



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 02:13 PM BST

PDB ID : 5XQO
Title : Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from *Penicillium chrysogenum* complexed with tetrameric substrate
Authors : Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on : 2017-06-07
Resolution : 3.20 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 ⓘ symbol.

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	:	2.13.1
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)	:	2.13.1

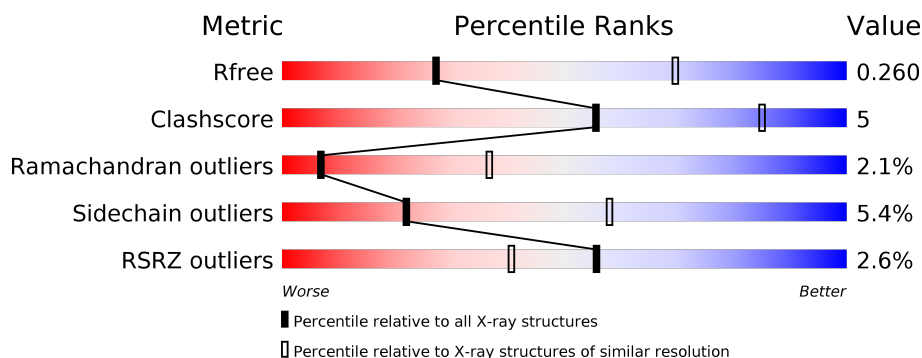
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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 $\leq 5\%$. 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	906	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	906	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
3	D	4	<div> <div>75%</div> <div>25%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14092 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.

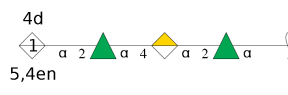
- Molecule 1 is a protein called Percglx protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	Se	0	0	0
			7017	4476	1178	1357	3	3			
1	B	881	Total	C	N	O	S	Se	0	0	0
			6870	4392	1153	1319	3	3			

There are 2 discrepancies between the modelled and reference sequences:

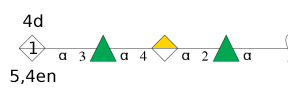
Chain	Residue	Modelled	Actual	Comment	Reference
A	458	PHE	TYR	engineered mutation	UNP A0A0C6EFY4
B	458	PHE	TYR	engineered mutation	UNP A0A0C6EFY4

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			44	24	20			

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



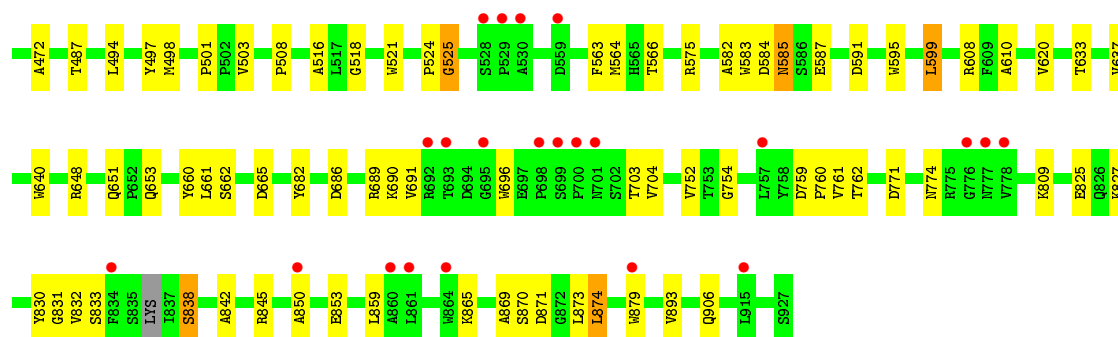
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	54	Total	O	0	0
			54	54		

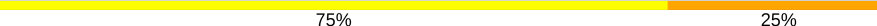


- Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose

Chain C: 

RAM1
ADA2
RAM3
GAD4

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

Chain D: 

RAM1
ADA2
RAM3
GAD4

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.44Å 166.44Å 171.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.58 – 3.20 48.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (119.58-3.20) 99.5 (48.56-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.40 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.191 , 0.264 0.195 , 0.260	Depositor DCC
R_{free} test set	2100 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14092	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: CA, RAM, GAD, ADA

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	0.54	0/7218	0.76	0/9854
1	B	0.57	0/7069	0.77	1/9655 (0.0%)
All	All	0.56	0/14287	0.77	1/19509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	ASP	CB-CG-OD1	5.36	123.13	118.30

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	7017	0	6566	68	0
1	B	6870	0	6391	70	0
2	C	44	0	32	5	0
3	D	44	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	61	0	0	3	0
5	B	54	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14092	0	13015	137	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 5.

The worst 5 of 137 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:24:CYS:SG	5:B:1114:HOH:O	2.34	0.84
1:A:157:ILE:HA	1:A:204:ILE:HD11	1.70	0.73
1:B:288:ILE:HD13	1:B:349:TYR:CE1	2.29	0.67
1:A:708:LEU:HG	1:A:755:SER:HA	1.78	0.66
1:B:825:GLU:CB	5:B:1149:HOH:O	2.46	0.63

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	893/906 (99%)	805 (90%)	74 (8%)	14 (2%)	9	43
1	B	873/906 (96%)	773 (88%)	77 (9%)	23 (3%)	5	31
All	All	1766/1812 (98%)	1578 (89%)	151 (9%)	37 (2%)	7	37

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	695	GLY
1	A	748	THR
1	A	774	ASN
1	B	231	ASP

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Mol	Chain	Res	Type
1	B	525	GLY

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	719/742 (97%)	677 (94%)	42 (6%)	20	55
1	B	694/742 (94%)	660 (95%)	34 (5%)	25	61
All	All	1413/1484 (95%)	1337 (95%)	76 (5%)	22	58

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	803	ASP
1	B	26	SER
1	B	620	VAL
1	A	804	ILE
1	A	862	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	810	GLN
1	A	902	ASN
1	B	391	GLN
1	A	746	ASN
1	B	203	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	RAM	C	1	2	11,11,11	0.62	0	15,16,16	1.55	4 (26%)
2	ADA	C	2	2	9,12,13	0.68	0	12,17,19	2.95	3 (25%)
2	RAM	C	3	2	10,10,11	0.76	0	14,14,16	1.71	5 (35%)
2	GAD	C	4	2	7,11,11	2.73	3 (42%)	8,15,15	2.87	3 (37%)
3	RAM	D	1	3	11,11,11	0.89	0	15,16,16	1.66	5 (33%)
3	ADA	D	2	1,3	9,12,13	0.77	0	12,17,19	2.19	4 (33%)
3	RAM	D	3	3	10,10,11	3.17	3 (30%)	14,14,16	5.87	9 (64%)
3	GAD	D	4	3	7,11,11	2.98	2 (28%)	8,15,15	5.04	4 (50%)

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	RAM	C2-C3	8.71	1.65	1.52
3	D	4	GAD	O5-C5	7.23	1.47	1.37
2	C	4	GAD	O5-C5	6.24	1.46	1.37
3	D	3	RAM	O3-C3	3.57	1.51	1.43
2	C	4	GAD	C4-C5	2.68	1.36	1.32

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	RAM	O3-C3-C2	13.43	135.71	109.99
3	D	3	RAM	C1-C2-C3	11.75	124.11	109.67
3	D	4	GAD	O5-C5-C4	-10.12	116.26	124.81
3	D	3	RAM	O5-C1-C2	-8.83	97.14	110.77
2	C	2	ADA	O4-C4-C5	8.69	126.65	110.05

There are no chirality outliers.

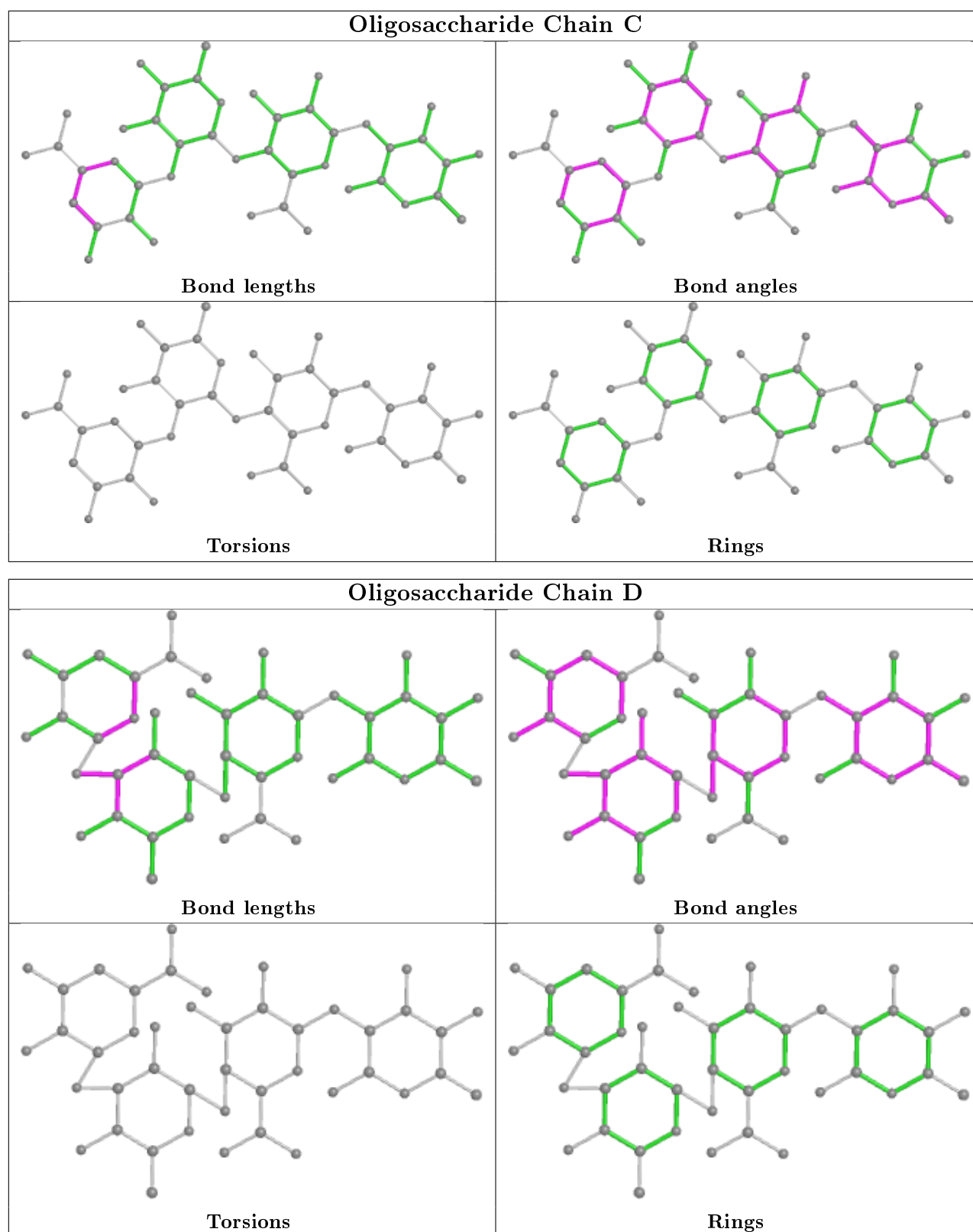
There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	RAM	2	0
3	D	4	GAD	1	0
2	C	1	RAM	3	0
2	C	2	ADA	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 ⓘ

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.

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, 95th 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 ²)	Q<0.9
1	A	896/906 (98%)	0.02	15 (1%) 70 57	62, 84, 111, 156	0
1	B	878/906 (96%)	0.16	31 (3%) 44 28	60, 90, 119, 159	0
All	All	1774/1812 (97%)	0.09	46 (2%) 56 40	60, 87, 117, 159	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	4.4
1	B	777	ASN	4.1
1	B	701	ASN	4.0
1	A	66	GLY	3.7
1	B	860	ALA	3.7

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, 95th 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.

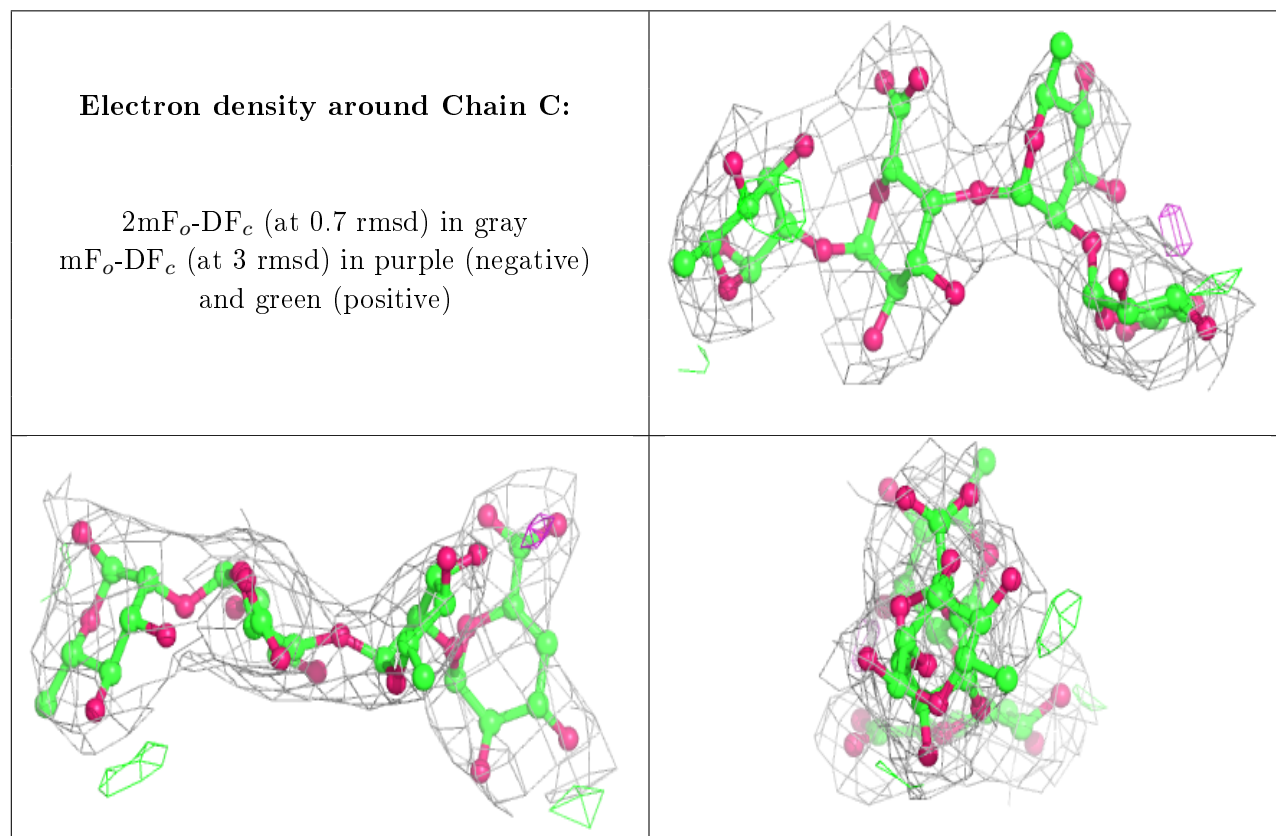
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	RAM	D	3	10/11	0.85	0.21	100,139,152,168	0
2	GAD	C	4	11/11	0.86	0.22	89,104,110,113	0
3	RAM	D	1	11/11	0.92	0.15	99,103,108,120	0
3	GAD	D	4	11/11	0.92	0.16	100,114,134,138	0
3	ADA	D	2	12/13	0.93	0.14	81,102,118,125	0

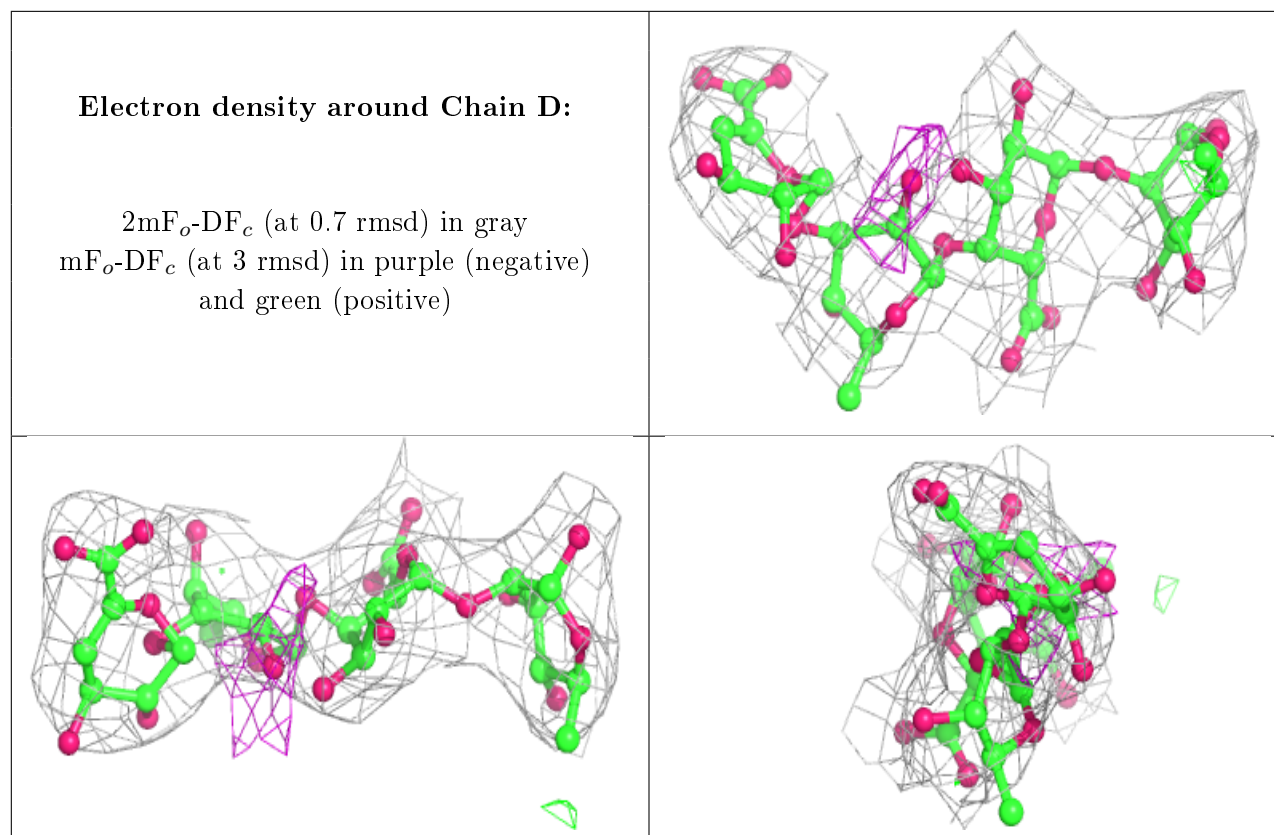
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RAM	C	3	10/11	0.93	0.18	104,106,115,125	0
2	ADA	C	2	12/13	0.94	0.18	73,84,88,103	0
2	RAM	C	1	11/11	0.96	0.20	73,76,83,84	0

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, 95th 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(\AA^2)	Q<0.9
4	CA	B	1001	1/1	0.98	0.27	57,57,57,57	0
4	CA	A	1001	1/1	0.99	0.25	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.