



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:44 AM UTC

PDB ID : 1I1C / pdb_00001i1c
Title : NON-FCRN BINDING FC FRAGMENT OF RAT IGG2A
Authors : Martin, W.L.; West Jr., A.P.; Gan, L.; Bjorkman, P.J.
Deposited on : 2001-01-31
Resolution : 2.70 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

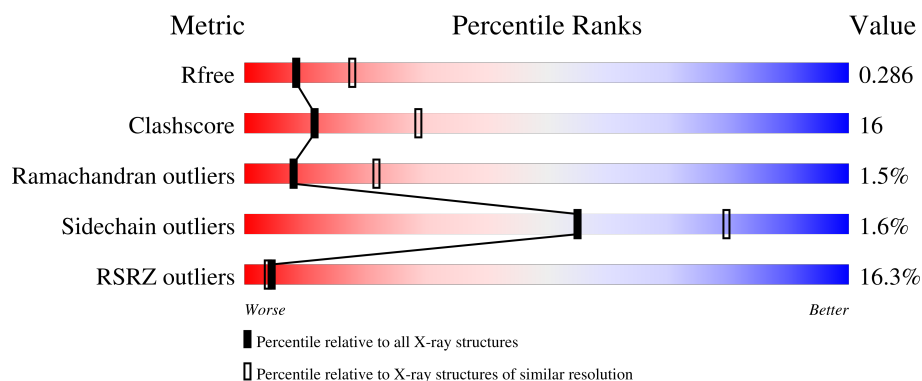
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	239	14% 57% 26% • 14%
1	B	239	14% 57% 27% • 14%
2	C	8	38% 38% 25%
3	D	8	38% 38% 25%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	D	8	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3440 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-2A CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1621	1027	268	317	9			
1	B	205	Total	C	N	O	S	0	0	0
			1621	1027	268	317	9			

There are 40 discrepancies between the modelled and reference sequences:

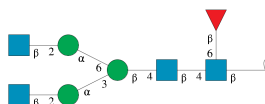
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	GLY	THR	engineered mutation	UNP P20760
A	253	GLY	ILE	engineered mutation	UNP P20760
A	254	GLY	THR	engineered mutation	UNP P20760
A	310	GLU	HIS	engineered mutation	UNP P20760
A	433	GLU	HIS	engineered mutation	UNP P20760
A	435	GLU	HIS	engineered mutation	UNP P20760
A	448	GLY	-	cloning artifact	UNP P20760
A	449	ILE	-	cloning artifact	UNP P20760
A	450	GLU	-	cloning artifact	UNP P20760
A	451	GLY	-	cloning artifact	UNP P20760
A	452	ARG	-	cloning artifact	UNP P20760
A	453	GLY	-	cloning artifact	UNP P20760
A	454	SER	-	cloning artifact	UNP P20760
A	455	SER	-	cloning artifact	UNP P20760
A	456	HIS	-	cloning artifact	UNP P20760
A	457	HIS	-	cloning artifact	UNP P20760
A	458	HIS	-	cloning artifact	UNP P20760
A	459	HIS	-	cloning artifact	UNP P20760
A	460	HIS	-	cloning artifact	UNP P20760
A	461	HIS	-	cloning artifact	UNP P20760
B	252	GLY	THR	engineered mutation	UNP P20760
B	253	GLY	ILE	engineered mutation	UNP P20760
B	254	GLY	THR	engineered mutation	UNP P20760
B	310	GLU	HIS	engineered mutation	UNP P20760
B	433	GLU	HIS	engineered mutation	UNP P20760

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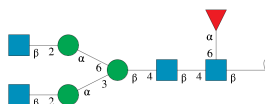
Chain	Residue	Modelled	Actual	Comment	Reference
B	435	GLU	HIS	engineered mutation	UNP P20760
B	448	GLY	-	cloning artifact	UNP P20760
B	449	ILE	-	cloning artifact	UNP P20760
B	450	GLU	-	cloning artifact	UNP P20760
B	451	GLY	-	cloning artifact	UNP P20760
B	452	ARG	-	cloning artifact	UNP P20760
B	453	GLY	-	cloning artifact	UNP P20760
B	454	SER	-	cloning artifact	UNP P20760
B	455	SER	-	cloning artifact	UNP P20760
B	456	HIS	-	cloning artifact	UNP P20760
B	457	HIS	-	cloning artifact	UNP P20760
B	458	HIS	-	cloning artifact	UNP P20760
B	459	HIS	-	cloning artifact	UNP P20760
B	460	HIS	-	cloning artifact	UNP P20760
B	461	HIS	-	cloning artifact	UNP P20760

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			

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

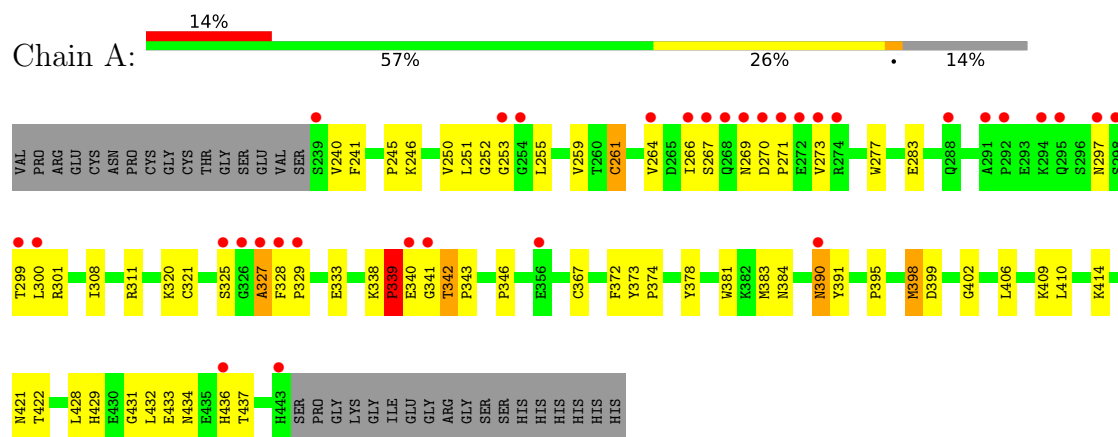


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

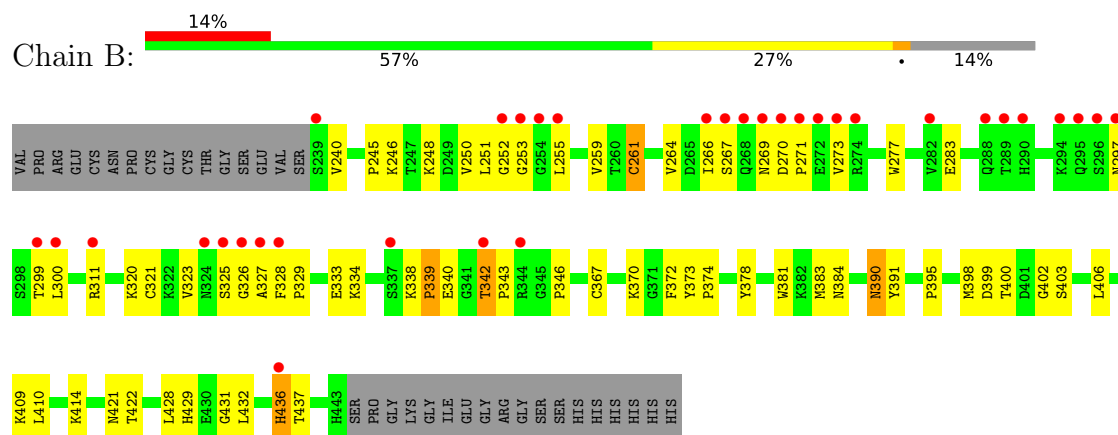
3 Residue-property plots

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.

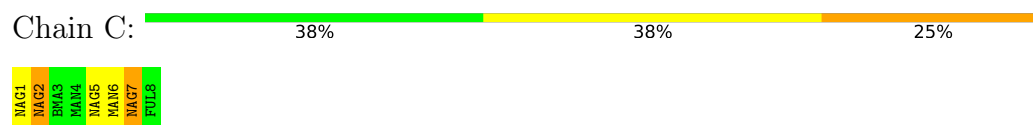
• Molecule 1: IG GAMMA-2A CHAIN C REGION



• Molecule 1: IG GAMMA-2A CHAIN C REGION



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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

Chain D:  38% 38% 25%

NA61	NA62	BR43	MA64	MA65	MA66	MA67	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.50Å 73.36Å 82.16Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	29.81 – 2.70 29.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.81-2.70) 98.5 (29.81-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.279 0.251 , 0.286	Depositor DCC
R_{free} test set	1375 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3440	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: BMA, NAG, FUL, FUC, 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	0.47	1/1666 (0.1%)	1.06	12/2267 (0.5%)
1	B	0.48	1/1666 (0.1%)	0.96	7/2267 (0.3%)
All	All	0.48	2/3332 (0.1%)	1.01	19/4534 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	C-N	6.03	1.42	1.33
1	A	398	MET	SD-CE	-5.03	1.67	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	N-CA-C	14.85	132.98	109.07
1	A	341	GLY	N-CA-C	9.68	128.14	112.84
1	A	339	PRO	CA-C-N	-7.42	112.76	123.00
1	A	339	PRO	C-N-CA	-7.42	112.76	123.00
1	B	342	THR	CA-C-N	7.41	127.33	119.85
1	B	342	THR	C-N-CA	7.41	127.33	119.85
1	A	342	THR	CA-C-N	7.24	127.16	119.85
1	A	342	THR	C-N-CA	7.24	127.16	119.85
1	A	390	ASN	N-CA-C	5.96	118.86	109.39
1	B	390	ASN	N-CA-C	5.59	118.27	109.39
1	A	340	GLU	CA-C-O	5.51	126.39	120.38
1	A	259	VAL	N-CA-C	-5.34	100.89	108.58
1	B	436	HIS	N-CA-C	5.32	116.61	108.42
1	A	327	ALA	N-CA-C	-5.24	105.55	112.94
1	A	436	HIS	N-CA-C	5.20	116.42	108.42
1	B	370	LYS	N-CA-C	5.14	117.49	109.52
1	A	308	ILE	N-CA-C	5.11	115.06	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	GLY	N-CA-C	-5.11	109.00	115.08
1	B	259	VAL	N-CA-C	-5.02	101.35	108.58

There are no chirality outliers.

There are no planarity outliers.

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	1621	0	1570	51	0
1	B	1621	0	1570	54	0
2	C	99	0	85	6	0
3	D	99	0	85	5	0
All	All	3440	0	3310	108	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 16.

All (108) 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:325:SER:HB2	1:A:328:PHE:HB2	1.36	1.06
1:B:325:SER:HB2	1:B:328:PHE:HB2	1.36	1.01
1:B:398:MET:HE1	1:B:402:GLY:C	1.99	0.86
1:B:248:LYS:HD2	1:B:378:TYR:CE1	2.10	0.86
1:A:398:MET:HE1	1:A:402:GLY:C	2.01	0.84
1:A:384:ASN:HD21	1:A:421:ASN:HD22	1.22	0.83
1:B:384:ASN:HD21	1:B:421:ASN:HD22	1.26	0.82
1:B:325:SER:CB	1:B:328:PHE:HB2	2.11	0.81
1:A:325:SER:CB	1:A:328:PHE:HB2	2.11	0.80
1:A:271:PRO:HB3	1:A:300:LEU:HD12	1.64	0.79
1:B:271:PRO:HB3	1:B:300:LEU:HD12	1.65	0.77
1:B:398:MET:HE1	1:B:402:GLY:O	1.86	0.74
1:A:398:MET:HE1	1:A:402:GLY:O	1.88	0.72
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:HIS:CD2	1:B:431:GLY:H	2.09	0.71
1:A:398:MET:HE3	1:A:399:ASP:H	1.56	0.71
1:A:429:HIS:CD2	1:A:431:GLY:H	2.10	0.70
1:A:246:LYS:HE2	2:C:7:NAG:O4	1.91	0.70
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.75	0.69
1:B:398:MET:HE3	1:B:399:ASP:H	1.62	0.65
1:A:398:MET:HE3	1:A:399:ASP:N	2.12	0.65
1:A:271:PRO:HB3	1:A:300:LEU:CD1	2.28	0.63
1:B:271:PRO:HB3	1:B:300:LEU:CD1	2.28	0.63
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.36	0.61
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.36	0.60
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.36	0.60
1:B:266:ILE:HB	1:B:300:LEU:HB2	1.83	0.59
1:B:311:ARG:HA	1:B:311:ARG:HE	1.68	0.59
1:A:266:ILE:HB	1:A:300:LEU:HB2	1.84	0.59
1:A:311:ARG:HA	1:A:311:ARG:HE	1.68	0.57
1:B:398:MET:HE3	1:B:399:ASP:N	2.20	0.56
1:B:390:ASN:O	1:B:410:LEU:HD12	2.07	0.55
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.40	0.55
1:A:429:HIS:HD2	1:A:431:GLY:H	1.54	0.55
1:A:266:ILE:HD13	1:A:273:VAL:HG21	1.88	0.54
1:B:248:LYS:HB2	1:B:378:TYR:CD1	2.43	0.54
1:A:406:LEU:C	1:A:406:LEU:HD12	2.33	0.54
1:A:390:ASN:O	1:A:410:LEU:HD12	2.07	0.54
1:B:429:HIS:HD2	1:B:431:GLY:H	1.54	0.53
1:B:432:LEU:HD13	1:B:437:THR:HG22	1.91	0.53
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.91	0.53
1:B:266:ILE:HD13	1:B:273:VAL:HG21	1.89	0.53
1:A:264:VAL:HG11	2:C:2:NAG:H2	1.90	0.52
1:B:406:LEU:HD12	1:B:406:LEU:C	2.35	0.52
1:B:297:ASN:O	1:B:299:THR:HG23	2.10	0.51
1:B:264:VAL:HG11	3:D:2:NAG:H2	1.91	0.51
1:A:301:ARG:NE	2:C:2:NAG:O7	2.39	0.49
1:B:248:LYS:HD2	1:B:378:TYR:CZ	2.46	0.49
1:A:297:ASN:O	1:A:299:THR:HG23	2.13	0.49
1:A:338:LYS:O	1:A:339:PRO:O	2.31	0.48
1:A:267:SER:C	1:A:269:ASN:H	2.22	0.48
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.48	0.48
1:B:267:SER:C	1:B:269:ASN:N	2.71	0.48
1:B:270:ASP:CG	1:B:327:ALA:HB2	2.39	0.47
1:B:328:PHE:CD2	1:B:329:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.50	0.47
1:A:270:ASP:CG	1:A:327:ALA:HB2	2.40	0.46
1:B:267:SER:C	1:B:269:ASN:H	2.23	0.46
1:B:246:LYS:HE2	3:D:7:NAG:O4	2.16	0.46
1:A:267:SER:C	1:A:269:ASN:N	2.70	0.46
1:A:320:LYS:HE2	1:A:333:GLU:OE2	2.16	0.45
1:B:320:LYS:HE2	1:B:333:GLU:OE2	2.16	0.45
1:A:328:PHE:CD2	1:A:329:PRO:HD2	2.52	0.45
1:A:338:LYS:C	1:A:339:PRO:O	2.60	0.45
2:C:2:NAG:H83	2:C:6:MAN:C3	2.47	0.45
1:A:320:LYS:HE2	1:A:333:GLU:CD	2.42	0.45
1:A:395:PRO:HD2	1:B:395:PRO:HD2	1.99	0.45
3:D:2:NAG:H83	3:D:6:MAN:C3	2.47	0.44
1:B:391:TYR:HA	1:B:409:LYS:O	2.17	0.44
1:B:383:MET:HA	1:B:422:THR:O	2.17	0.44
1:B:251:LEU:O	1:B:253:GLY:N	2.50	0.44
1:B:338:LYS:O	1:B:339:PRO:O	2.36	0.44
1:A:391:TYR:HA	1:A:409:LYS:O	2.18	0.44
1:A:342:THR:HA	1:A:343:PRO:HD3	1.74	0.44
1:B:270:ASP:OD2	1:B:327:ALA:HB2	2.17	0.44
3:D:2:NAG:H83	3:D:6:MAN:H3	1.99	0.43
1:B:320:LYS:HE2	1:B:333:GLU:CD	2.43	0.43
1:B:373:TYR:HA	1:B:374:PRO:C	2.42	0.43
1:B:384:ASN:ND2	1:B:421:ASN:HD22	2.06	0.43
1:B:398:MET:HE2	1:B:399:ASP:O	2.18	0.43
1:A:378:TYR:HB3	1:A:428:LEU:HB2	2.00	0.43
2:C:5:NAG:H61	3:D:8:FUC:H4	1.98	0.43
1:A:373:TYR:HA	1:A:374:PRO:C	2.43	0.43
1:A:270:ASP:OD2	1:A:327:ALA:HB2	2.19	0.42
1:A:245:PRO:HB2	1:A:250:VAL:CG2	2.49	0.42
1:A:374:PRO:O	1:A:429:HIS:HE1	2.02	0.42
1:A:383:MET:HA	1:A:422:THR:O	2.19	0.42
2:C:2:NAG:H83	2:C:6:MAN:H3	1.99	0.42
1:A:251:LEU:O	1:A:253:GLY:N	2.53	0.42
1:B:240:VAL:HG21	1:B:323:VAL:CG1	2.49	0.42
1:B:342:THR:HA	1:B:343:PRO:HD3	1.70	0.42
1:B:374:PRO:O	1:B:429:HIS:HE1	2.02	0.42
1:A:277:TRP:O	1:A:283:GLU:HA	2.19	0.42
1:A:384:ASN:ND2	1:A:421:ASN:HD22	2.02	0.42
1:B:251:LEU:C	1:B:253:GLY:H	2.28	0.42
1:B:428:LEU:HD23	1:B:436:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:PRO:HB2	1:B:250:VAL:CG2	2.49	0.42
1:B:277:TRP:O	1:B:283:GLU:HA	2.20	0.41
1:B:325:SER:C	1:B:327:ALA:H	2.28	0.41
1:A:251:LEU:C	1:A:253:GLY:H	2.29	0.41
1:A:433:GLU:O	1:A:434:ASN:HB2	2.20	0.41
1:A:325:SER:C	1:A:327:ALA:H	2.28	0.41
1:A:266:ILE:CD1	1:A:273:VAL:HG21	2.51	0.41
1:B:334:LYS:HD3	1:B:334:LYS:HA	1.87	0.41
1:A:240:VAL:HG12	1:A:241:PHE:N	2.37	0.40
1:A:390:ASN:ND2	1:B:400:THR:HG21	2.36	0.40
1:B:338:LYS:C	1:B:339:PRO:O	2.63	0.40
1:B:398:MET:HE3	1:B:403:SER:O	2.21	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	203/239 (85%)	190 (94%)	10 (5%)	3 (2%)	8	22
1	B	203/239 (85%)	190 (94%)	10 (5%)	3 (2%)	8	22
All	All	406/478 (85%)	380 (94%)	20 (5%)	6 (2%)	8	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	B	255	LEU
1	A	252	GLY
1	A	339	PRO
1	B	252	GLY
1	B	339	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	188/216 (87%)	185 (98%)	3 (2%)	55	80
1	B	188/216 (87%)	185 (98%)	3 (2%)	55	80
All	All	376/432 (87%)	370 (98%)	6 (2%)	55	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	CYS
1	A	321	CYS
1	A	414	LYS
1	B	261	CYS
1	B	321	CYS
1	B	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	390	ASN
1	A	421	ASN
1	A	429	HIS
1	A	434	ASN
1	B	268	GLN
1	B	360	GLN
1	B	390	ASN
1	B	421	ASN
1	B	429	HIS
1	B	434	ASN

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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	0.73	1 (5%)
2	BMA	C	3	2	11,11,12	0.42	0	15,15,17	0.67	0
2	MAN	C	4	2	11,11,12	0.50	0	15,15,17	0.45	0
2	NAG	C	5	2	14,14,15	0.51	0	17,19,21	0.63	0
2	MAN	C	6	2	11,11,12	0.50	0	15,15,17	0.55	0
2	NAG	C	7	2	14,14,15	0.51	0	17,19,21	0.70	1 (5%)
2	FUL	C	8	2	10,10,11	0.47	0	14,14,16	0.29	0
3	NAG	D	1	3,1	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
3	BMA	D	3	3	11,11,12	0.41	0	15,15,17	0.66	0
3	MAN	D	4	3	11,11,12	0.50	0	15,15,17	0.43	0
3	NAG	D	5	3	14,14,15	0.53	0	17,19,21	0.62	0
3	MAN	D	6	3	11,11,12	0.51	0	15,15,17	0.50	0
3	NAG	D	7	3	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
3	FUC	D	8	3	10,10,11	0.41	0	14,14,16	0.31	0

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	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	NAG	C	5	2	-	3/6/23/26	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	C	7	2	-	4/6/23/26	0/1/1/1
2	FUL	C	8	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	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	-	3/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	NAG	D	7	3	-	4/6/23/26	0/1/1/1
3	FUC	D	8	3	1/1/4/5	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C2-N2-C7	-2.29	119.83	122.90
2	C	2	NAG	C2-N2-C7	-2.28	119.84	122.90
3	D	2	NAG	C2-N2-C7	-2.21	119.94	122.90
3	D	7	NAG	C2-N2-C7	-2.20	119.95	122.90
2	C	1	NAG	C2-N2-C7	-2.13	120.05	122.90
2	C	7	NAG	C2-N2-C7	-2.10	120.09	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	8	FUC	C1

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2

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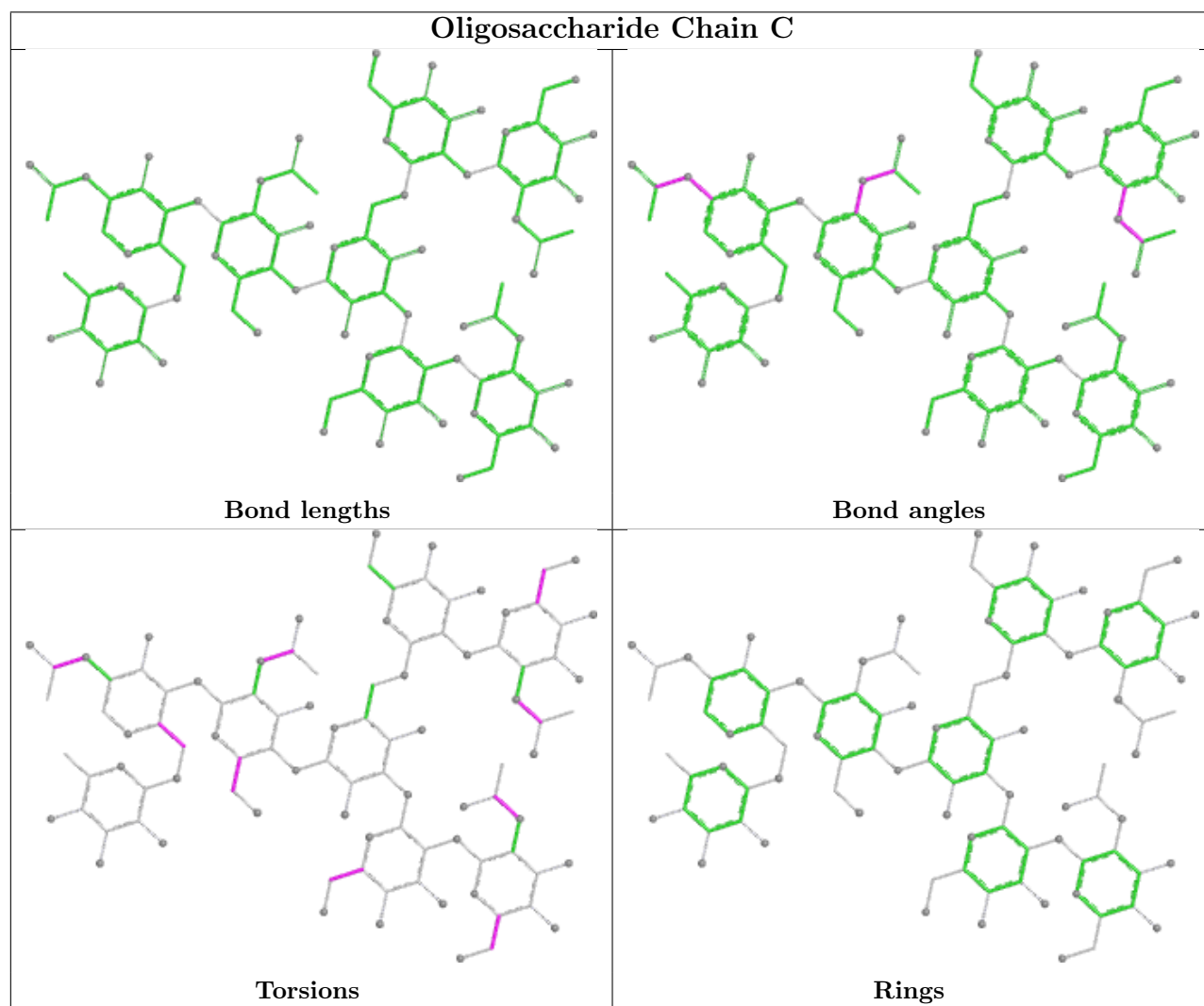
Mol	Chain	Res	Type	Atoms
2	C	7	NAG	C8-C7-N2-C2
2	C	7	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	7	NAG	O5-C5-C6-O6
3	D	7	NAG	O5-C5-C6-O6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

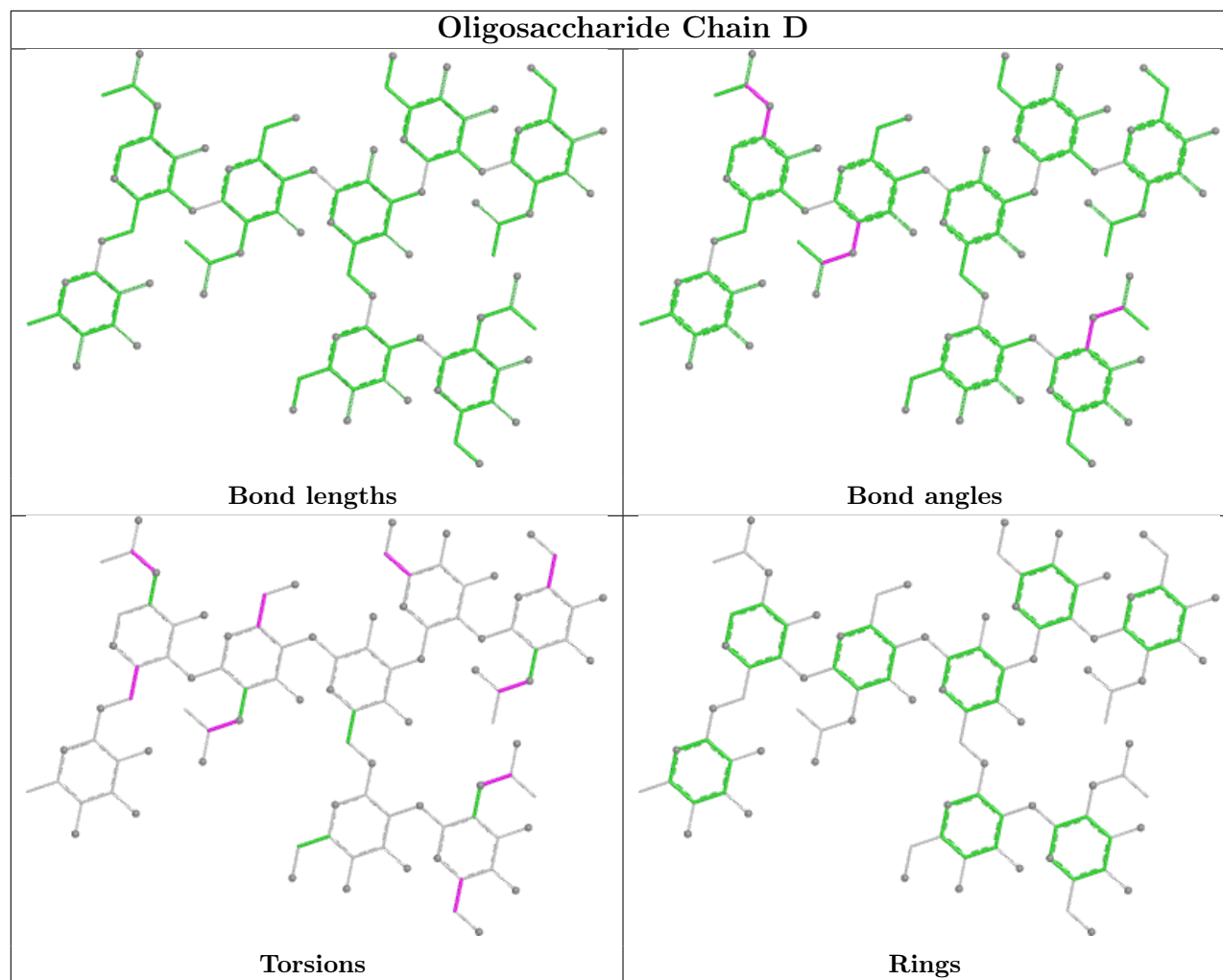
There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	7	NAG	1	0
3	D	8	FUC	1	0
3	D	2	NAG	3	0
2	C	6	MAN	2	0
2	C	7	NAG	1	0
3	D	6	MAN	2	0
2	C	5	NAG	1	0
2	C	2	NAG	4	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	205/239 (85%)	0.69	33 (16%) 4 4	11, 32, 86, 119	0
1	B	205/239 (85%)	0.74	34 (16%) 4 4	7, 34, 81, 116	0
All	All	410/478 (85%)	0.71	67 (16%) 4 4	7, 33, 86, 119	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	PHE	6.9
1	A	271	PRO	6.7
1	B	253	GLY	5.9
1	A	341	GLY	5.8
1	A	325	SER	5.3
1	B	273	VAL	5.1
1	B	325	SER	5.1
1	B	436	HIS	4.2
1	A	328	PHE	4.2
1	A	340	GLU	4.1
1	B	326	GLY	4.1
1	A	270	ASP	4.1
1	A	272	GLU	4.0
1	B	272	GLU	4.0
1	B	271	PRO	3.9
1	B	296	SER	3.7
1	A	300	LEU	3.6
1	A	326	GLY	3.4
1	B	252	GLY	3.3
1	A	436	HIS	3.3
1	A	267	SER	3.3
1	B	342	THR	3.2
1	B	254	GLY	3.2
1	A	266	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	298	SER	3.1
1	A	291	ALA	3.0
1	A	269	ASN	3.0
1	A	356	GLU	2.9
1	B	270	ASP	2.9
1	A	299	THR	2.9
1	A	292	PRO	2.9
1	B	311	ARG	2.9
1	B	295	GLN	2.8
1	B	288	GLN	2.8
1	A	327	ALA	2.8
1	B	255	LEU	2.8
1	B	324	ASN	2.7
1	A	268	GLN	2.7
1	A	239	SER	2.7
1	B	300	LEU	2.6
1	A	273	VAL	2.6
1	B	268	GLN	2.6
1	A	329	PRO	2.6
1	B	327	ALA	2.5
1	A	295	GLN	2.5
1	A	253	GLY	2.4
1	A	297	ASN	2.4
1	B	290	HIS	2.4
1	B	299	THR	2.3
1	A	443	HIS	2.3
1	B	269	ASN	2.3
1	A	254	GLY	2.3
1	B	344	ARG	2.3
1	A	294	LYS	2.2
1	B	266	ILE	2.2
1	B	282	VAL	2.2
1	A	390	ASN	2.2
1	A	288	GLN	2.2
1	B	297	ASN	2.2
1	B	289	THR	2.1
1	A	264	VAL	2.1
1	B	239	SER	2.0
1	B	267	SER	2.0
1	B	337	SER	2.0
1	A	274	ARG	2.0
1	B	274	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	294	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](#)

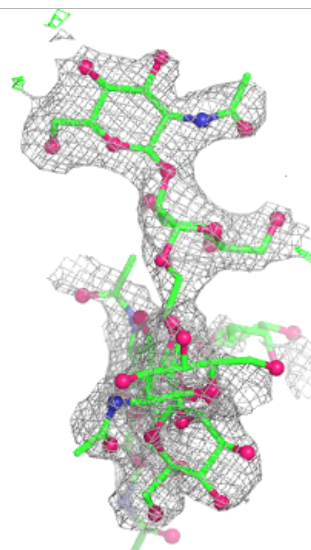
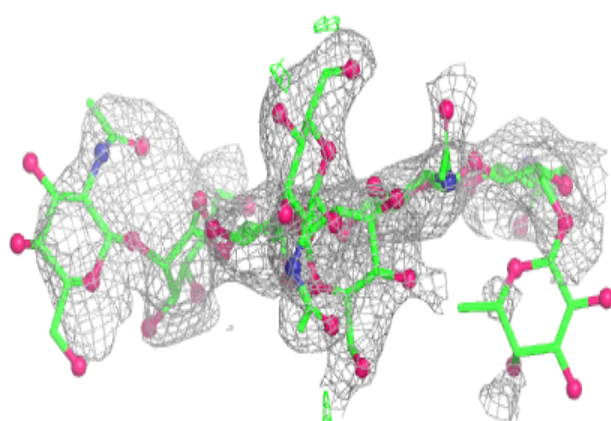
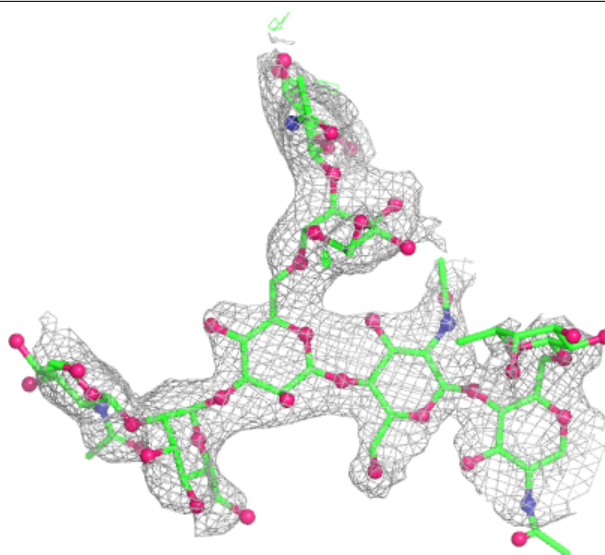
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

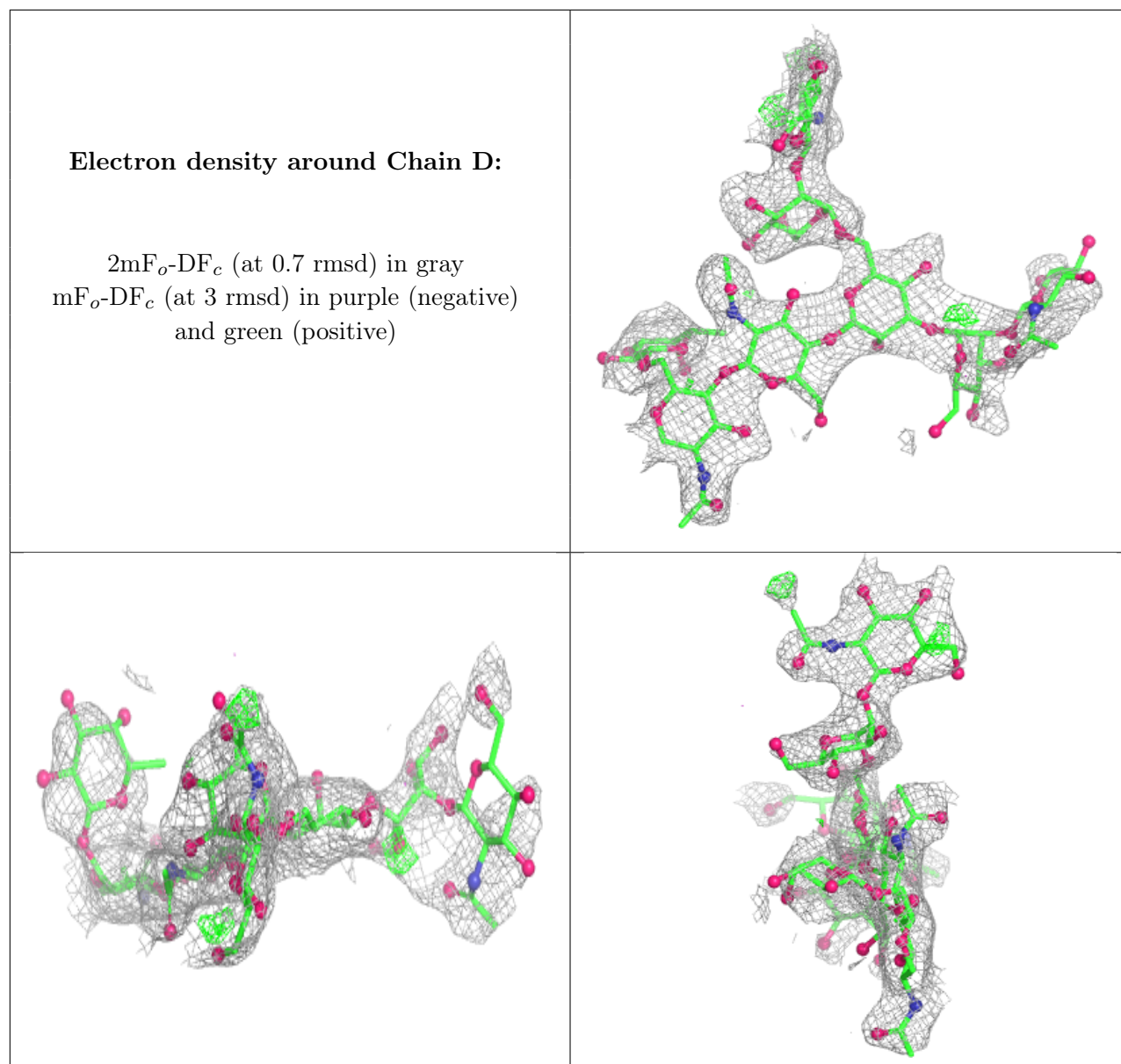
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	5	14/15	0.27	0.25	113,119,121,121	0
2	FUL	C	8	10/11	0.29	0.25	128,130,131,132	0
3	FUC	D	8	10/11	0.48	0.23	117,121,123,124	0
3	MAN	D	4	11/12	0.62	0.20	105,110,114,118	0
2	MAN	C	4	11/12	0.63	0.15	88,92,94,98	0
2	NAG	C	5	14/15	0.64	0.18	93,103,106,106	0
2	NAG	C	1	14/15	0.65	0.18	100,112,117,123	0
3	NAG	D	7	14/15	0.76	0.23	78,80,88,89	0
2	NAG	C	7	14/15	0.77	0.14	46,65,74,77	0
2	NAG	C	2	14/15	0.77	0.17	78,86,90,91	0
3	NAG	D	1	14/15	0.79	0.19	87,96,104,112	0
3	BMA	D	3	11/12	0.81	0.18	83,98,102,108	0
3	NAG	D	2	14/15	0.83	0.19	80,94,101,104	0
3	MAN	D	6	11/12	0.83	0.17	72,75,79,80	0
2	MAN	C	6	11/12	0.84	0.10	60,62,64,64	0
2	BMA	C	3	11/12	0.85	0.14	65,76,77,82	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.