



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:57 PM UTC

PDB ID : 4QGT / pdb_00004qgt
Title : The Crystal Structure of Human IgG Fc Domain with Enhanced Aromatic Sequon
Authors : Kong, L.; Connelly, S.C.; Wilson, I.A.
Deposited on : 2014-05-25
Resolution : 2.99 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

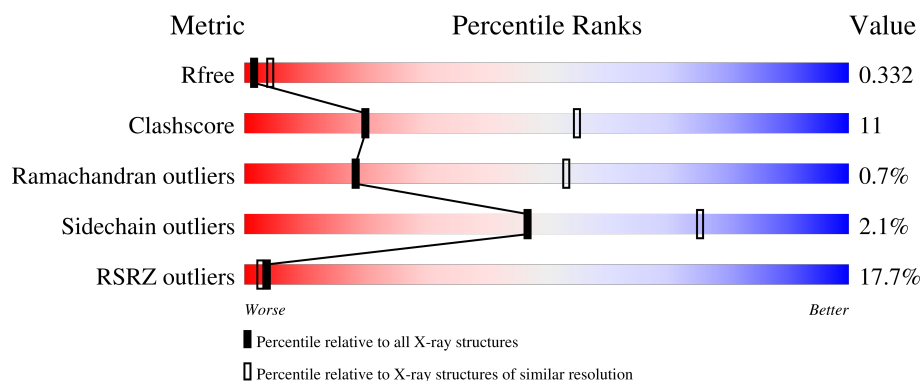
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	233	15% 63% 22% • 12%
1	B	233	16% 69% 19% • 11%
2	C	5	60% 40%
3	D	8	88% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3463 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 Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1637	1044	274	312	7			
1	B	207	Total	C	N	O	S	0	0	0
			1654	1054	278	315	7			

There are 6 discrepancies between the modelled and reference sequences:

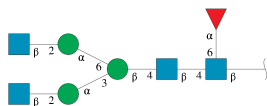
Chain	Residue	Modelled	Actual	Comment	Reference
A	215	PHE	-	expression tag	UNP Q6PYX1
A	295	PHE	GLN	engineered mutation	UNP Q6PYX1
A	296	ALA	TYR	engineered mutation	UNP Q6PYX1
B	215	PHE	-	expression tag	UNP Q6PYX1
B	295	PHE	GLN	engineered mutation	UNP Q6PYX1
B	296	ALA	TYR	engineered mutation	UNP Q6PYX1

- Molecule 2 is an oligosaccharide called 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



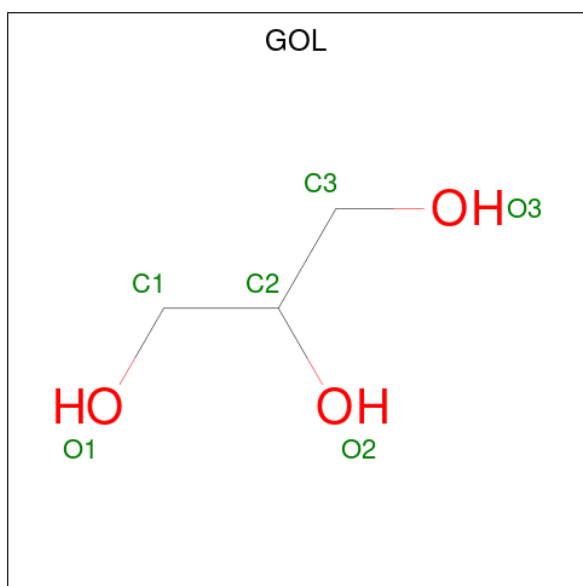
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			64	36	3	25			

- 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			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

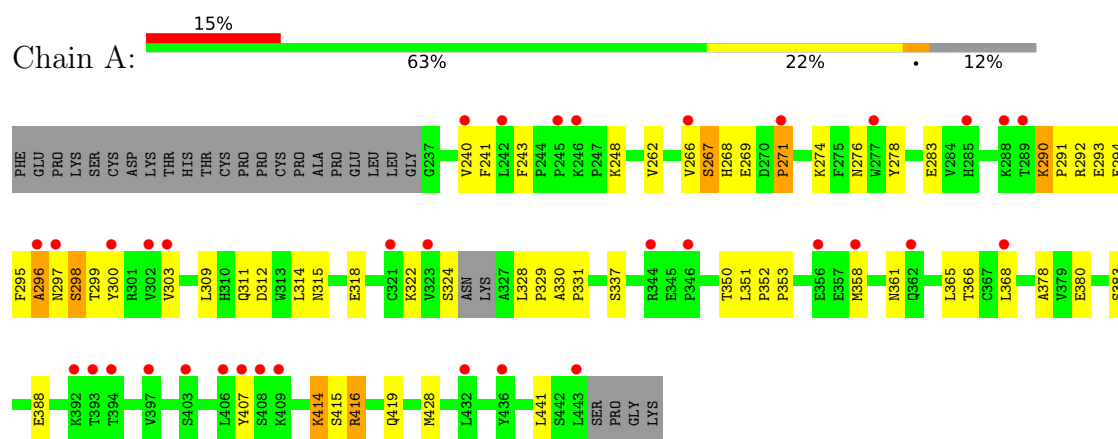
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			1	1		

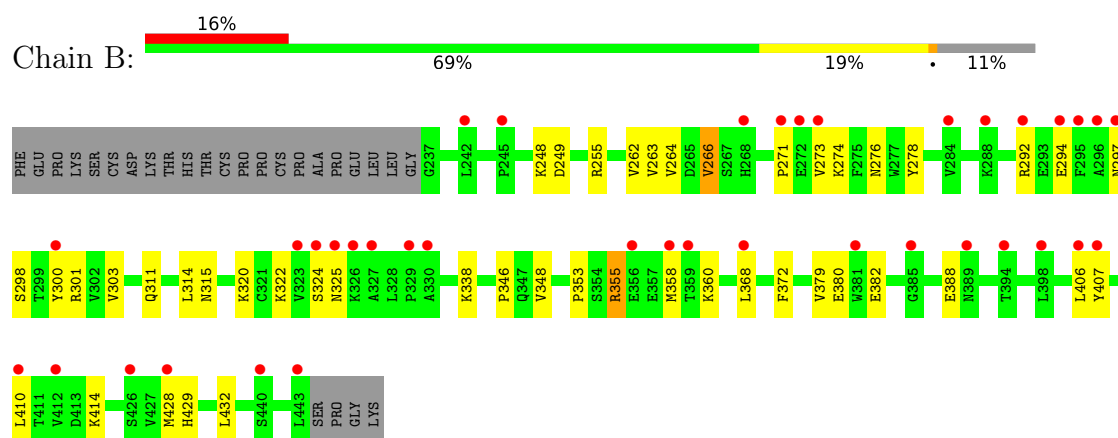
3 Residue-property plots [i](#)

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: Hepatitis B virus receptor binding protein



- Molecule 1: Hepatitis B virus receptor binding protein



- Molecule 2: 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)-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:  88% 12%

NAG1	NAG2	BR43	MAN4	MAN5	MAN6	MAN7	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.07Å 49.19Å 75.54Å 90.00° 104.21° 90.00°	Depositor
Resolution (Å)	46.85 – 2.99 46.85 – 2.99	Depositor EDS
% Data completeness (in resolution range)	87.9 (46.85-2.99) 88.0 (46.85-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.298 , 0.326 0.302 , 0.332	Depositor DCC
R_{free} test set	520 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.0	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	0.83	EDS
Total number of atoms	3463	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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 48.10 % 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 9.0296e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, FUC, BMA, NAG, 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	0.33	0/1682	0.83	4/2290 (0.2%)
1	B	0.27	0/1700	0.74	0/2315
All	All	0.30	0/3382	0.78	4/4605 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ALA	N-CA-C	7.87	120.48	109.31
1	A	298	SER	N-CA-C	-6.86	105.53	114.04
1	A	243	PHE	CA-C-N	5.71	126.26	120.38
1	A	243	PHE	C-N-CA	5.71	126.26	120.38

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	1637	0	1603	44	0
1	B	1654	0	1621	34	0
2	C	64	0	55	3	0
3	D	99	0	85	1	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	3463	0	3372	78	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 11.

All (78) 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:297:ASN:HD21	2:C:1:NAG:C1	1.02	1.54
1:A:297:ASN:ND2	2:C:1:NAG:C1	1.87	1.37
1:B:358:MET:O	1:B:414:LYS:NZ	1.62	1.32
1:A:358:MET:O	1:A:414:LYS:NZ	1.94	1.00
1:A:296:ALA:HB3	1:A:299:THR:C	2.01	0.84
1:A:268:HIS:O	1:A:269:GLU:HB2	1.81	0.81
1:A:296:ALA:HB3	1:A:299:THR:O	1.81	0.80
1:B:266:VAL:CG1	1:B:300:TYR:O	2.36	0.74
1:B:271:PRO:HB3	1:B:292:ARG:HH12	1.53	0.73
1:A:294:GLU:HG2	1:A:300:TYR:H	1.54	0.73
1:B:266:VAL:HG12	1:B:300:TYR:O	1.90	0.72
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.72	0.72
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.24	0.71
1:A:297:ASN:OD1	1:A:298:SER:N	2.24	0.70
1:A:383:SER:HB2	1:A:388:GLU:OE2	1.92	0.70
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.74	0.68
1:A:361:ASN:HA	1:A:414:LYS:HE2	1.76	0.67
1:A:268:HIS:O	1:A:269:GLU:CB	2.43	0.66
1:B:294:GLU:HB2	1:B:300:TYR:HE1	1.62	0.64
1:A:291:PRO:HB3	1:A:300:TYR:CZ	2.35	0.61
1:B:360:LYS:O	1:B:414:LYS:NZ	2.34	0.61
1:A:266:VAL:O	1:A:267:SER:CB	2.49	0.60
1:B:294:GLU:CB	1:B:300:TYR:HE1	2.16	0.59
1:A:248:LYS:NZ	1:A:380:GLU:OE2	2.26	0.58
1:B:314:LEU:O	1:B:338:LYS:NZ	2.36	0.58
1:A:297:ASN:CG	1:A:298:SER:H	2.12	0.57
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.87	0.56
1:A:383:SER:CB	1:A:388:GLU:OE2	2.54	0.56
1:A:378:ALA:HB3	1:A:428:MET:HB2	1.89	0.55
1:A:351:LEU:HB2	1:A:366:THR:HB	1.90	0.54
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:NZ	1:B:380:GLU:OE2	2.31	0.53
1:A:266:VAL:O	1:A:267:SER:HB3	2.08	0.52
1:B:266:VAL:HG13	1:B:300:TYR:O	2.10	0.52
1:B:248:LYS:HG3	1:B:428:MET:HE1	1.92	0.52
1:A:291:PRO:HB3	1:A:300:TYR:OH	2.11	0.51
1:A:240:VAL:C	1:A:241:PHE:HD2	2.19	0.51
1:B:294:GLU:CG	1:B:300:TYR:HE1	2.24	0.51
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.45	0.51
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.94	0.50
1:B:429:HIS:H	1:B:432:LEU:HD12	1.77	0.50
1:B:355:ARG:HA	1:B:358:MET:HG2	1.95	0.49
1:B:273:VAL:HG12	1:B:325:ASN:HD22	1.77	0.49
1:A:295:PHE:H	1:A:300:TYR:HB3	1.78	0.49
1:A:352:PRO:HG3	1:A:441:LEU:HD11	1.95	0.49
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.95	0.48
1:A:241:PHE:HE1	2:C:3:BMA:H2	1.80	0.47
1:A:309:LEU:HB2	1:A:312:ASP:HB2	1.95	0.47
1:A:291:PRO:O	1:A:292:ARG:HB2	2.13	0.47
1:B:388:GLU:HG3	1:B:410:LEU:HD11	1.97	0.47
1:B:294:GLU:HG3	1:B:300:TYR:CE1	2.50	0.46
1:B:274:LYS:NZ	1:B:276:ASN:OD1	2.49	0.46
1:B:262:VAL:HG22	1:B:303:VAL:HG13	1.97	0.46
1:A:318:GLU:HA	1:A:337:SER:HB3	1.98	0.45
1:B:249:ASP:OD1	1:B:255:ARG:NH2	2.45	0.45
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.98	0.45
1:A:350:THR:HB	1:A:441:LEU:HD22	1.99	0.44
1:A:278:TYR:HA	1:A:283:GLU:HA	1.99	0.44
1:A:295:PHE:CD2	1:A:295:PHE:O	2.70	0.44
1:A:297:ASN:OD1	1:A:297:ASN:N	2.51	0.44
1:B:294:GLU:CG	1:B:300:TYR:CE1	3.02	0.43
1:A:290:LYS:HB2	1:A:291:PRO:HD3	2.00	0.43
1:A:271:PRO:HB2	1:A:293:GLU:HG2	2.01	0.43
1:A:311:GLN:O	1:A:315:ASN:N	2.47	0.42
1:B:379:VAL:HG21	1:B:406:LEU:HD11	2.02	0.42
1:B:311:GLN:O	1:B:315:ASN:N	2.48	0.42
1:B:353:PRO:HG2	1:B:358:MET:HE1	2.01	0.42
1:B:353:PRO:CG	1:B:358:MET:HE1	2.50	0.42
1:A:274:LYS:HE2	1:A:324:SER:HB2	2.01	0.41
1:A:276:ASN:HB2	1:A:322:LYS:HB3	2.02	0.41
1:A:330:ALA:HA	1:A:331:PRO:HD3	1.90	0.41
1:A:415:SER:O	1:A:419:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LYS:HB3	1:B:338:LYS:HE2	1.84	0.41
1:B:297:ASN:OD1	3:D:8:FUC:H61	2.21	0.41
1:B:294:GLU:HB2	1:B:300:TYR:CE1	2.49	0.40
1:A:262:VAL:HA	1:A:303:VAL:HG22	2.03	0.40
1:A:311:GLN:HA	1:A:314:LEU:HB2	2.04	0.40
1:B:278:TYR:HB2	1:B:320:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/233 (86%)	188 (94%)	10 (5%)	3 (2%)	8	35
1	B	205/233 (88%)	199 (97%)	6 (3%)	0	100	100
All	All	406/466 (87%)	387 (95%)	16 (4%)	3 (1%)	18	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	A	290	LYS
1	A	271	PRO

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	190/215 (88%)	188 (99%)	2 (1%)	65	83
1	B	192/215 (89%)	186 (97%)	6 (3%)	35	68
All	All	382/430 (89%)	374 (98%)	8 (2%)	47	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	414	LYS
1	A	416	ARG
1	B	263	VAL
1	B	266	VAL
1	B	298	SER
1	B	348	VAL
1	B	355	ARG
1	B	382	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	419	GLN
1	B	311	GLN
1	B	347	GLN
1	B	389	ASN
1	B	433	HIS

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 ⓘ

13 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	2	14,14,15	0.75	0	17,19,21	1.19	1 (5%)
2	NAG	C	2	2	14,14,15	0.77	0	17,19,21	1.00	1 (5%)
2	BMA	C	3	2	11,11,12	0.60	0	15,15,17	1.54	3 (20%)
2	MAN	C	4	2	11,11,12	0.75	0	15,15,17	1.37	1 (6%)
2	NAG	C	5	2	14,14,15	0.94	1 (7%)	17,19,21	1.24	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.73	0	17,19,21	1.18	1 (5%)
3	NAG	D	2	3	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
3	BMA	D	3	3	11,11,12	0.58	0	15,15,17	1.55	3 (20%)
3	MAN	D	4	3	11,11,12	0.59	0	15,15,17	1.34	1 (6%)
3	NAG	D	5	3	14,14,15	0.47	0	17,19,21	1.12	2 (11%)
3	MAN	D	6	3	11,11,12	0.76	0	15,15,17	1.37	1 (6%)
3	NAG	D	7	3	14,14,15	0.94	1 (7%)	17,19,21	1.23	2 (11%)
3	FUC	D	8	3	10,10,11	0.57	0	14,14,16	1.09	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
2	NAG	C	1	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	4/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	NAG	D	7	3	-	0/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	NAG	O5-C5	-2.15	1.39	1.43
3	D	7	NAG	O5-C5	-2.14	1.39	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	MAN	C1-O5-C5	4.58	118.32	112.19
2	C	4	MAN	C1-O5-C5	4.57	118.31	112.19
3	D	4	MAN	C1-O5-C5	3.77	117.25	112.19
3	D	3	BMA	O3-C3-C4	-3.28	102.64	110.38
2	C	3	BMA	O3-C3-C4	-3.28	102.65	110.38
3	D	5	NAG	C1-O5-C5	3.21	116.49	112.19
2	C	5	NAG	O4-C4-C3	3.21	117.94	110.38
3	D	7	NAG	O4-C4-C3	3.19	117.91	110.38
3	D	3	BMA	C1-O5-C5	3.00	116.21	112.19
2	C	3	BMA	C1-O5-C5	2.98	116.18	112.19
2	C	3	BMA	O6-C6-C5	-2.71	102.09	111.33
3	D	3	BMA	O6-C6-C5	-2.70	102.14	111.33
2	C	2	NAG	C8-C7-N2	-2.23	112.42	116.12
3	D	2	NAG	C8-C7-N2	-2.23	112.42	116.12
2	C	1	NAG	C1-O5-C5	2.14	115.06	112.19
3	D	1	NAG	C1-O5-C5	2.09	114.99	112.19
3	D	5	NAG	O5-C1-C2	2.07	114.49	111.29
3	D	8	FUC	O2-C2-C1	2.06	113.94	109.22
2	C	5	NAG	O5-C5-C4	-2.04	105.87	110.83
3	D	7	NAG	O5-C5-C4	-2.01	105.95	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

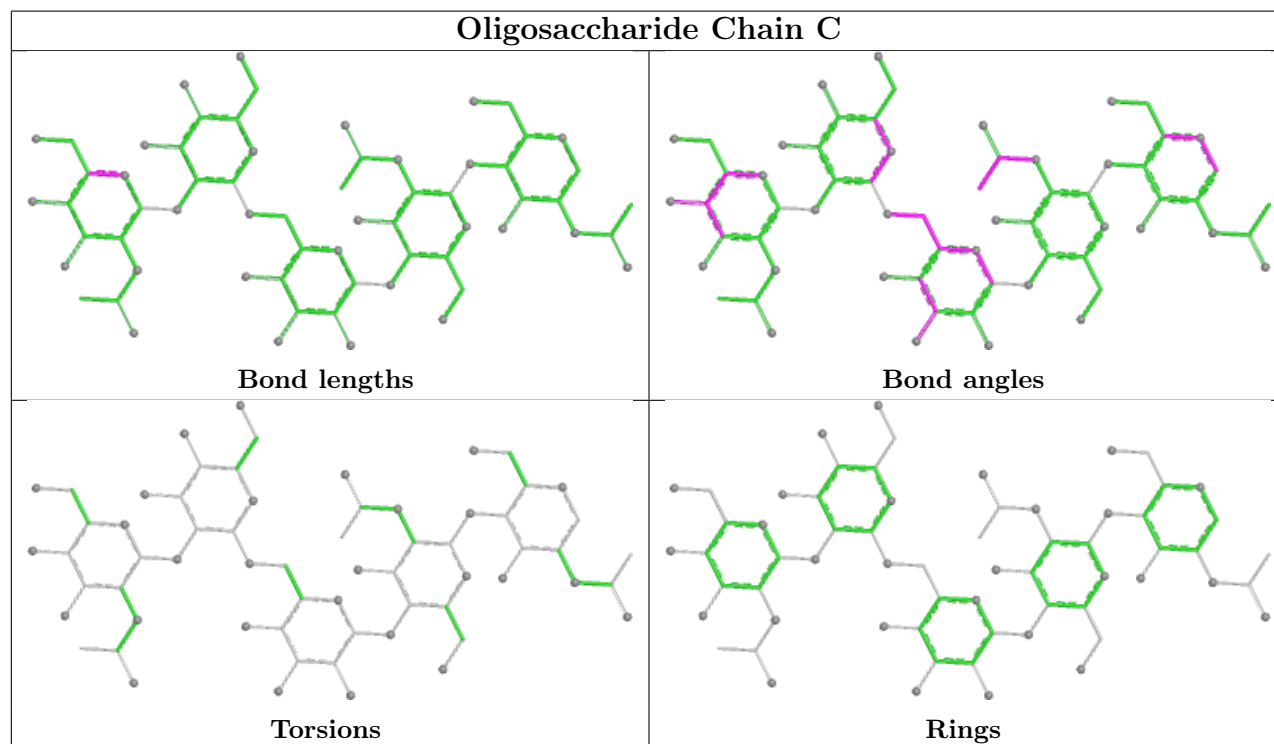
Mol	Chain	Res	Type	Atoms
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	5	NAG	C4-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6

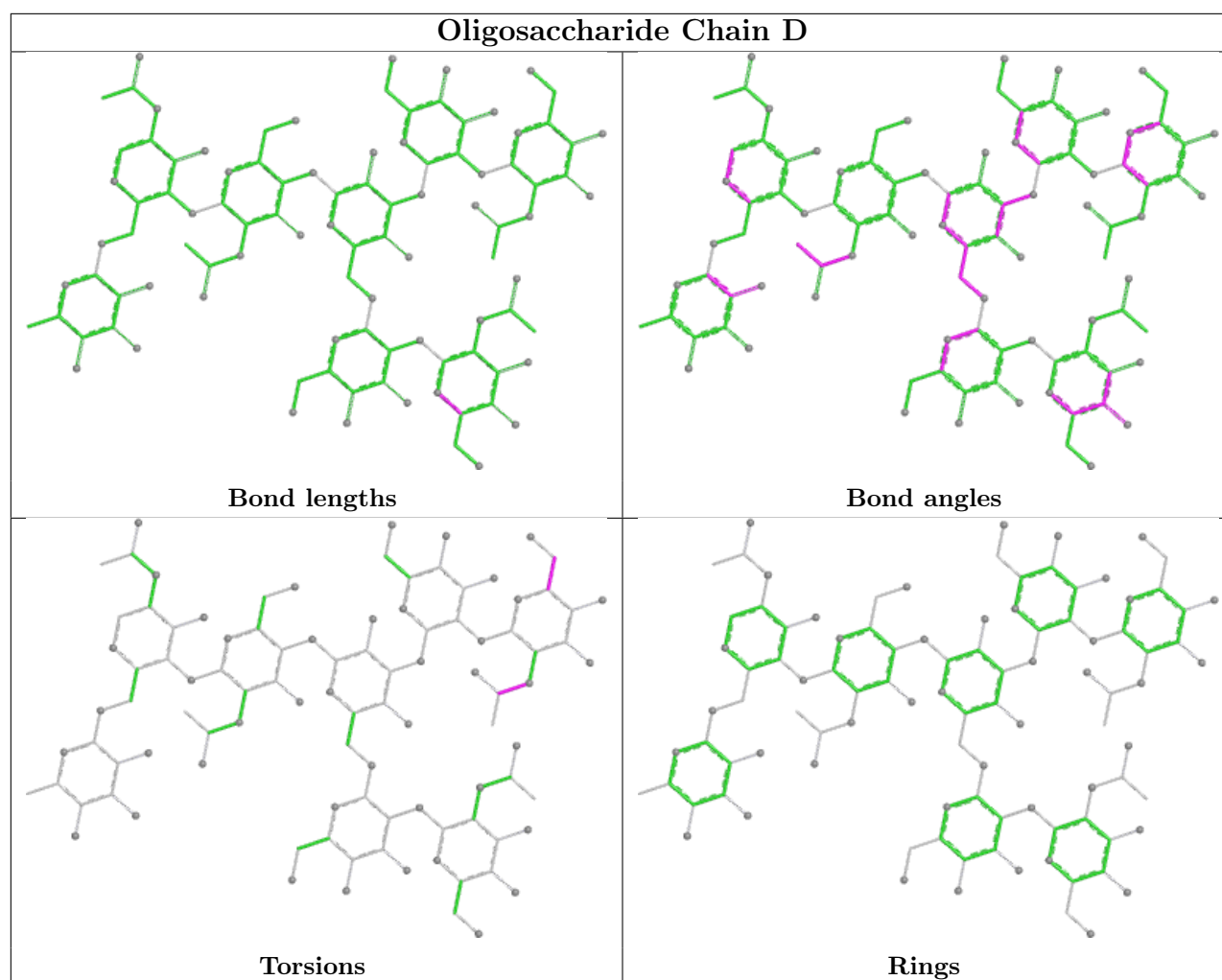
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	1	0
2	C	1	NAG	2	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](#)

1 ligand is 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	$\# Z > 2$
4	GOL	B	509	-	5,5,5	0.37	0	5,5,5	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
4	GOL	B	509	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	509	GOL	O1-C1-C2-O2
4	B	509	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	205/233 (87%)	1.15	35 (17%) 4 3	31, 67, 130, 143	0
1	B	207/233 (88%)	1.24	38 (18%) 3 2	31, 66, 106, 127	0
All	All	412/466 (88%)	1.19	73 (17%) 4 2	31, 67, 123, 143	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	4.4
1	A	303	VAL	4.3
1	B	389	ASN	4.2
1	B	385	GLY	4.2
1	B	295	PHE	4.1
1	B	271	PRO	4.1
1	A	240	VAL	4.0
1	A	288	LYS	3.6
1	A	408	SER	3.5
1	A	443	LEU	3.5
1	A	407	TYR	3.5
1	A	394	THR	3.4
1	B	406	LEU	3.4
1	B	407	TYR	3.4
1	B	300	TYR	3.2
1	B	273	VAL	3.1
1	B	359	THR	3.1
1	A	321	CYS	3.1
1	A	358	MET	3.0
1	A	297	ASN	3.0
1	B	296	ALA	3.0
1	B	368	LEU	3.0
1	A	285	HIS	2.9
1	B	440	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	436	TYR	2.7
1	A	403	SER	2.7
1	A	246	LYS	2.6
1	B	326	LYS	2.6
1	A	356	GLU	2.6
1	B	245	PRO	2.6
1	B	426	SER	2.5
1	A	266	VAL	2.5
1	B	284	VAL	2.5
1	B	325	ASN	2.5
1	B	268	HIS	2.5
1	A	242	LEU	2.5
1	B	292	ARG	2.5
1	A	277	TRP	2.4
1	B	410	LEU	2.4
1	B	381	TRP	2.4
1	A	289	THR	2.4
1	A	392	LYS	2.3
1	B	428	MET	2.3
1	A	409	LYS	2.3
1	B	330	ALA	2.2
1	A	432	LEU	2.2
1	B	242	LEU	2.2
1	A	271	PRO	2.2
1	A	397	VAL	2.2
1	B	358	MET	2.2
1	B	288	LYS	2.2
1	B	272	GLU	2.2
1	B	443	LEU	2.2
1	A	302	VAL	2.2
1	B	412	VAL	2.2
1	A	344	ARG	2.1
1	A	362	GLN	2.1
1	A	346	PRO	2.1
1	A	393	THR	2.1
1	A	296	ALA	2.1
1	A	245	PRO	2.1
1	A	323	VAL	2.1
1	B	329	PRO	2.1
1	B	398	LEU	2.1
1	B	294	GLU	2.1
1	B	324	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	GLU	2.1
1	A	406	LEU	2.1
1	A	300	TYR	2.1
1	B	297	ASN	2.1
1	A	368	LEU	2.0
1	B	394	THR	2.0
1	B	323	VAL	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](#)

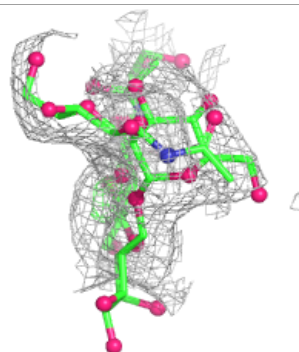
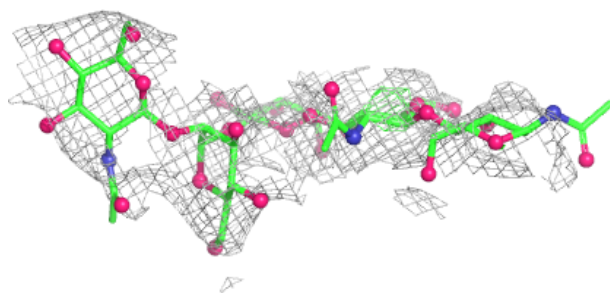
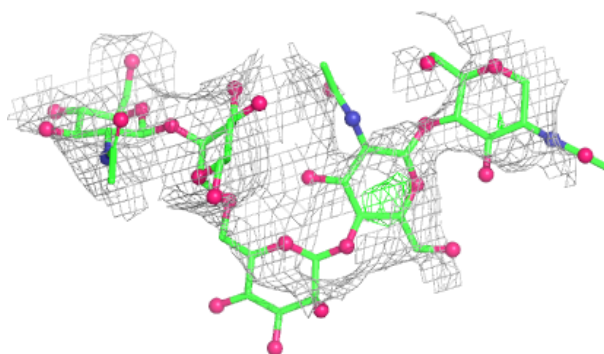
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

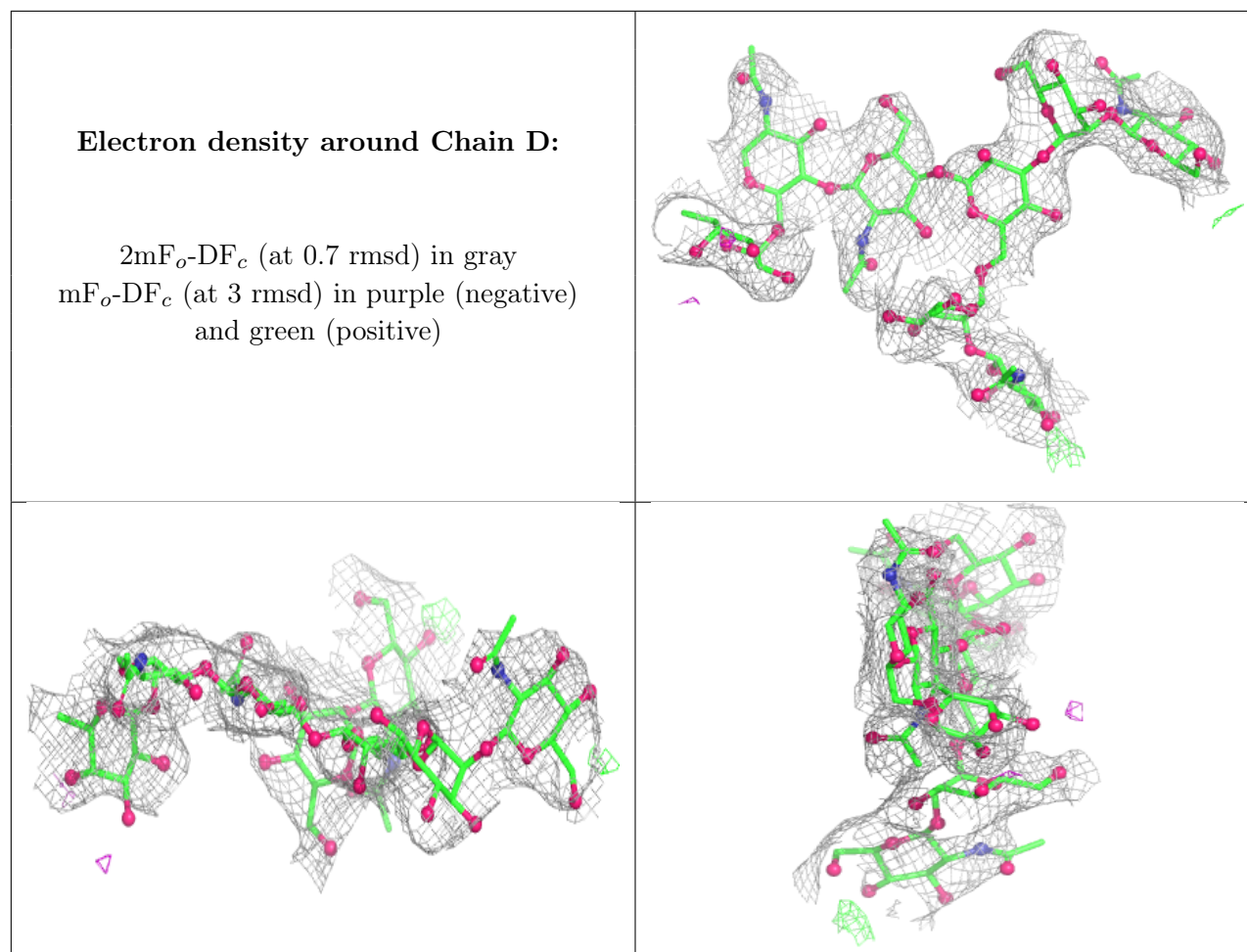
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.23	0.21	194,302,322,324	0
2	NAG	C	1	14/15	0.39	0.26	280,327,380,388	0
3	FUC	D	8	10/11	0.54	0.21	87,99,110,115	0
3	MAN	D	4	11/12	0.59	0.14	107,111,116,116	0
3	NAG	D	5	14/15	0.60	0.16	104,111,116,120	0
2	NAG	C	2	14/15	0.61	0.21	249,308,346,366	0
3	MAN	D	6	11/12	0.73	0.13	90,95,98,103	0
2	NAG	C	5	14/15	0.75	0.23	81,105,130,142	0
2	MAN	C	4	11/12	0.78	0.15	123,146,164,167	0
3	NAG	D	1	14/15	0.79	0.12	87,98,103,109	0
3	NAG	D	7	14/15	0.82	0.17	66,90,109,110	0
3	NAG	D	2	14/15	0.85	0.11	89,99,103,104	0
3	BMA	D	3	11/12	0.86	0.12	80,100,108,110	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](#)

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
4	GOL	B	509	6/6	0.58	0.27	61,83,85,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.