



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:18 PM BST

PDB ID : 2VZV
Title : Substrate Complex of Amycolatopsis orientalis exo-chitosanase CsxA E541A with chitosan
Authors : Lammerts van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B.
Deposited on : 2008-08-05
Resolution : 2.70 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

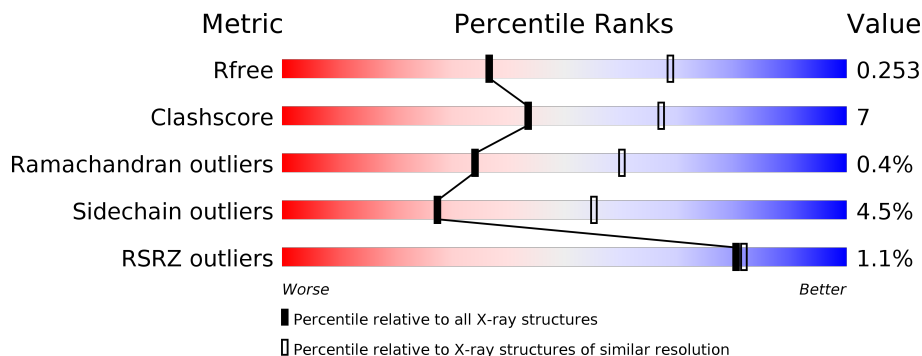
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	1032	
1	B	1032	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13565 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.

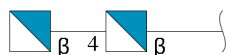
- Molecule 1 is a protein called EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6548	4113	1133	1285	17	4	0	1
1	B	858	6548	4113	1133	1285	17	4	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	ALA	GLU	engineered mutation	UNP Q56F26
A	750	ASN	TRP	conflict	UNP Q56F26
B	541	ALA	GLU	engineered mutation	UNP Q56F26
B	750	ASN	TRP	conflict	UNP Q56F26

- Molecule 2 is an oligosaccharide called 2-amino-2-deoxy-beta-D-glucopyranose-(1-4)-2-amino-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	23	12	2	9	0	0	0
2	D	2	23	12	2	9	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total	O	0	0
			212	212		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	211	Total 211	O 211	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.86Å 121.41Å 184.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	185.70 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (185.70-2.70) 91.6 (19.97-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.71Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.255 0.184 , 0.253	Depositor DCC
R_{free} test set	2545 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13565	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.86% 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: GCS

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	3/6711 (0.0%)	0.66	5/9158 (0.1%)
1	B	0.52	3/6711 (0.0%)	0.66	8/9158 (0.1%)
All	All	0.53	6/13422 (0.0%)	0.66	13/18316 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	16.66	1.83	1.52
1	B	430	GLU	CB-CG	10.96	1.73	1.52
1	B	246	ASP	CB-CG	7.18	1.66	1.51
1	B	296	ASP	CB-CG	6.59	1.65	1.51
1	A	246	ASP	CB-CG	6.17	1.64	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASP	CB-CG-OD1	15.77	132.49	118.30
1	B	246	ASP	CB-CG-OD1	15.13	131.92	118.30
1	B	296	ASP	CB-CG-OD1	14.89	131.71	118.30
1	A	296	ASP	CB-CG-OD2	11.98	129.08	118.30
1	A	430	GLU	CA-CB-CG	-11.08	89.02	113.40

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	6548	0	6327	81	9
1	B	6548	0	6327	92	9
2	C	23	0	23	0	0
2	D	23	0	23	2	0
3	A	212	0	0	9	0
3	B	211	0	0	17	0
All	All	13565	0	12700	173	9

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 7.

The worst 5 of 173 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:201:TRP:HE1	1:B:212:ASN:HD21	1.00	0.93
1:B:310:HIS:CE1	3:B:2079:HOH:O	2.23	0.90
1:B:577:ARG:HG2	1:B:583:PHE:O	1.75	0.85
1:B:244:HIS:HE2	1:B:246:ASP:CG	1.82	0.80
1:B:115:ALA:O	1:B:118:SER:HB2	1.82	0.79

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASP:OD2	1:B:296:ASP:OD1[3_554]	1.58	0.62
1:A:296:ASP:OD2	1:B:246:ASP:OD1[3_554]	1.61	0.59
1:A:296:ASP:OD2	1:B:246:ASP:OD2[3_554]	1.61	0.59
1:A:246:ASP:OD1	1:B:296:ASP:OD1[3_554]	1.75	0.45
1:A:246:ASP:OD2	1:B:296:ASP:CG[3_554]	1.82	0.38

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	856/1032 (83%)	811 (95%)	42 (5%)	3 (0%)	34	60
1	B	856/1032 (83%)	810 (95%)	42 (5%)	4 (0%)	29	54
All	All	1712/2064 (83%)	1621 (95%)	84 (5%)	7 (0%)	34	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	LYS
1	B	202	ILE
1	A	202	ILE
1	A	205	ALA
1	B	205	ALA

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	701/833 (84%)	672 (96%)	29 (4%)	30	59
1	B	701/833 (84%)	667 (95%)	34 (5%)	25	52
All	All	1402/1666 (84%)	1339 (96%)	63 (4%)	27	55

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	895	THR
1	B	237	LYS
1	B	808	ASN
1	B	118	SER
1	B	144	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	796	ASN
1	B	178	HIS
1	B	796	ASN
1	B	128	ASN
1	B	169	HIS

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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GCS	C	1	2	12,12,12	1.69	4 (33%)	16,17,17	1.39	3 (18%)
2	GCS	C	2	2	11,11,12	0.61	0	12,15,17	1.60	2 (16%)
2	GCS	D	1	2	12,12,12	1.39	1 (8%)	16,17,17	1.54	2 (12%)
2	GCS	D	2	2	11,11,12	0.82	0	12,15,17	1.85	1 (8%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCS	C	1	2	-	1/2/22/22	0/1/1/1
2	GCS	C	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCS	D	1	2	-	2/2/22/22	0/1/1/1
2	GCS	D	2	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GCS	O4-C4	2.76	1.49	1.43
2	D	1	GCS	O4-C4	2.75	1.49	1.43
2	C	1	GCS	O5-C5	2.32	1.50	1.44
2	C	1	GCS	C6-C5	2.24	1.59	1.51
2	C	1	GCS	C4-C5	2.16	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GCS	C1-O5-C5	5.90	120.19	112.19
2	D	1	GCS	O5-C5-C4	4.53	117.92	109.69
2	C	2	GCS	C1-O5-C5	3.62	117.09	112.19
2	C	2	GCS	O5-C5-C6	-3.61	101.55	107.20
2	C	1	GCS	O1-C1-C2	2.71	114.55	108.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

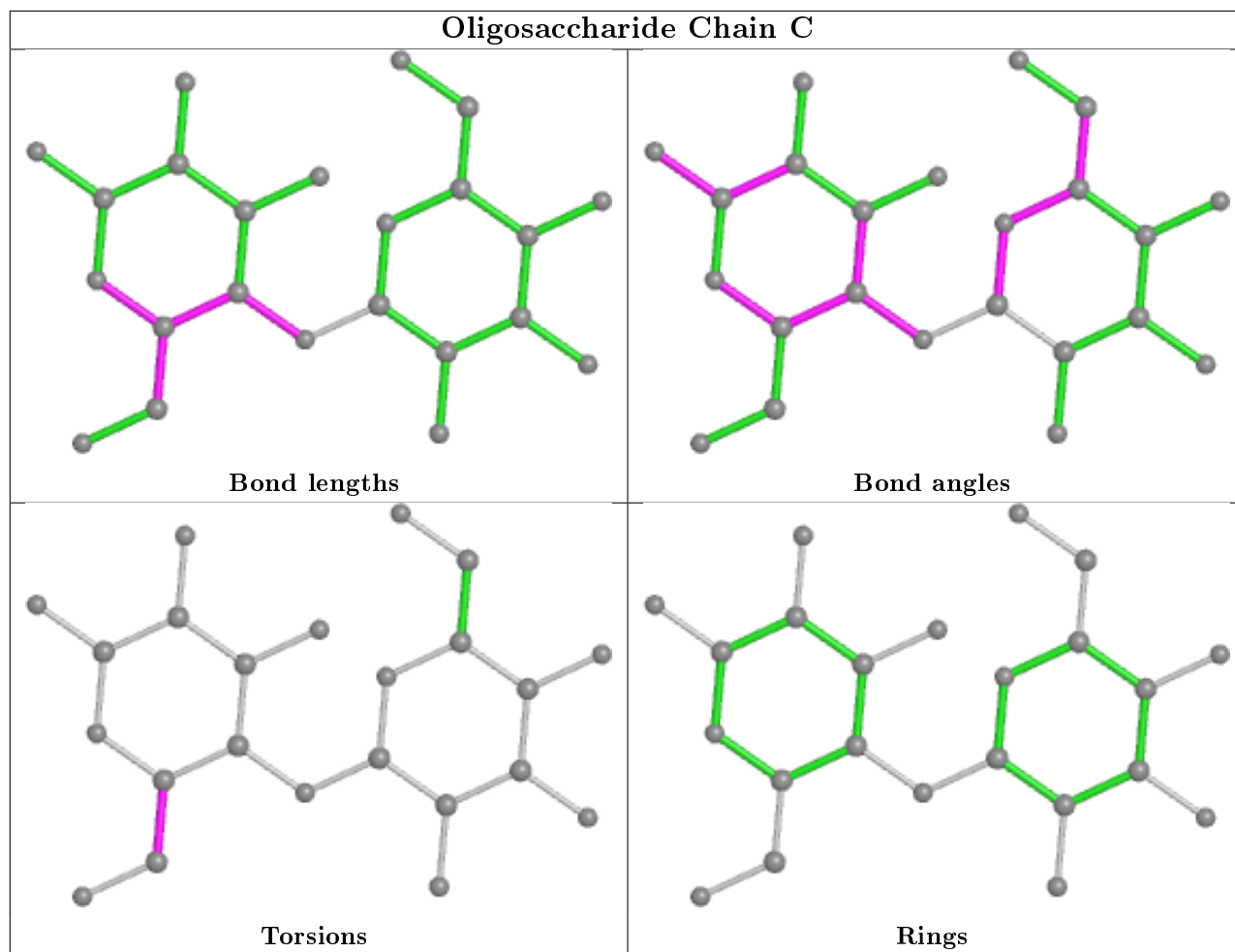
Mol	Chain	Res	Type	Atoms
2	D	1	GCS	C4-C5-C6-O6
2	C	1	GCS	O5-C5-C6-O6
2	D	1	GCS	O5-C5-C6-O6

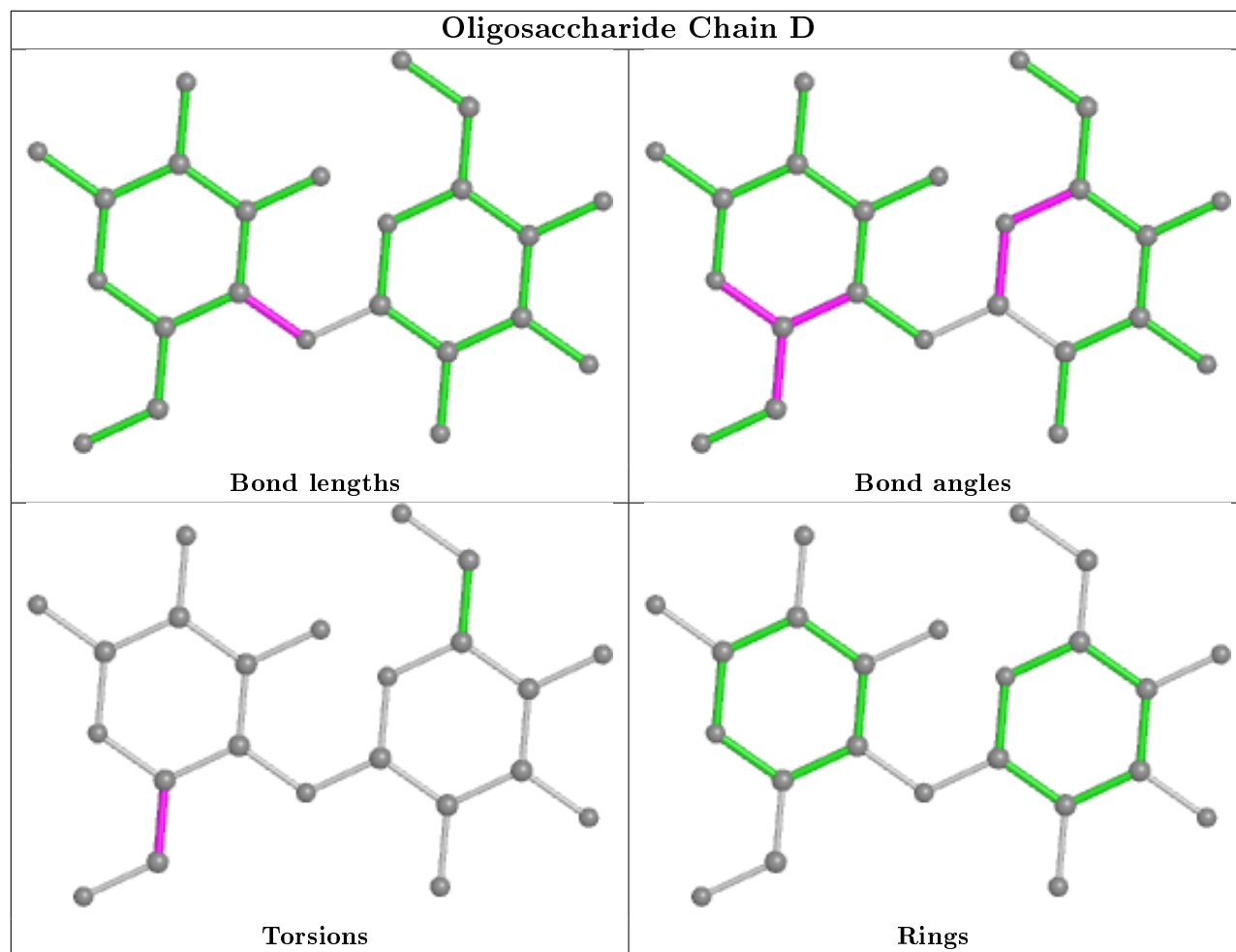
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GCS	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](#)

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](#)

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	858/1032 (83%)	-0.46	10 (1%) 79 80	3, 15, 27, 66	1 (0%)
1	B	858/1032 (83%)	-0.46	9 (1%) 82 83	3, 15, 25, 68	1 (0%)
All	All	1716/2064 (83%)	-0.46	19 (1%) 80 82	3, 15, 26, 68	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	SER	8.0
1	A	47	ALA	6.1
1	A	45	GLY	5.7
1	A	44	VAL	5.6
1	B	46	ALA	5.2

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

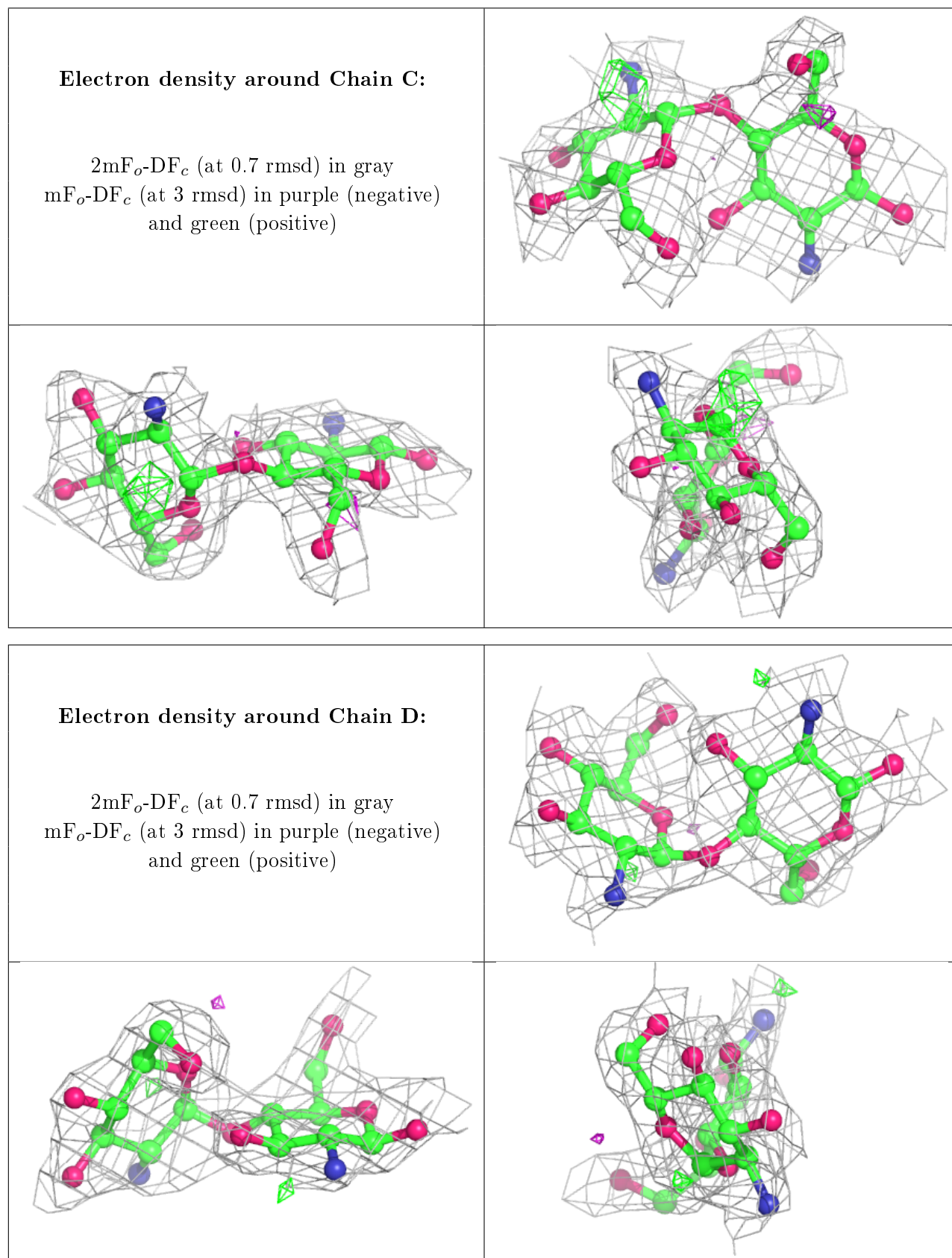
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	GCS	C	1	12/12	0.88	0.20	26,28,28,29	0
2	GCS	D	1	12/12	0.90	0.21	28,33,34,35	0
2	GCS	D	2	11/12	0.95	0.15	19,22,23,24	0
2	GCS	C	2	11/12	0.96	0.15	15,19,21,22	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.