



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:16 PM EDT

PDB ID : 6YSC / pdb_00006ysc
Title : GLYCOSYLATED KNOB-HOLE/DUMMY FC FRAGMENT
Authors : Kuglstatter, A.; Leibrock, L.; Benz, J.
Deposited on : 2020-04-22
Resolution : 2.05 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

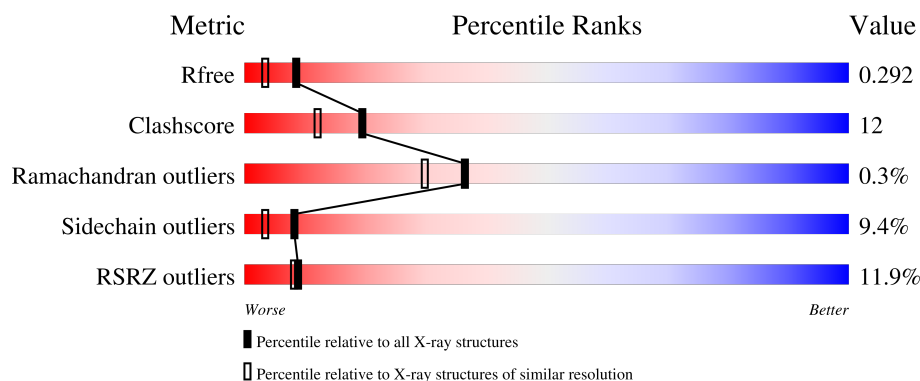
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 ≥ 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	232	5% 69% 21% • 9%
2	B	245	16% 51% 27% • 18%
3	C	8	100%
3	D	8	62% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3573 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	5	0
			1698	1083	286	322	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	CYS	SER	engineered mutation	UNP P0DOX5
A	366	TRP	THR	engineered mutation	UNP P0DOX5

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	5	0
			1602	1026	269	300	7			

There are 18 discrepancies between the modelled and reference sequences:

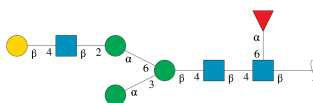
Chain	Residue	Modelled	Actual	Comment	Reference
B	357	LYS	GLU	engineered mutation	UNP P0DOX5
B	366	SER	THR	engineered mutation	UNP P0DOX5
B	368	ALA	LEU	engineered mutation	UNP P0DOX5
B	407	VAL	TYR	engineered mutation	UNP P0DOX5
B	448	GLY	-	expression tag	UNP P0DOX5
B	449	GLY	-	expression tag	UNP P0DOX5
B	450	GLY	-	expression tag	UNP P0DOX5
B	451	GLY	-	expression tag	UNP P0DOX5
B	452	SER	-	expression tag	UNP P0DOX5
B	453	HIS	-	expression tag	UNP P0DOX5
B	454	HIS	-	expression tag	UNP P0DOX5
B	455	HIS	-	expression tag	UNP P0DOX5
B	456	HIS	-	expression tag	UNP P0DOX5
B	457	HIS	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	458	HIS	-	expression tag	UNP P0DOX5
B	459	HIS	-	expression tag	UNP P0DOX5
B	460	HIS	-	expression tag	UNP P0DOX5
B	461	CYS	-	expression tag	UNP P0DOX5

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			96	54	3	39			
3	D	8	Total	C	N	O	0	0	0
			96	54	3	39			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	33	Total	O	0	0
			33	33		

ido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



MAG1
MAG2
EMA3
MAM4
MAG5
GAL6
MAM7
FUC8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.36Å 80.36Å 141.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.01 – 2.05 70.91 – 2.05	Depositor EDS
% Data completeness (in resolution range)	72.5 (71.01-2.05) 72.6 (70.91-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.230 , 0.293 0.230 , 0.292	Depositor DCC
R_{free} test set	1265 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3573	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, MAN, GAL

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	0.77	2/1741 (0.1%)	1.22	8/2364 (0.3%)
2	B	0.63	0/1645	1.19	6/2232 (0.3%)
All	All	0.70	2/3386 (0.1%)	1.21	14/4596 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ASN	C-N	12.83	1.52	1.33
1	A	297	ASN	CG-OD1	5.01	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	PRO	CB-CA-C	-9.72	98.92	111.46
2	B	376	ASP	CB-CA-C	-9.01	97.19	110.16
1	A	395	PRO	CB-CA-C	-8.33	103.56	111.39
1	A	335	THR	CA-CB-OG1	-6.93	99.20	109.60
1	A	437	THR	CA-CB-OG1	-6.75	99.47	109.60
2	B	342	GLN	CB-CA-C	-5.96	99.92	109.69
2	B	395	PRO	CB-CA-C	-5.80	103.84	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	297	ASN	CA-C-N	5.31	129.67	122.19
1	A	297	ASN	C-N-CA	5.31	129.67	122.19
2	B	306	LEU	CA-C-N	5.06	128.06	120.87
2	B	306	LEU	C-N-CA	5.06	128.06	120.87
1	A	297	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	350	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ARG	Sidechain
2	B	265	ASP	Peptide
2	B	292	ARG	Sidechain

5.2 Too-close contacts

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	1698	0	1653	30	0
2	B	1602	0	1570	48	0
3	C	96	0	82	0	0
3	D	96	0	82	3	0
4	A	48	0	0	3	0
4	B	33	0	0	1	0
All	All	3573	0	3387	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 12.

All (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:A:286:ASN:HD22	1:A:286:ASN:H	1.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:LYS:HD3	2:B:361:ASN:H	1.30	0.94
2:B:421:ASN:HD22	2:B:421:ASN:H	1.14	0.89
2:B:328:LEU:HG	2:B:329:PRO:HD2	1.56	0.86
2:B:296:TYR:HB2	3:D:8:FUC:H62	1.61	0.83
1:A:286:ASN:H	1:A:286:ASN:ND2	1.79	0.81
2:B:360:LYS:HD3	2:B:361:ASN:N	1.98	0.78
2:B:390:ASN:OD1	2:B:411:THR:HB	1.84	0.78
1:A:286:ASN:HD22	1:A:286:ASN:N	1.82	0.74
2:B:295:GLN:NE2	3:D:1:NAG:H62	2.05	0.72
1:A:366[A]:TRP:CH2	1:A:409:LYS:HD3	2.27	0.70
2:B:360:LYS:CD	2:B:361:ASN:H	2.06	0.68
2:B:283:GLU:HG3	2:B:284:VAL:N	2.08	0.68
2:B:421:ASN:H	2:B:421:ASN:ND2	1.90	0.66
2:B:238:PRO:HD2	2:B:328:LEU:HB2	1.76	0.66
2:B:289:THR:HG22	2:B:290:LYS:N	2.11	0.65
2:B:289:THR:HG22	2:B:290:LYS:H	1.61	0.64
1:A:416:ARG:HD3	4:A:636:HOH:O	2.00	0.61
1:A:407[A]:TYR:CZ	2:B:407[A]:VAL:HG11	2.37	0.59
1:A:406:LEU:C	1:A:406:LEU:HD12	2.29	0.57
2:B:318:GLU:OE2	2:B:335:THR:HG21	2.05	0.57
2:B:422:VAL:HA	2:B:442:SER:HB3	1.86	0.57
1:A:417:TRP:CZ3	1:A:442:SER:HA	2.40	0.57
1:A:338:LYS:NZ	1:A:430:GLU:OE1	2.35	0.57
2:B:421:ASN:HD22	2:B:421:ASN:N	1.94	0.56
1:A:272:GLU:OE2	1:A:326:LYS:NZ	2.39	0.56
2:B:241:PHE:CE1	3:D:2:NAG:H4	2.40	0.56
2:B:289:THR:CG2	2:B:290:LYS:H	2.20	0.55
1:A:355:ARG:O	1:A:358:LEU:HB2	2.07	0.55
1:A:428:MET:HG2	4:A:645:HOH:O	2.06	0.55
2:B:265:ASP:H	2:B:299:THR:HG23	1.73	0.54
2:B:328:LEU:CG	2:B:329:PRO:HD2	2.34	0.54
1:A:407[A]:TYR:CE2	2:B:407[A]:VAL:HG11	2.43	0.54
2:B:238:PRO:CD	2:B:328:LEU:HB2	2.38	0.53
2:B:248:LYS:HD2	2:B:428:MET:HE1	1.91	0.53
2:B:265:ASP:H	2:B:299:THR:CG2	2.22	0.53
2:B:365:LEU:HD13	2:B:441:LEU:HD23	1.90	0.53
2:B:289:THR:CG2	2:B:290:LYS:N	2.73	0.51
2:B:390:ASN:O	2:B:410:LEU:HD12	2.12	0.50
2:B:312:ASP:HB3	2:B:319:TYR:OH	2.11	0.50
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.93	0.49
2:B:406:LEU:HD12	2:B:406:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:VAL:HG12	2:B:334:LYS:HG3	1.95	0.49
1:A:418:GLN:C	1:A:420:GLY:N	2.72	0.48
2:B:436:TYR:C	2:B:436:TYR:CD1	2.92	0.47
1:A:442:SER:HB2	4:A:624:HOH:O	2.14	0.46
1:A:418:GLN:C	1:A:420:GLY:H	2.23	0.46
2:B:266:VAL:HG13	2:B:300:TYR:HB2	1.96	0.46
2:B:441:LEU:HD12	2:B:441:LEU:HA	1.83	0.46
2:B:423:PHE:O	2:B:441:LEU:N	2.47	0.46
2:B:247:PRO:O	2:B:251:LEU:HG	2.17	0.45
2:B:342:GLN:HE21	2:B:342:GLN:CA	2.30	0.45
1:A:283:GLU:HG2	1:A:285:HIS:CE1	2.52	0.45
2:B:417:TRP:O	2:B:443:LEU:HD23	2.18	0.44
1:A:434:ASN:O	1:A:435:HIS:HB2	2.17	0.44
2:B:423:PHE:N	2:B:441:LEU:O	2.33	0.44
2:B:343:PRO:HA	2:B:373:TYR:O	2.18	0.44
2:B:325:ASN:CG	2:B:326:LYS:H	2.26	0.43
1:A:433:HIS:C	1:A:435:HIS:H	2.27	0.43
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.89	0.43
1:A:353:PRO:HG3	1:A:365:LEU:HD23	2.01	0.42
2:B:338:LYS:HE3	4:B:604:HOH:O	2.20	0.42
2:B:421:ASN:ND2	2:B:421:ASN:N	2.59	0.42
1:A:361:ASN:ND2	1:A:361:ASN:C	2.77	0.42
2:B:415:SER:O	2:B:418:GLN:CB	2.68	0.41
1:A:347:GLN:OE1	1:A:370:LYS:HE3	2.20	0.41
2:B:434:ASN:O	2:B:435:HIS:HB2	2.20	0.41
2:B:436:TYR:CE1	2:B:438:GLN:HG3	2.56	0.41
1:A:358:LEU:HG	1:A:414:LYS:HD2	2.03	0.41
1:A:379:VAL:C	1:A:380:GLU:HG2	2.45	0.41
1:A:415:SER:O	1:A:418:GLN:N	2.52	0.41
2:B:360:LYS:O	2:B:414:LYS:HD2	2.21	0.41
2:B:418:GLN:NE2	2:B:418:GLN:HA	2.35	0.40
1:A:381:TRP:CE3	1:A:410:LEU:HD22	2.56	0.40
1:A:433:HIS:C	1:A:435:HIS:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	200/232 (86%)	191 (96%)	9 (4%)	0	100	100
2	B	188/245 (77%)	176 (94%)	11 (6%)	1 (0%)	24	16
All	All	388/477 (81%)	367 (95%)	20 (5%)	1 (0%)	36	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	329	PRO

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	197/214 (92%)	184 (93%)	13 (7%)	15	9
2	B	186/223 (83%)	163 (88%)	23 (12%)	4	1
All	All	383/437 (88%)	347 (91%)	36 (9%)	8	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	290	LYS
1	A	292	ARG
1	A	336	ILE
1	A	343	PRO

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	358	LEU
1	A	361	ASN
1	A	363	VAL
1	A	383	SER
1	A	386	GLN
1	A	418	GLN
1	A	443	LEU
2	B	239	SER
2	B	252	MET
2	B	274	LYS
2	B	278	TYR
2	B	283	GLU
2	B	284	VAL
2	B	292	ARG
2	B	293	GLU
2	B	298	SER
2	B	307	THR
2	B	324	SER
2	B	336	ILE
2	B	342	GLN
2	B	344	ARG
2	B	368[B]	LEU
2	B	383	SER
2	B	389	ASN
2	B	408	SER
2	B	421	ASN
2	B	422	VAL
2	B	440	SER
2	B	443	LEU
2	B	444	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
1	A	286	ASN
1	A	419	GLN
2	B	276	ASN
2	B	342	GLN
2	B	418	GLN
2	B	421	ASN

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Mol	Chain	Res	Type
2	B	438	GLN

5.3.3 RNA ⓘ

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 ⓘ

16 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	3,1	14,14,15	3.22	2 (14%)	17,19,21	3.66	8 (47%)
3	NAG	C	2	3	14,14,15	0.71	0	17,19,21	1.83	3 (17%)
3	BMA	C	3	3	11,11,12	0.65	0	15,15,17	1.79	5 (33%)
3	MAN	C	4	3	11,11,12	0.75	0	15,15,17	2.63	5 (33%)
3	NAG	C	5	3	14,14,15	0.88	0	17,19,21	1.50	5 (29%)
3	GAL	C	6	3	11,11,12	1.12	0	15,15,17	1.76	4 (26%)
3	MAN	C	7	3	11,11,12	1.10	1 (9%)	15,15,17	1.93	5 (33%)
3	FUC	C	8	3	10,10,11	1.23	1 (10%)	14,14,16	2.05	6 (42%)
3	NAG	D	1	3,2	14,14,15	0.58	0	17,19,21	1.54	5 (29%)
3	NAG	D	2	3	14,14,15	0.51	0	17,19,21	1.31	3 (17%)
3	BMA	D	3	3	11,11,12	0.59	0	15,15,17	2.24	5 (33%)
3	MAN	D	4	3	11,11,12	0.30	0	15,15,17	1.60	3 (20%)
3	NAG	D	5	3	14,14,15	0.59	0	17,19,21	1.52	2 (11%)
3	GAL	D	6	3	11,11,12	0.73	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	7	3	11,11,12	1.12	1 (9%)	15,15,17	1.74	5 (33%)
3	FUC	D	8	3	10,10,11	0.66	0	14,14,16	1.23	2 (14%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	10.30	1.61	1.43
3	C	1	NAG	C1-C2	6.00	1.60	1.52
3	D	7	MAN	C2-C3	2.41	1.56	1.52
3	C	7	MAN	O2-C2	2.13	1.47	1.43
3	C	8	FUC	O2-C2	-2.11	1.38	1.43

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-C2-N2	-10.78	93.45	110.43
3	C	1	NAG	C1-O5-C5	-6.95	102.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	5.87	120.05	112.19
3	C	4	MAN	O3-C3-C4	-5.46	97.51	110.38
3	C	1	NAG	O5-C1-C2	-5.23	103.20	111.29
3	D	3	BMA	C1-C2-C3	5.11	117.08	109.64
3	C	7	MAN	O4-C4-C5	-4.72	97.69	109.32
3	C	8	FUC	C2-C3-C4	4.06	117.99	110.86
3	C	6	GAL	O4-C4-C3	4.05	119.92	110.38
3	D	5	NAG	C2-N2-C7	-3.98	117.56	122.90
3	C	3	BMA	C1-O5-C5	3.98	117.52	112.19
3	C	2	NAG	C2-N2-C7	-3.78	117.84	122.90
3	D	3	BMA	O4-C4-C3	-3.58	101.93	110.38
3	D	7	MAN	C1-O5-C5	-3.54	107.45	112.19
3	D	5	NAG	O5-C1-C2	-3.43	105.99	111.29
3	C	2	NAG	O6-C6-C5	-3.42	99.70	111.33
3	C	4	MAN	O2-C2-C3	-3.33	103.25	110.15
3	C	6	GAL	C3-C4-C5	-3.29	104.27	110.23
3	C	1	NAG	C3-C4-C5	-3.27	104.31	110.23
3	C	4	MAN	C3-C4-C5	3.24	116.11	110.23
3	C	8	FUC	O2-C2-C3	3.20	116.78	110.15
3	C	3	BMA	O6-C6-C5	-3.03	101.01	111.33
3	C	4	MAN	O6-C6-C5	-3.03	101.02	111.33
3	D	2	NAG	C2-N2-C7	-3.00	118.87	122.90
3	D	3	BMA	C1-O5-C5	-2.98	108.19	112.19
3	D	8	FUC	C1-O5-C5	2.97	119.96	112.97
3	D	7	MAN	O2-C2-C3	2.96	116.27	110.15
3	C	8	FUC	O4-C4-C5	-2.93	103.27	109.74
3	C	7	MAN	O4-C4-C3	-2.88	103.58	110.38
3	D	1	NAG	C1-O5-C5	-2.81	108.42	112.19
3	D	3	BMA	C2-C3-C4	2.80	115.79	110.86
3	C	5	NAG	C6-C5-C4	2.80	119.90	113.02
3	C	2	NAG	O4-C4-C5	-2.77	102.51	109.32
3	D	7	MAN	C2-C3-C4	2.76	115.71	110.86
3	C	5	NAG	O3-C3-C2	-2.70	103.80	109.40
3	C	5	NAG	O5-C1-C2	-2.68	107.14	111.29
3	D	4	MAN	C1-O5-C5	2.68	115.78	112.19
3	C	1	NAG	C2-N2-C7	-2.68	119.31	122.90
3	D	4	MAN	O5-C5-C4	2.63	117.23	110.83
3	D	3	BMA	O3-C3-C2	2.61	115.37	110.05
3	C	8	FUC	C3-C4-C5	2.59	113.76	109.81
3	C	6	GAL	O3-C3-C4	2.59	116.48	110.38
3	D	1	NAG	C1-C2-N2	2.58	114.50	110.43
3	C	3	BMA	O4-C4-C3	-2.53	104.42	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O5-C5-C6	2.42	112.38	107.66
3	C	7	MAN	O6-C6-C5	-2.40	103.16	111.33
3	D	7	MAN	O6-C6-C5	-2.38	103.22	111.33
3	D	1	NAG	C3-C4-C5	-2.35	105.97	110.23
3	D	8	FUC	C1-C2-C3	-2.34	106.24	109.64
3	C	5	NAG	O4-C4-C5	-2.29	103.68	109.32
3	C	3	BMA	O3-C3-C2	2.29	114.72	110.05
3	D	4	MAN	C6-C5-C4	-2.27	107.44	113.02
3	C	8	FUC	O2-C2-C1	2.25	114.38	109.22
3	D	6	GAL	O2-C2-C1	2.20	114.26	109.22
3	C	1	NAG	C6-C5-C4	-2.19	107.65	113.02
3	D	2	NAG	C3-C4-C5	-2.16	106.31	110.23
3	C	7	MAN	O2-C2-C1	2.11	114.05	109.22
3	C	1	NAG	O7-C7-N2	-2.11	118.26	121.98
3	D	1	NAG	C2-N2-C7	-2.10	120.08	122.90
3	D	7	MAN	O5-C1-C2	-2.06	105.87	110.79
3	C	5	NAG	O5-C5-C4	-2.06	105.83	110.83
3	C	7	MAN	O2-C2-C3	2.05	114.39	110.15
3	C	8	FUC	O5-C5-C6	2.05	111.84	107.40
3	C	3	BMA	O2-C2-C1	-2.03	104.57	109.22
3	D	2	NAG	C1-O5-C5	2.03	114.90	112.19
3	C	6	GAL	C2-C3-C4	2.02	114.41	110.86
3	C	1	NAG	C4-C3-C2	2.01	113.96	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	MAN	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
3	C	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6

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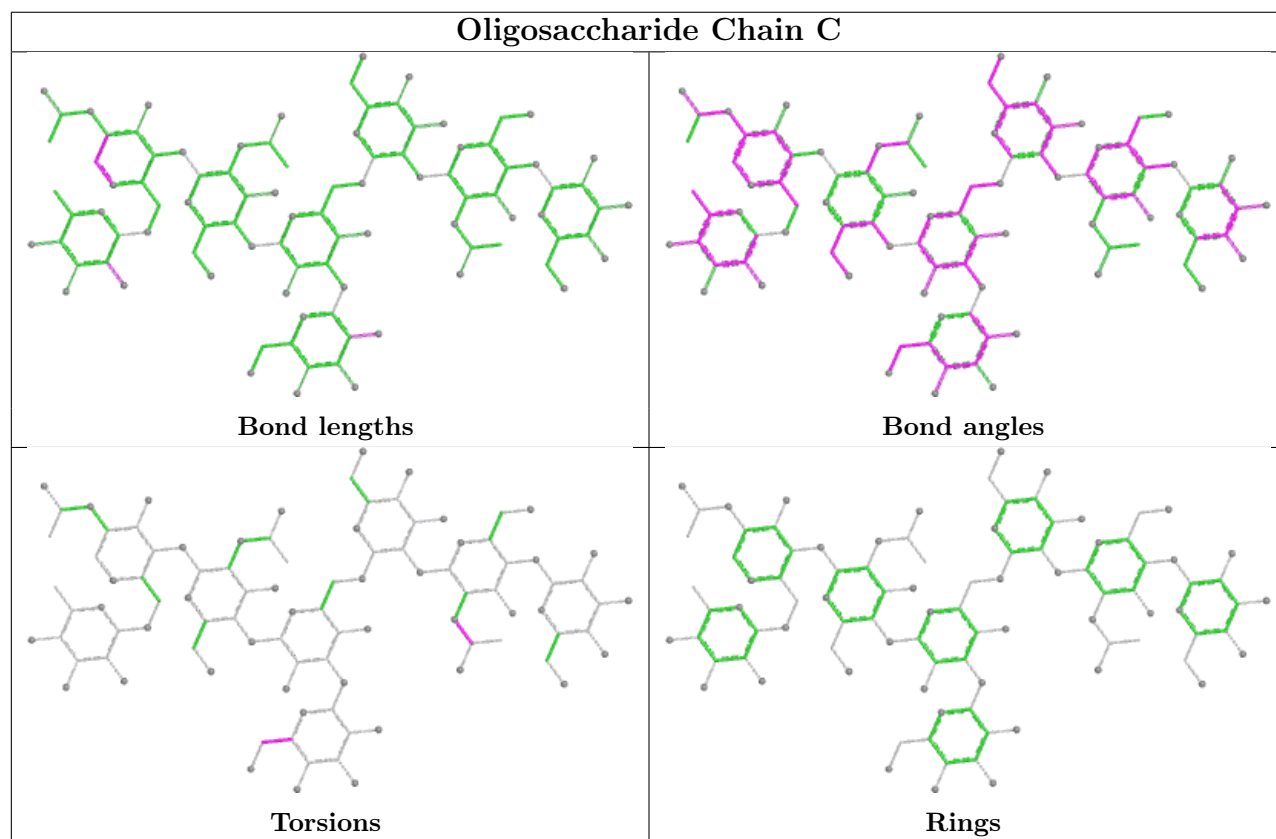
Mol	Chain	Res	Type	Atoms
3	C	5	NAG	O7-C7-N2-C2

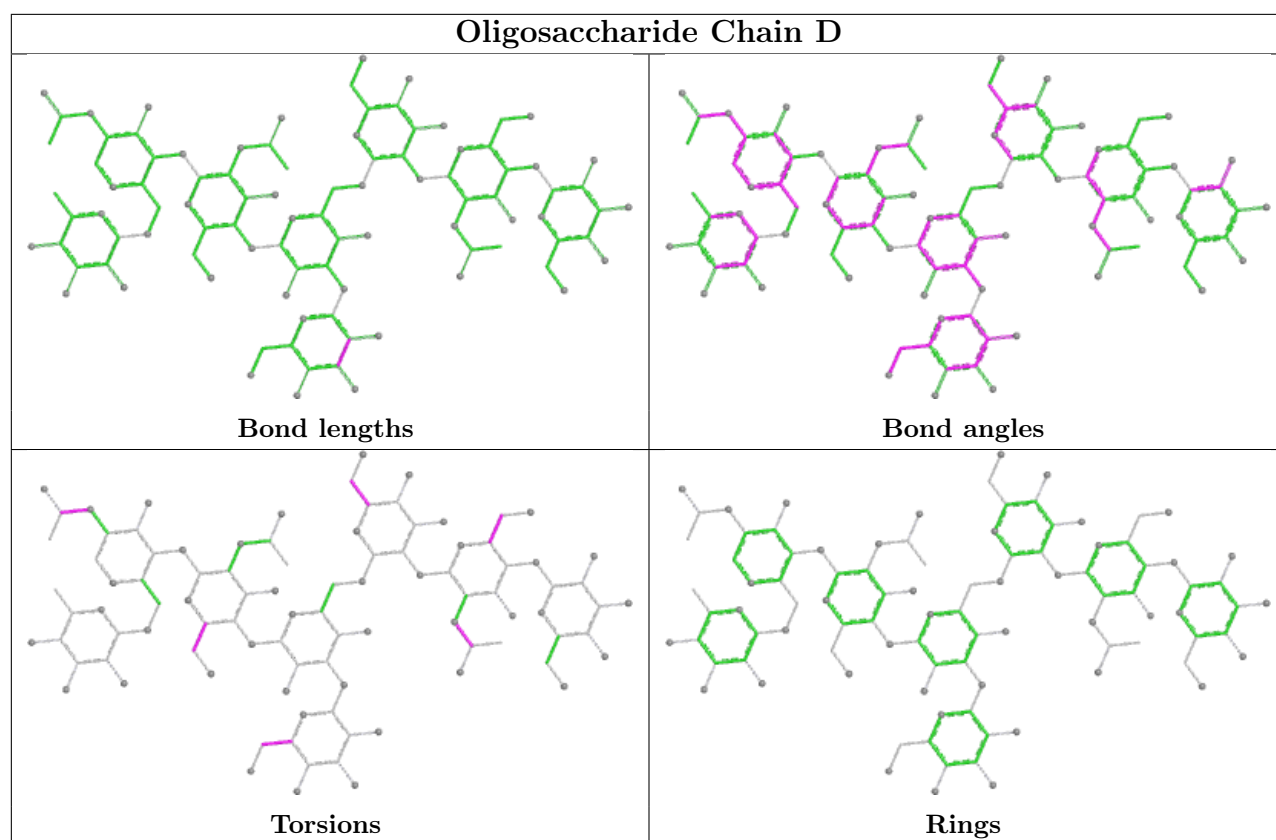
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	D	2	NAG	1	0
3	D	8	FUC	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	202/232 (87%)	0.08	8 (3%) 42 42	21, 37, 72, 115	0
2	B	192/245 (78%)	0.89	36 (18%) 3 2	20, 49, 91, 113	1 (0%)
All	All	394/477 (82%)	0.47	44 (11%) 9 9	20, 43, 89, 115	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	328	LEU	5.4
2	B	300	TYR	5.3
2	B	327	ALA	4.7
2	B	296	TYR	4.5
2	B	266	VAL	4.4
2	B	299	THR	3.8
1	A	443	LEU	3.7
2	B	329	PRO	3.5
2	B	237	GLY	3.3
1	A	358	LEU	3.1
2	B	282	VAL	3.0
2	B	303	VAL	3.0
2	B	292	ARG	2.9
2	B	302	VAL	2.9
2	B	419	GLN	2.8
2	B	238	PRO	2.6
1	A	361	ASN	2.6
2	B	281	GLY	2.6
2	B	420	GLY	2.6
2	B	442	SER	2.5
2	B	443	LEU	2.5
2	B	418	GLN	2.4
2	B	278	TYR	2.4
2	B	326	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	420	GLY	2.4
2	B	323	VAL	2.4
2	B	275	PHE	2.3
1	A	359	THR	2.3
1	A	422	VAL	2.3
2	B	423	PHE	2.2
2	B	263	VAL	2.2
2	B	425	CYS	2.2
2	B	325	ASN	2.2
2	B	284	VAL	2.2
2	B	318	GLU	2.2
2	B	349	TYR	2.2
2	B	360	LYS	2.1
2	B	414	LYS	2.1
1	A	441	LEU	2.1
2	B	361	ASN	2.1
2	B	265	ASP	2.1
1	A	363	VAL	2.1
2	B	330	ALA	2.0
2	B	288	LYS	2.0

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.

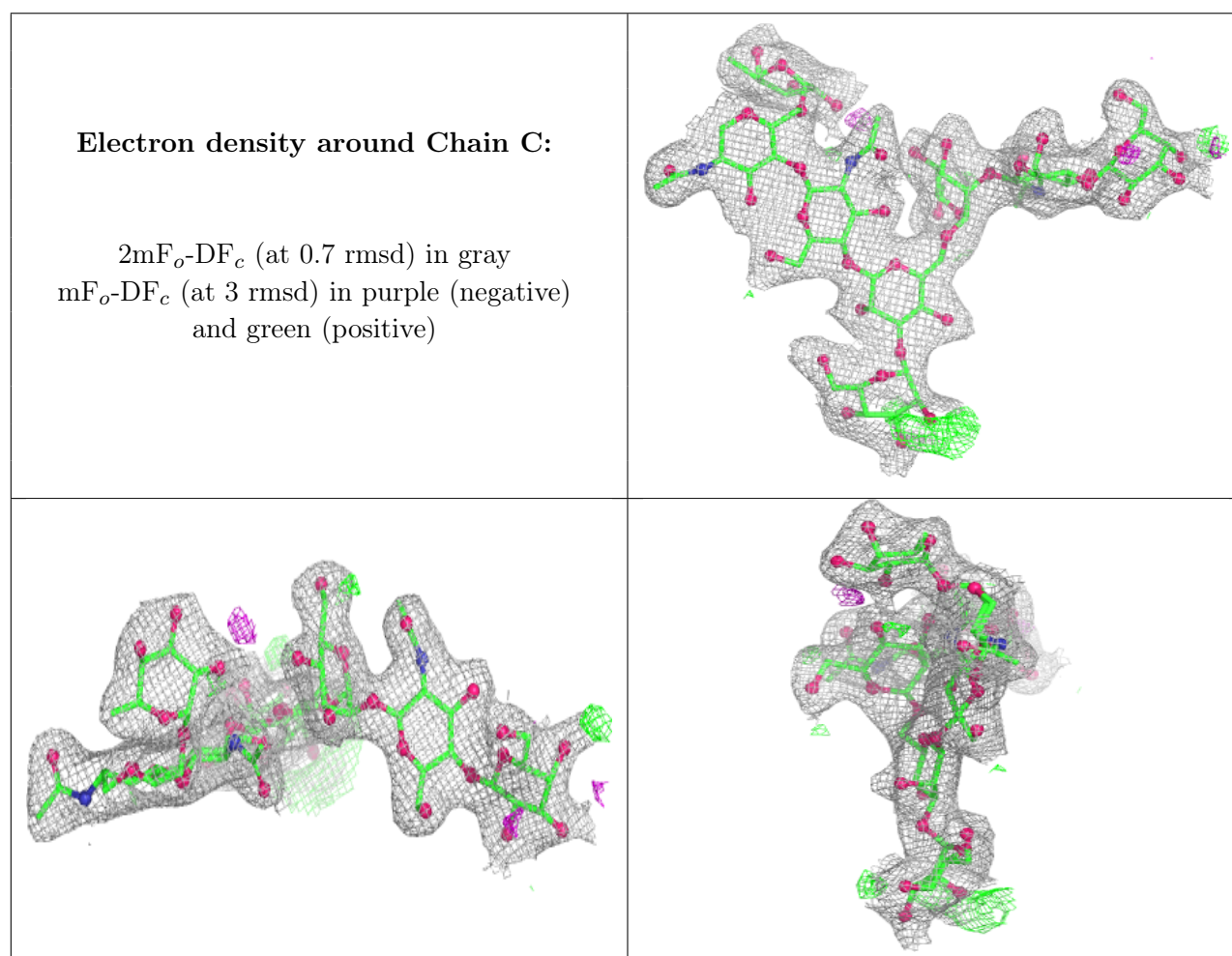
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	D	8	10/11	0.64	0.14	90,96,109,112	0
3	MAN	D	7	11/12	0.77	0.13	57,68,72,75	0
3	MAN	C	7	11/12	0.77	0.14	53,55,62,72	0
3	NAG	D	1	14/15	0.78	0.13	80,93,100,105	0
3	BMA	D	3	11/12	0.83	0.13	65,76,84,87	0
3	NAG	D	2	14/15	0.84	0.12	77,87,89,90	0
3	MAN	D	4	11/12	0.86	0.10	59,67,74,76	0
3	NAG	D	5	14/15	0.86	0.11	52,63,81,86	0

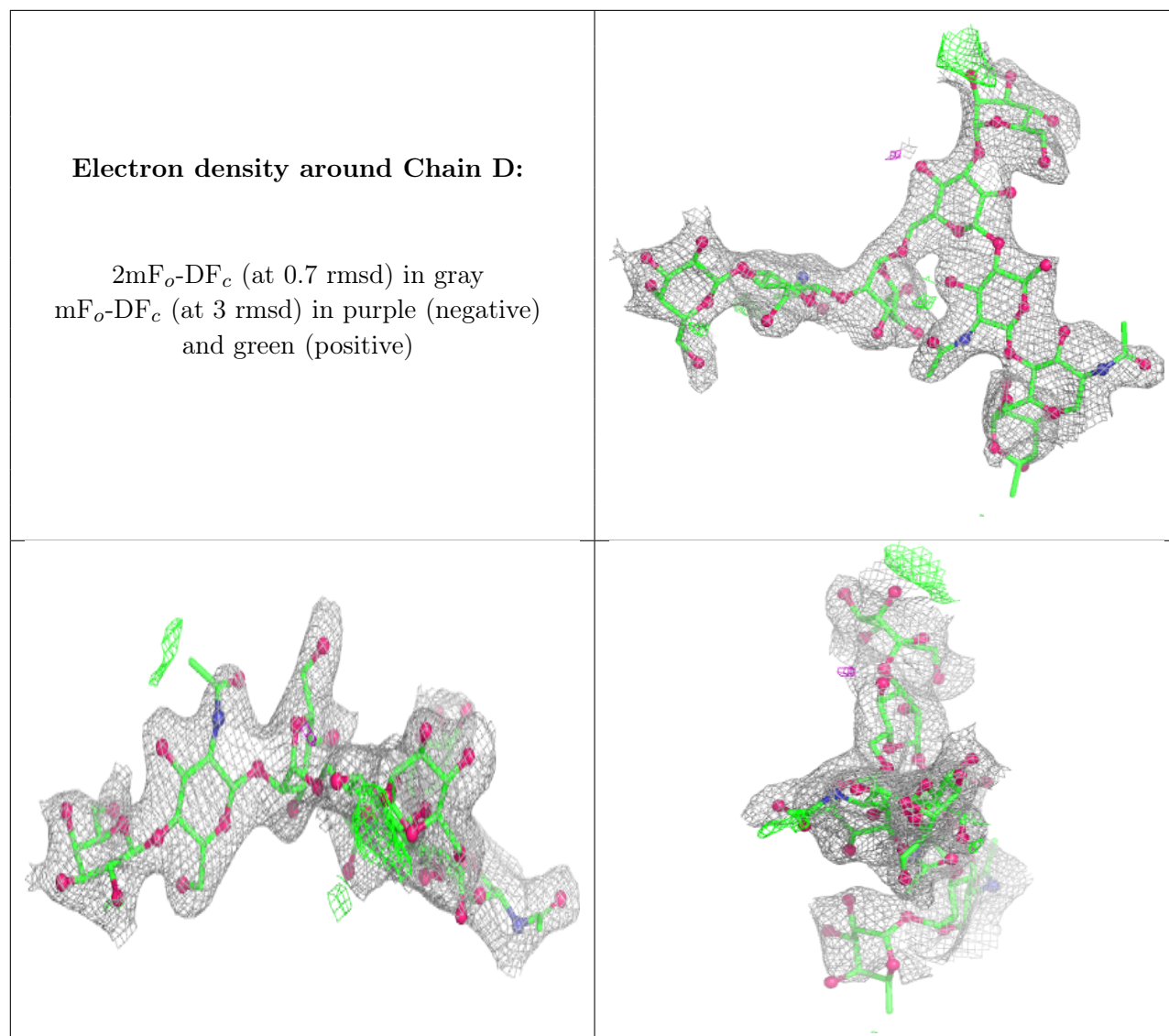
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	D	6	11/12	0.87	0.13	64,75,81,82	0
3	MAN	C	4	11/12	0.88	0.09	36,39,42,42	0
3	FUC	C	8	10/11	0.88	0.11	46,54,57,59	0
3	GAL	C	6	11/12	0.89	0.14	40,54,60,64	0
3	NAG	C	5	14/15	0.93	0.08	38,45,57,60	0
3	NAG	C	1	14/15	0.94	0.08	38,45,55,56	0
3	BMA	C	3	11/12	0.95	0.06	35,38,47,48	0
3	NAG	C	2	14/15	0.95	0.07	31,41,43,49	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.