



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:50 AM BST

PDB ID : 5M3V
Title : BEAT Fc
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Deposited on : 2016-10-17
Resolution : 1.97 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 ⓘ 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

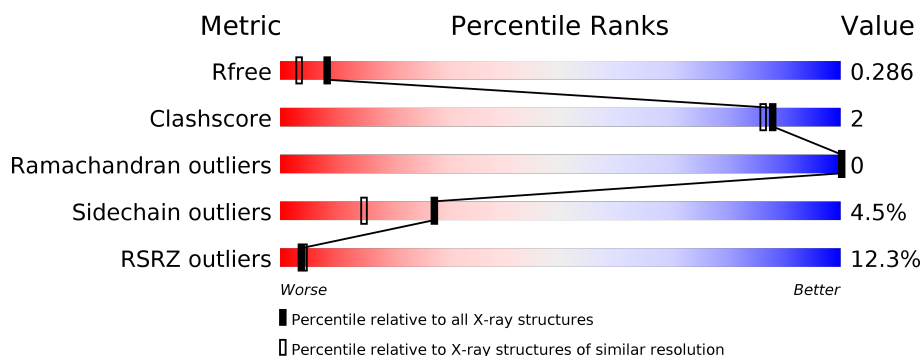
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	233	
2	B	227	
3	C	9	
3	D	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	1	-	-	-	X
3	NAG	D	2	-	-	-	X
3	MAN	D	7	-	-	-	X
3	NAG	D	8	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3820 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 Ig gamma-1 chain C region,Ig gamma-3 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1673	1066	280	318	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LYS	SER	engineered mutation	UNP P01860
A	366	VAL	THR	engineered mutation	UNP P01860
A	370	THR	LYS	engineered mutation	UNP P01860
A	392	TYR	ASN	engineered mutation	UNP P01860
A	405	SER	PHE	engineered mutation	UNP P01860
A	407	VAL	TYR	engineered mutation	UNP P01860
A	409	TRP	LYS	engineered mutation	UNP P01860
A	411	ASN	THR	engineered mutation	UNP P01860
A	448	HIS	-	expression tag	UNP P01860
A	449	HIS	-	expression tag	UNP P01860
A	450	HIS	-	expression tag	UNP P01860
A	451	HIS	-	expression tag	UNP P01860
A	452	HIS	-	expression tag	UNP P01860
A	453	HIS	-	expression tag	UNP P01860

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	4	0
			1434	911	244	272	7			

There are 13 discrepancies between the modelled and reference sequences:

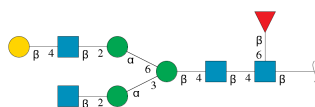
Chain	Residue	Modelled	Actual	Comment	Reference
B	347	GLU	GLN	engineered mutation	UNP P01857
B	349	ALA	TYR	engineered mutation	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
B	351	PHE	LEU	engineered mutation	UNP P01857
B	364	THR	SER	engineered mutation	UNP P01857
B	366	VAL	THR	engineered mutation	UNP P01857
B	370	THR	LYS	engineered mutation	UNP P01857
B	394	ASP	THR	engineered mutation	UNP P01857
B	397	LEU	VAL	engineered mutation	UNP P01857
B	399	GLU	ASP	engineered mutation	UNP P01857
B	405	ALA	PHE	engineered mutation	UNP P01857
B	407	SER	TYR	engineered mutation	UNP P01857
B	409	ARG	LYS	engineered mutation	UNP P01857
B	411	ARG	THR	engineered mutation	UNP P01857

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

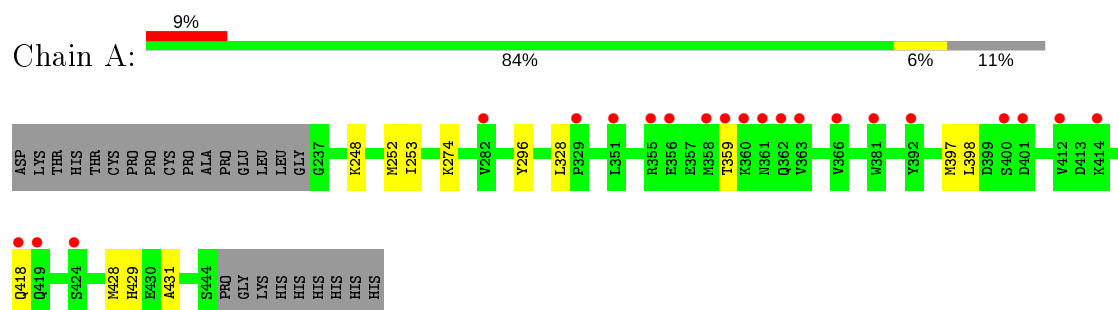
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total	O	0	0
			285	285		
4	B	208	Total	O	0	0
			208	208		

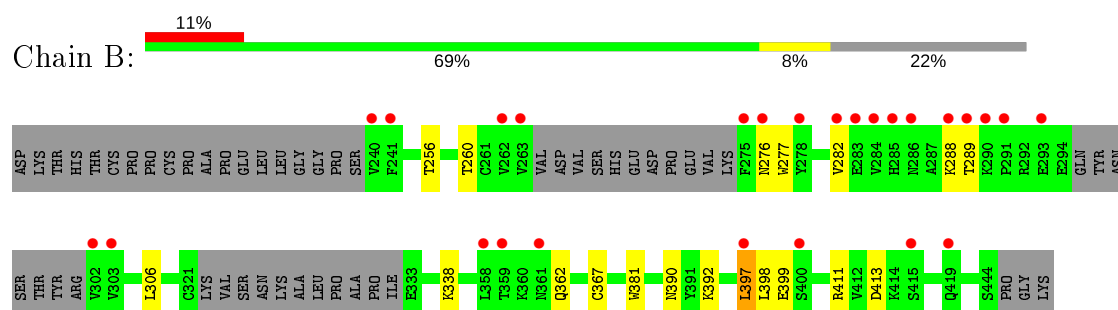
3 Residue-property plots [i](#)

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: Ig gamma-1 chain C region,Ig gamma-3 chain C region



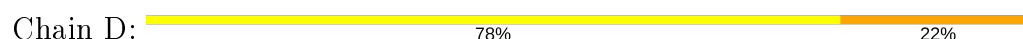
- Molecule 2: Ig gamma-1 chain C region



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BM43
MAN4
MAG5
GAL6
MAN7
MAG8
FUL9

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.78 Å 73.65 Å 141.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.97 29.60 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-1.97) 99.0 (29.60-1.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.210 , 0.279 0.221 , 0.286	Depositor DCC
R_{free} test set	1883 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3820	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1848e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: BMA, NAG, GAL, MLZ, FUL, MLY, MAN

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	0.55	0/1700	0.70	0/2316
2	B	0.51	0/1469	0.71	1/1994 (0.1%)
All	All	0.53	0/3169	0.70	1/4310 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	LEU	CA-CB-CG	5.07	126.96	115.30

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	1673	0	1641	7	0
2	B	1434	0	1410	7	0
3	C	110	0	94	0	0
3	D	110	0	93	1	0
4	A	285	0	0	1	2
4	B	208	0	0	1	2
All	All	3820	0	3238	13	2

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 2.

All (13) 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:A:248:MLY:HG2	1:A:428[B]:MET:HE1	1.67	0.75
1:A:248:MLY:CG	1:A:428[B]:MET:HE1	2.24	0.67
1:A:252:MET:SD	4:A:1225:HOH:O	2.54	0.64
3:D:4:MAN:O2	3:D:5:NAG:H83	2.10	0.52
1:A:429:HIS:CD2	1:A:431:ALA:H	2.29	0.51
2:B:367:CYS:HB2	2:B:381:TRP:CZ2	2.47	0.50
2:B:338:LYS:NZ	4:B:1105:HOH:O	2.46	0.48
2:B:398:LEU:HD23	2:B:399:GLU:O	2.14	0.47
1:A:397:MET:CE	2:B:392:LYS:HB3	2.46	0.45
1:A:397:MET:HE3	2:B:392:LYS:HB3	1.99	0.43
2:B:277:TRP:CE3	2:B:306:LEU:HD22	2.54	0.42
1:A:429:HIS:HD2	1:A:431:ALA:H	1.66	0.42
2:B:390[B]:ASN:HA	2:B:390[B]:ASN:HD22	1.58	0.41

All (2) 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)
4:A:1140:HOH:O	4:B:1193:HOH:O[3_654]	2.06	0.14
4:A:1112:HOH:O	4:B:1133:HOH:O[3_654]	2.14	0.06

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	205/233 (88%)	203 (99%)	2 (1%)	0	100	100
2	B	171/227 (75%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	376/460 (82%)	371 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	193/214 (90%)	187 (97%)	6 (3%)	40	28
2	B	166/207 (80%)	156 (94%)	10 (6%)	19	8
All	All	359/421 (85%)	343 (96%)	16 (4%)	27	15

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	296	TYR
1	A	328	LEU
1	A	359	THR
1	A	398	LEU
1	A	418	GLN
2	B	256	THR
2	B	260	THR
2	B	276	ASN
2	B	282	VAL
2	B	288	LYS
2	B	289	THR
2	B	362	GLN
2	B	397	LEU
2	B	411	ARG
2	B	413	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	276	ASN
1	A	310	HIS
1	A	429	HIS
2	B	310	HIS
2	B	315	ASN
2	B	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	MLY	B	248	2	9,10,11	0.54	0	6,11,13	0.88	0
1	MLY	A	248	1	9,10,11	0.52	0	6,11,13	0.87	0
1	MLZ	A	274	1	8,9,10	0.60	0	4,9,11	1.29	1 (25%)

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	MLY	B	248	2	-	1/8/9/11	-
1	MLY	A	248	1	-	0/8/9/11	-
1	MLZ	A	274	1	-	0/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	MLZ	CM-NZ-CE	2.55	119.31	111.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	248	MLY	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	248	MLY	2	0

5.5 Carbohydrates [i](#)

18 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	0.72	0
3	BMA	C	3	3	11,11,12	0.52	0	15,15,17	1.26	2 (13%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	2.18	4 (26%)
3	NAG	C	5	3	14,14,15	0.38	0	17,19,21	1.42	3 (17%)
3	GAL	C	6	3	11,11,12	0.63	0	15,15,17	1.20	1 (6%)
3	MAN	C	7	3	11,11,12	0.43	0	15,15,17	1.03	1 (6%)
3	NAG	C	8	3	14,14,15	0.55	0	17,19,21	1.46	3 (17%)
3	FUL	C	9	3	10,10,11	0.60	0	14,14,16	1.49	3 (21%)
3	NAG	D	1	3	14,14,15	0.68	0	17,19,21	1.85	5 (29%)
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	1.89	3 (17%)
3	BMA	D	3	3	11,11,12	0.94	1 (9%)	15,15,17	2.13	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	4	3	11,11,12	0.45	0	15,15,17	2.04	4 (26%)
3	NAG	D	5	3	14,14,15	0.50	0	17,19,21	1.93	4 (23%)
3	GAL	D	6	3	11,11,12	0.65	0	15,15,17	1.29	2 (13%)
3	MAN	D	7	3	11,11,12	0.51	0	15,15,17	2.22	2 (13%)
3	NAG	D	8	3	14,14,15	0.43	0	17,19,21	1.42	2 (11%)
3	FUL	D	9	3	10,10,11	0.43	0	14,14,16	1.00	1 (7%)

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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	GAL	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	NAG	C	8	3	-	4/6/23/26	0/1/1/1
3	FUL	C	9	3	-	-	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	1/6/23/26	0/1/1/1
3	FUL	D	9	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	C2-C3	2.52	1.56	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	MAN	C1-O5-C5	7.24	122.00	112.19
3	D	3	BMA	C1-C2-C3	6.63	117.81	109.67
3	D	2	NAG	C1-O5-C5	5.62	119.81	112.19
3	C	4	MAN	C1-O5-C5	4.76	118.65	112.19
3	D	4	MAN	O5-C1-C2	4.64	117.94	110.77
3	D	5	NAG	C2-N2-C7	4.61	129.47	122.90
3	D	1	NAG	O5-C1-C2	4.48	118.36	111.29
3	C	4	MAN	O5-C1-C2	4.29	117.40	110.77
3	D	4	MAN	C1-O5-C5	4.23	117.93	112.19
3	C	4	MAN	C1-C2-C3	4.16	114.78	109.67
3	D	5	NAG	C8-C7-N2	4.15	123.13	116.10
3	D	8	NAG	O5-C1-C2	-3.74	105.39	111.29
3	C	5	NAG	C2-N2-C7	3.53	127.92	122.90
3	C	1	NAG	O5-C5-C6	3.31	112.40	107.20
3	D	3	BMA	C2-C3-C4	3.09	116.23	110.89
3	C	6	GAL	O5-C5-C6	3.06	112.00	107.20
3	D	8	NAG	C1-C2-N2	3.01	115.64	110.49
3	D	7	MAN	C3-C4-C5	3.00	115.59	110.24
3	D	2	NAG	C4-C3-C2	-2.95	106.70	111.02
3	C	9	FUL	C1-O5-C5	2.86	119.26	112.78
3	C	8	NAG	C3-C4-C5	2.85	115.32	110.24
3	C	8	NAG	C2-N2-C7	2.84	126.95	122.90
3	D	1	NAG	C3-C4-C5	-2.79	105.26	110.24
3	D	6	GAL	C1-C2-C3	2.76	113.05	109.67
3	D	5	NAG	C1-C2-N2	2.74	115.18	110.49
3	D	1	NAG	C1-C2-N2	-2.70	105.88	110.49
3	D	2	NAG	C1-C2-N2	2.68	115.07	110.49
3	C	8	NAG	C8-C7-N2	2.63	120.55	116.10
3	C	3	BMA	C1-O5-C5	2.50	115.58	112.19
3	C	3	BMA	C1-C2-C3	2.47	112.70	109.67
3	D	4	MAN	C3-C4-C5	2.46	114.62	110.24
3	D	4	MAN	C1-C2-C3	2.44	112.67	109.67
3	D	9	FUL	O5-C1-C2	-2.26	107.28	110.77
3	C	9	FUL	O5-C5-C4	2.23	113.52	109.52
3	C	5	NAG	O4-C4-C3	-2.20	105.27	110.35
3	C	5	NAG	C6-C5-C4	2.19	118.13	113.00
3	D	1	NAG	O5-C5-C6	2.18	110.62	107.20
3	D	5	NAG	O7-C7-C8	-2.18	118.01	122.06
3	C	7	MAN	C1-O5-C5	2.13	115.08	112.19
3	D	1	NAG	O5-C5-C4	-2.12	105.66	110.83
3	D	3	BMA	O5-C5-C4	-2.08	105.76	110.83
3	C	9	FUL	C1-C2-C3	2.07	112.22	109.67
3	C	4	MAN	O2-C2-C3	-2.02	106.09	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	GAL	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

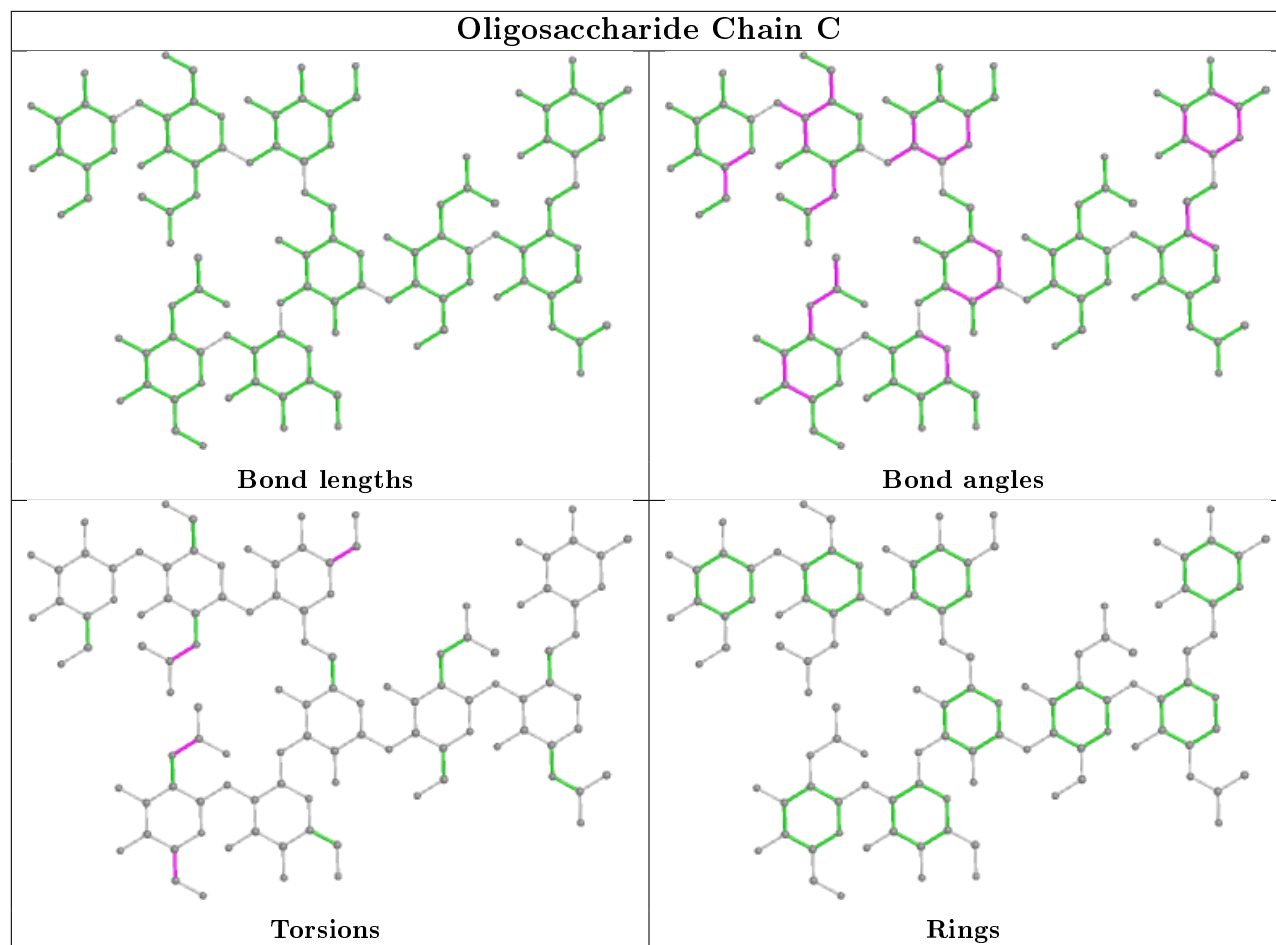
Mol	Chain	Res	Type	Atoms
3	D	7	MAN	O5-C5-C6-O6
3	C	8	NAG	O5-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
3	C	8	NAG	C4-C5-C6-O6
3	C	5	NAG	C8-C7-N2-C2
3	C	5	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	C	8	NAG	C8-C7-N2-C2
3	C	8	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	8	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

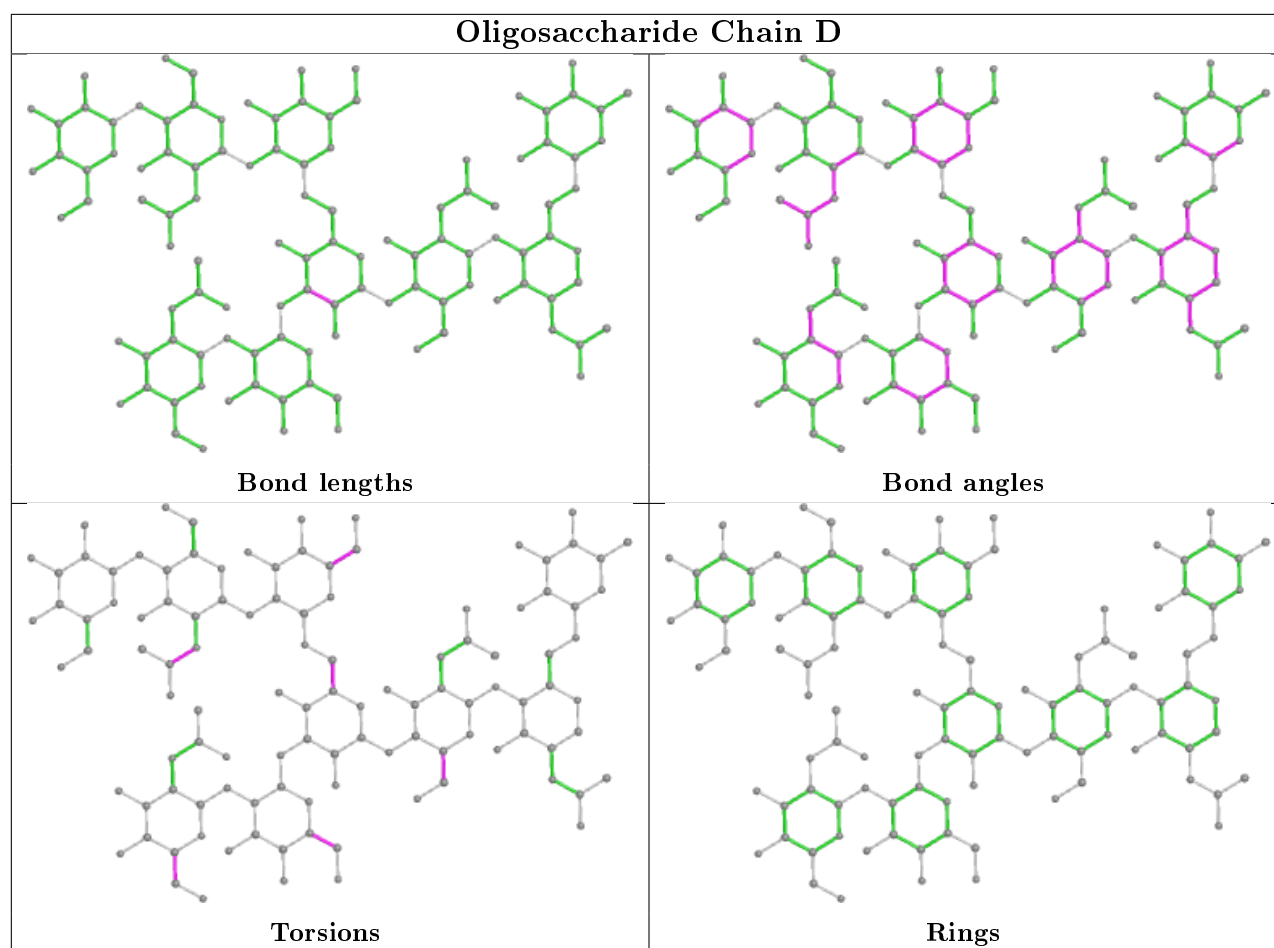
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	NAG	1	0
3	D	4	MAN	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	206/233 (88%)	0.55	21 (10%) 6 7	30, 45, 82, 125	0
2	B	175/227 (77%)	0.85	26 (14%) 2 2	28, 51, 106, 153	0
All	All	381/460 (82%)	0.69	47 (12%) 4 4	28, 47, 100, 153	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	263	VAL	11.1
1	A	358	MET	7.5
2	B	303	VAL	6.2
2	B	291	PRO	5.7
1	A	356	GLU	5.7
2	B	275	PHE	5.4
1	A	359	THR	5.4
1	A	361	ASN	5.3
2	B	262	VAL	4.8
2	B	293	GLU	4.5
2	B	302	VAL	4.5
2	B	241	PHE	4.3
2	B	282	VAL	4.3
2	B	361	ASN	4.1
2	B	289	THR	3.8
2	B	359	THR	3.6
2	B	285	HIS	3.6
1	A	355	ARG	3.5
1	A	351	LEU	3.4
1	A	418	GLN	3.2
1	A	419	GLN	3.2
1	A	381	TRP	3.0
2	B	278	TYR	2.9
2	B	400	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	360	LYS	2.8
1	A	392	TYR	2.8
2	B	240	VAL	2.8
2	B	290	LYS	2.7
2	B	397	LEU	2.7
2	B	276	ASN	2.5
2	B	415	SER	2.5
2	B	419	GLN	2.5
2	B	286	ASN	2.3
2	B	284	VAL	2.3
1	A	401	ASP	2.3
1	A	424	SER	2.2
2	B	358	LEU	2.2
1	A	282	VAL	2.2
1	A	400	SER	2.2
1	A	363	VAL	2.2
1	A	414	LYS	2.1
2	B	288	LYS	2.1
1	A	362	GLN	2.1
1	A	366	VAL	2.1
1	A	329	PRO	2.1
1	A	412	VAL	2.0
2	B	283	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	A	248	11/12	0.95	0.14	32,36,40,41	0
1	MLZ	A	274	10/11	0.95	0.10	38,40,48,50	0
2	MLY	B	248	11/12	0.97	0.14	33,34,37,39	0

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

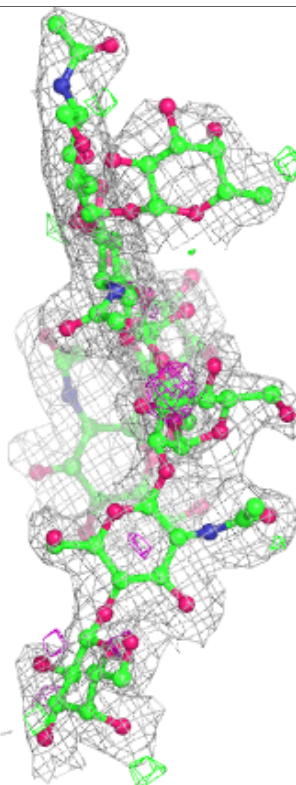
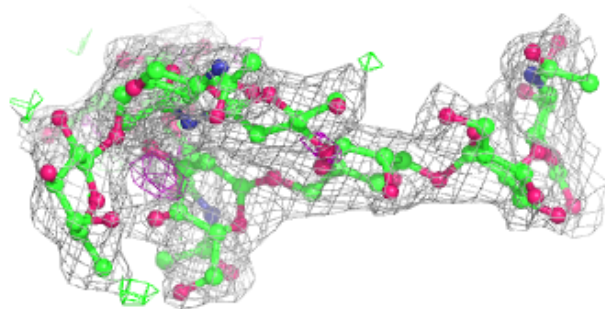
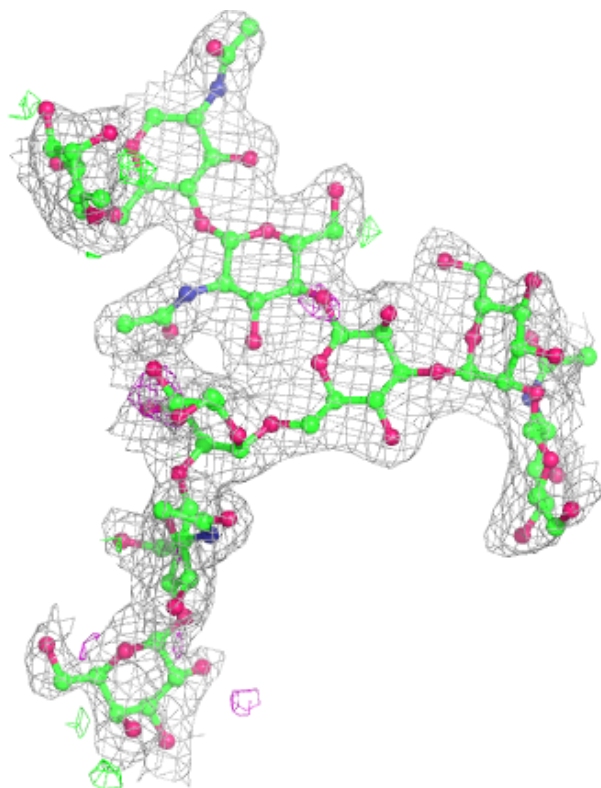
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

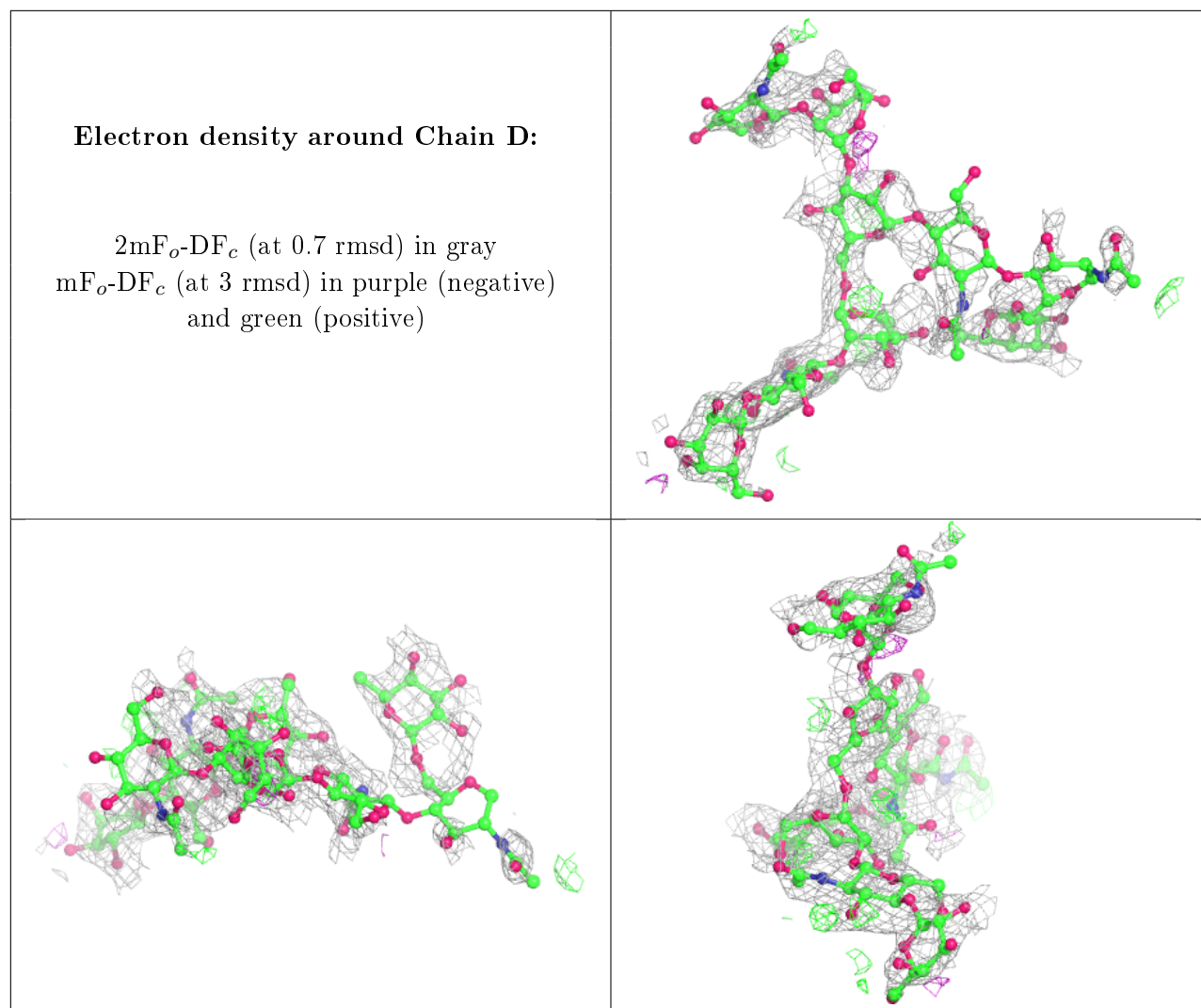
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	D	3	11/12	0.15	0.30	120,130,142,145	0
3	NAG	D	1	14/15	0.43	0.44	136,150,161,166	0
3	NAG	D	8	14/15	0.48	0.50	129,136,139,139	0
3	NAG	D	2	14/15	0.63	0.47	136,143,151,153	0
3	MAN	D	7	11/12	0.65	0.43	141,144,149,150	0
3	MAN	D	4	11/12	0.68	0.28	111,120,125,126	0
3	FUL	D	9	10/11	0.74	0.27	115,128,140,141	0
3	NAG	C	8	14/15	0.77	0.24	91,96,98,100	0
3	GAL	C	6	11/12	0.82	0.17	52,56,60,63	0
3	NAG	D	5	14/15	0.84	0.17	84,98,104,108	0
3	NAG	C	2	14/15	0.86	0.11	46,50,53,54	0
3	FUL	C	9	10/11	0.87	0.13	72,77,82,83	0
3	GAL	D	6	11/12	0.87	0.21	75,81,88,90	0
3	MAN	C	7	11/12	0.88	0.27	74,81,88,90	0
3	MAN	C	4	11/12	0.89	0.22	51,54,62,65	0
3	BMA	C	3	11/12	0.92	0.12	50,53,58,66	0
3	NAG	C	5	14/15	0.93	0.14	50,52,62,62	0
3	NAG	C	1	14/15	0.94	0.10	51,53,58,60	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.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.