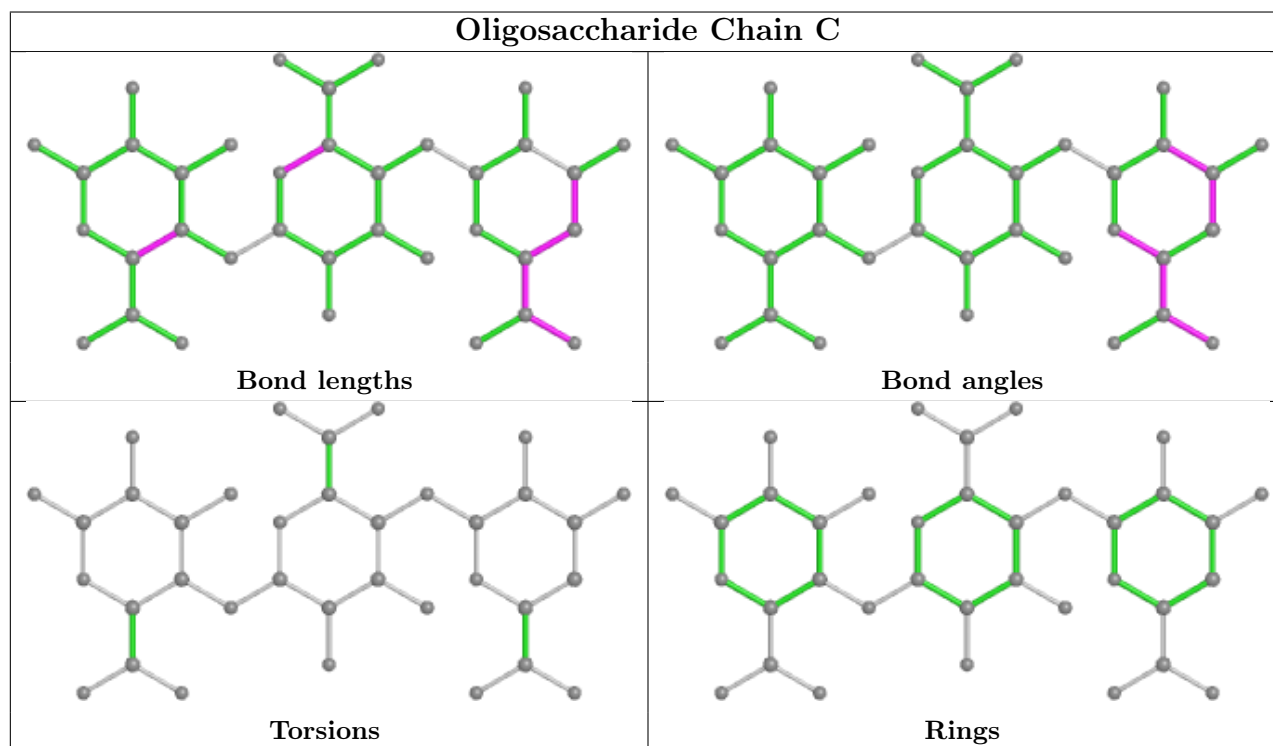
Mol	Chain	Res	Type	Atoms
2	D	2	ADA	C4-C5-C6-O6B

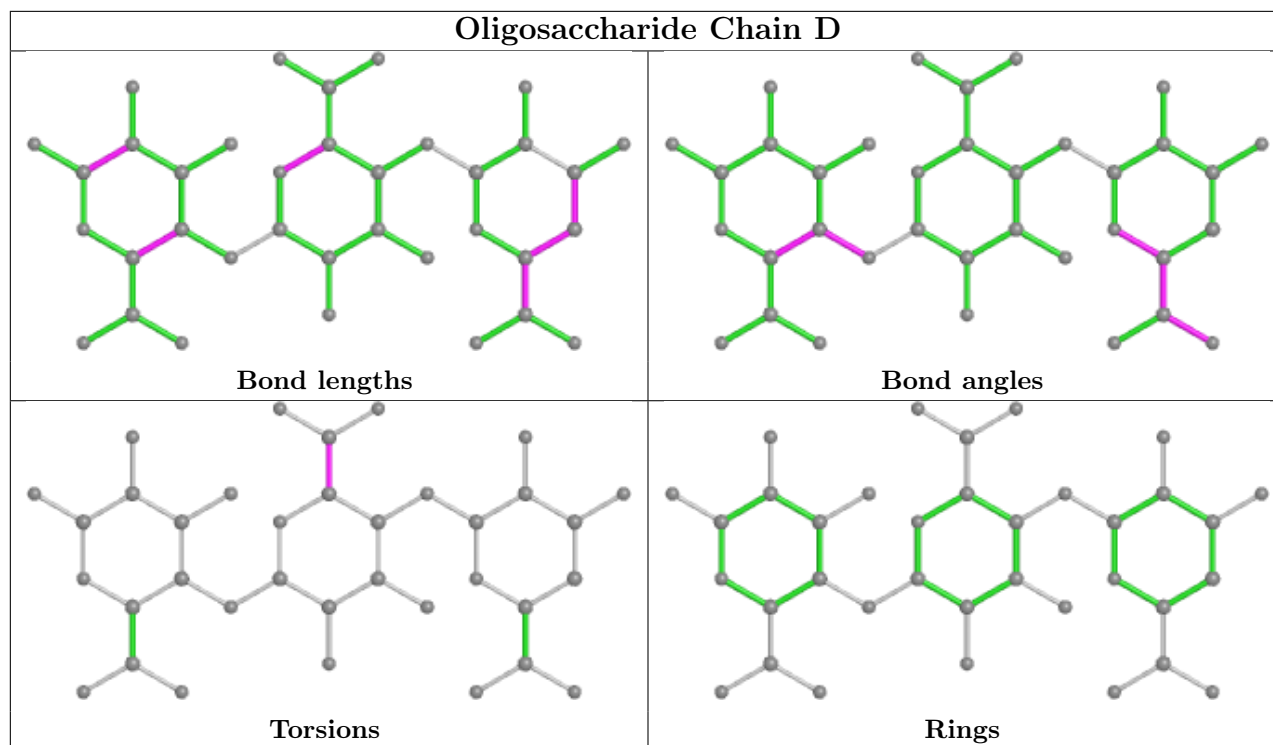
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	GAD	2	0
2	C	3	GAD	2	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](#)

9 ligands 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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	TLA	B	806	-	9,9,9	1.11	0	12,12,12	1.01	0
4	GOL	B	802	-	5,5,5	0.95	0	5,5,5	1.49	1 (20%)
5	TLA	A	803	-	9,9,9	1.18	0	12,12,12	1.14	1 (8%)
3	EPE	A	801	-	15,15,15	0.89	1 (6%)	18,20,20	1.73	5 (27%)
4	GOL	B	803	-	5,5,5	0.76	0	5,5,5	1.20	0
3	EPE	B	801	-	15,15,15	0.90	1 (6%)	18,20,20	2.18	6 (33%)
4	GOL	A	802	-	5,5,5	0.42	0	5,5,5	0.91	0
4	GOL	B	804	-	5,5,5	0.81	0	5,5,5	1.12	0
4	GOL	B	805	-	5,5,5	0.79	0	5,5,5	1.20	1 (20%)

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
5	TLA	B	806	-	-	7/12/12/12	-
4	GOL	B	802	-	-	2/4/4/4	-
5	TLA	A	803	-	-	10/12/12/12	-
3	EPE	A	801	-	-	3/9/19/19	0/1/1/1
4	GOL	B	803	-	-	4/4/4/4	-
3	EPE	B	801	-	-	3/9/19/19	0/1/1/1
4	GOL	A	802	-	-	1/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
4	GOL	B	805	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	EPE	C10-S	2.93	1.81	1.77
3	B	801	EPE	C10-S	2.84	1.81	1.77

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	EPE	C5-N4-C3	4.42	118.77	108.83
3	B	801	EPE	C5-N4-C3	4.38	118.68	108.83
3	B	801	EPE	O2S-S-C10	4.19	111.97	106.92
3	B	801	EPE	C7-N4-C3	3.78	120.89	111.23
3	B	801	EPE	O3S-S-C10	3.18	110.91	105.77

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	GOL	C1-C2-C3-O3
5	A	803	TLA	O1-C1-C2-O2
5	A	803	TLA	O11-C1-C2-O2
5	A	803	TLA	C1-C2-C3-C4
5	A	803	TLA	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	803	TLA	1	0
3	A	801	EPE	3	0
3	B	801	EPE	1	0
4	A	802	GOL	1	0
4	B	804	GOL	1	0
4	B	805	GOL	3	0

## 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](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	609/619 (98%)	0.24	16 (2%) 56 59	25, 35, 51, 62	0
1	B	609/619 (98%)	0.26	19 (3%) 49 52	28, 36, 52, 65	0
All	All	1218/1238 (98%)	0.25	35 (2%) 51 55	25, 36, 52, 65	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	ARG	3.5
1	A	305	LEU	3.1
1	B	190	LYS	3.0
1	A	193	GLN	2.9
1	A	308	LYS	2.9

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

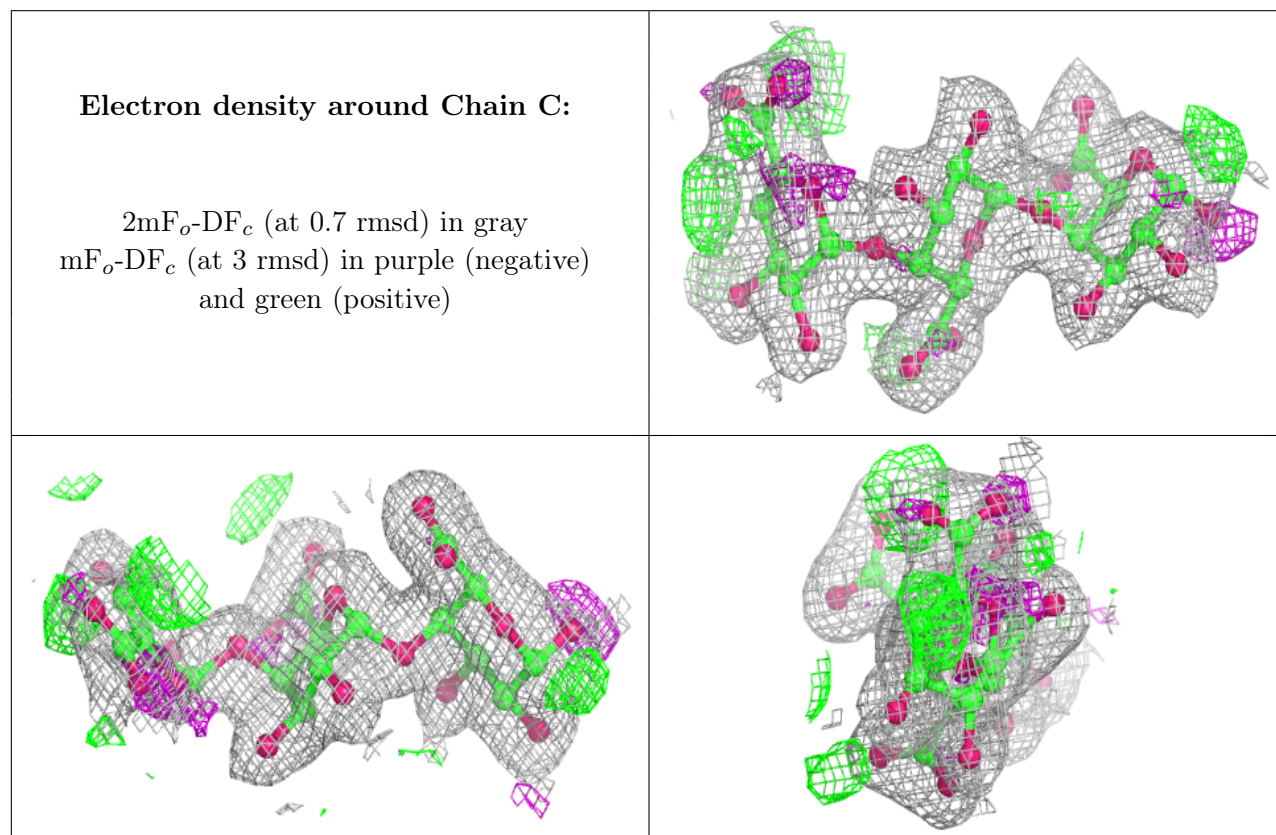
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GAD	D	3	11/11	0.84	0.13	34,38,45,47	0
2	GAD	C	3	11/11	0.88	0.14	32,36,43,45	0
2	ADA	D	2	12/13	0.92	0.13	25,30,32,32	0
2	ADA	C	2	12/13	0.93	0.12	24,28,29,30	0
2	ADA	C	1	13/13	0.94	0.14	23,26,29,34	0

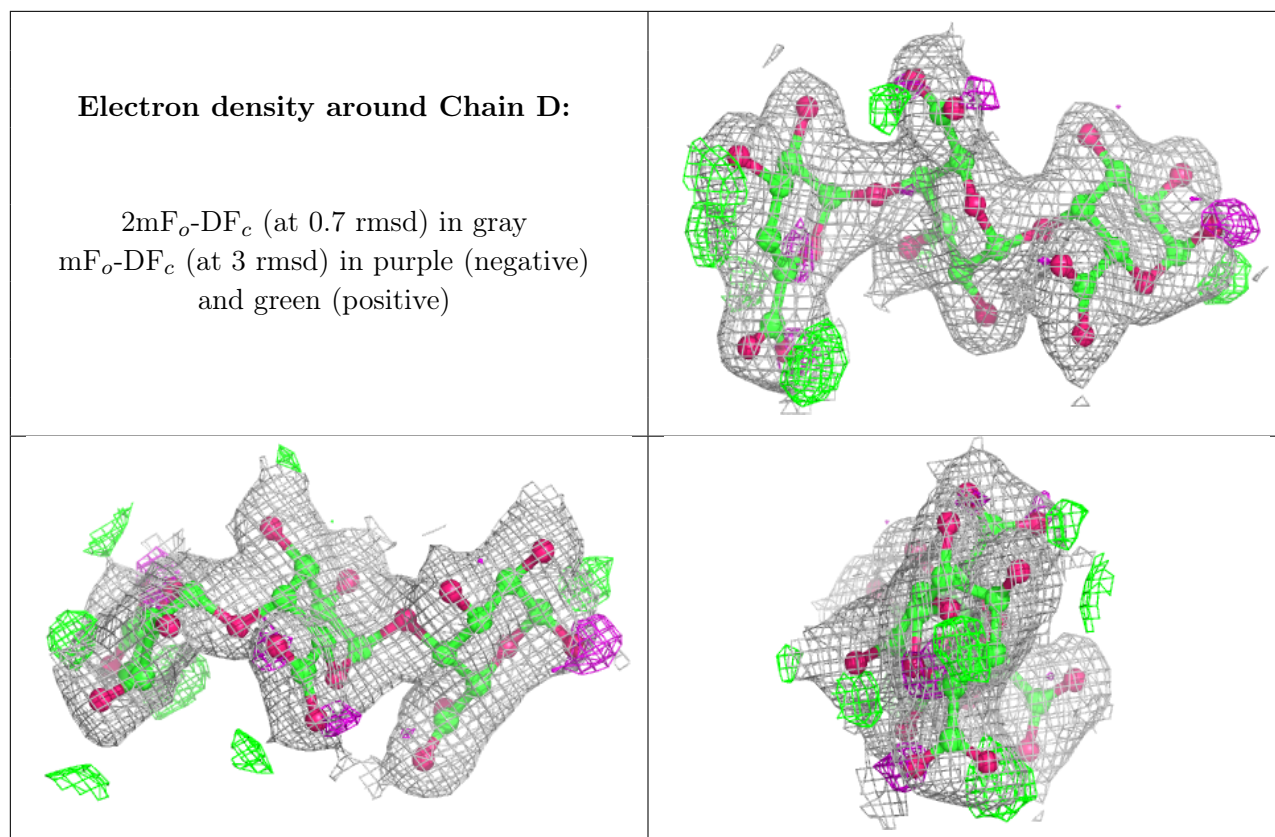
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADA	D	1	13/13	0.94	0.15	26,28,30,36	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	802	6/6	0.59	0.30	41,42,45,49	0
3	EPE	A	801	15/15	0.64	0.27	39,56,85,90	0
4	GOL	B	804	6/6	0.72	0.31	48,54,57,60	0
4	GOL	B	803	6/6	0.78	0.25	47,48,51,53	0
5	TLA	A	803	10/10	0.80	0.27	44,51,55,59	0
4	GOL	B	805	6/6	0.83	0.20	41,42,45,46	0
3	EPE	B	801	15/15	0.84	0.23	42,58,69,69	0
4	GOL	B	802	6/6	0.85	0.17	42,47,49,50	0
5	TLA	B	806	10/10	0.88	0.27	49,51,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.