



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 AM UTC

PDB ID : 5F7N / pdb_00005f7n
Title : Blood group antigen binding adhesin BabA of Helicobacter pylori strain 17875
in complex with blood group A Lewis b pentasaccharide
Authors : Moonens, K.; Gideonsson, P.; Subedi, S.; Romao, E.; Oscarson, S.; Muylder-
mans, S.; Boren, T.; Remaut, H.
Deposited on : 2015-12-08
Resolution : 2.28 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

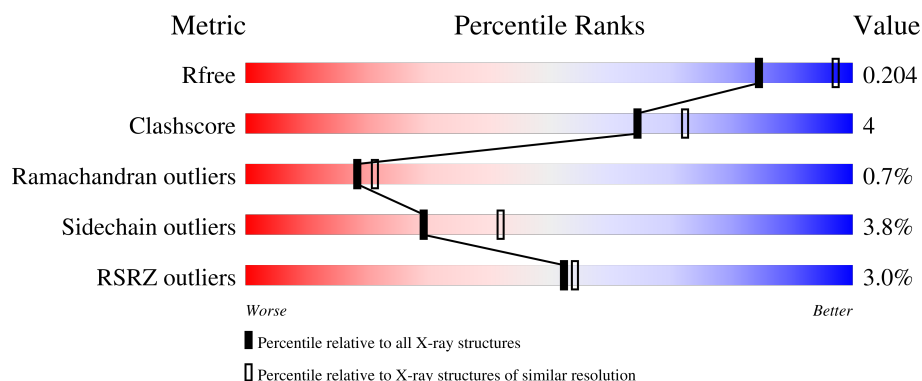
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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.



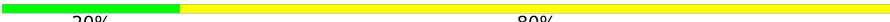
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	466	4% 79% 9% • 11%
1	B	466	3% 80% 9% • 10%
2	C	120	• 78% 15% • 6%
2	D	120	2% 87% 8% • •
3	E	5	100%

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Mol	Chain	Length	Quality of chain
3	F	5	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment on the left representing 20% and a yellow segment on the right representing 80%. The labels '20%' and '80%' are positioned below their respective segments.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8323 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 Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3098	1910	535	640	13			
1	B	420	Total	C	N	O	S	0	1	0
			3132	1930	540	649	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	461	GLY	-	expression tag	UNP O52269
A	462	SER	-	expression tag	UNP O52269
A	463	HIS	-	expression tag	UNP O52269

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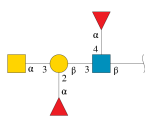
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Chain	Residue	Modelled	Actual	Comment	Reference
A	464	HIS	-	expression tag	UNP O52269
A	465	HIS	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
B	3	ALA	-	expression tag	UNP O52269
B	4	SER	-	expression tag	UNP O52269
B	5	TRP	-	expression tag	UNP O52269
B	6	SER	-	expression tag	UNP O52269
B	7	HIS	-	expression tag	UNP O52269
B	8	PRO	-	expression tag	UNP O52269
B	9	GLN	-	expression tag	UNP O52269
B	10	PHE	-	expression tag	UNP O52269
B	11	GLU	-	expression tag	UNP O52269
B	12	LYS	-	expression tag	UNP O52269
B	13	SER	-	expression tag	UNP O52269
B	14	GLY	-	expression tag	UNP O52269
B	15	GLY	-	expression tag	UNP O52269
B	16	GLY	-	expression tag	UNP O52269
B	17	GLY	-	expression tag	UNP O52269
B	18	GLY	-	expression tag	UNP O52269
B	19	LEU	-	expression tag	UNP O52269
B	20	VAL	-	expression tag	UNP O52269
B	21	PRO	-	expression tag	UNP O52269
B	22	ARG	-	expression tag	UNP O52269
B	23	GLY	-	expression tag	UNP O52269
B	24	SER	-	expression tag	UNP O52269
B	461	GLY	-	expression tag	UNP O52269
B	462	SER	-	expression tag	UNP O52269
B	463	HIS	-	expression tag	UNP O52269
B	464	HIS	-	expression tag	UNP O52269
B	465	HIS	-	expression tag	UNP O52269
B	466	HIS	-	expression tag	UNP O52269
B	467	HIS	-	expression tag	UNP O52269
B	468	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanobody Nb-ER19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	S	0	0	0
			863	540	155	163	5			
2	D	115	Total	C	N	O	S	0	0	0
			883	552	161	165	5			

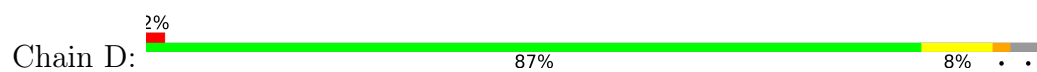
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



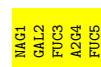
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			60	34	2	24			
3	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	71	Total	O	0	0
			71	71		
4	C	21	Total	O	0	0
			21	21		
4	D	54	Total	O	0	0
			54	54		



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.85Å 131.95Å 123.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	33.20 – 2.28 33.20 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.20-2.28) 98.5 (33.20-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.171 , 0.197 0.183 , 0.204	Depositor DCC
R_{free} test set	3651 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8323	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, GAL, A2G, FUC

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	1.28	3/3143 (0.1%)	1.15	15/4270 (0.4%)
1	B	1.24	4/3178 (0.1%)	1.10	9/4319 (0.2%)
2	C	1.25	1/882 (0.1%)	1.09	2/1195 (0.2%)
2	D	1.39	4/904 (0.4%)	1.10	1/1225 (0.1%)
All	All	1.27	12/8107 (0.1%)	1.12	27/11009 (0.2%)

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	B	0	1
2	D	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	CYS	C-O	-6.19	1.21	1.23
2	D	108	GLY	C-O	-5.91	1.15	1.23
2	D	72	ARG	C-O	-5.55	1.17	1.23
1	B	427	GLU	N-CA	-5.55	1.39	1.46
2	C	5	LEU	N-CA	-5.53	1.39	1.46
1	B	362	ALA	C-O	-5.47	1.17	1.24
1	A	47	ASN	N-CA	-5.23	1.40	1.46
2	D	45	LEU	CA-C	-5.19	1.46	1.53
2	D	62	ASP	C-O	-5.17	1.17	1.24
1	B	83	TYR	CA-CB	-5.12	1.45	1.53
1	A	104	THR	C-O	-5.11	1.17	1.24
1	A	101	GLY	C-O	-5.06	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	GLY	N-CA-C	-8.68	104.29	113.58
1	B	410	PRO	CA-C-N	-7.48	111.92	119.92
1	B	410	PRO	C-N-CA	-7.48	111.92	119.92
1	A	410	PRO	CA-C-N	-6.55	113.03	119.78
1	A	410	PRO	C-N-CA	-6.55	113.03	119.78
1	A	202	THR	N-CA-CB	-6.25	102.27	110.59
1	B	221	LYS	N-CA-C	6.23	118.24	108.96
2	C	49	VAL	N-CA-CB	-6.09	106.64	111.64
1	A	110	ALA	CA-C-N	-6.08	112.56	122.65
1	A	110	ALA	C-N-CA	-6.08	112.56	122.65
1	A	288	GLY	N-CA-C	5.78	124.13	112.34
1	A	340	LYS	N-CA-C	-5.77	102.81	110.07
1	A	243	VAL	N-CA-C	5.76	117.97	108.99
2	C	16	GLY	N-CA-C	-5.75	107.85	114.69
1	A	306	SER	CB-CA-C	-5.71	101.31	110.79
1	B	222	THR	N-CA-C	5.50	117.67	109.25
1	A	222	THR	N-CA-C	5.50	117.19	108.67
1	B	110	ALA	CA-C-N	-5.50	113.53	122.65
1	B	110	ALA	C-N-CA	-5.50	113.53	122.65
1	A	238	GLY	N-CA-C	-5.45	102.33	112.37
1	A	320	ASN	N-CA-C	5.40	117.92	111.71
1	A	292	GLU	N-CA-C	5.37	117.98	109.40
1	B	200	LYS	N-CA-CB	5.28	117.98	110.16
1	A	202	THR	CB-CA-C	5.22	117.49	109.03
2	D	29	ILE	CB-CA-C	-5.16	105.10	112.22
1	B	236	ALA	N-CA-C	-5.05	103.38	110.50
1	A	274	ASN	N-CA-C	5.01	116.75	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	286	SER	Peptide
2	D	3	VAL	Peptide

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	3098	0	3028	23	0
1	B	3132	0	3057	28	0
2	C	863	0	845	8	0
2	D	883	0	859	2	0
3	E	60	0	53	0	0
3	F	60	0	53	0	0
4	A	81	0	0	1	0
4	B	71	0	0	1	0
4	C	21	0	0	1	0
4	D	54	0	0	0	0
All	All	8323	0	7895	61	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 4.

All (61) 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:279:TYR:OH	1:A:295:ARG:NH1	1.99	0.95
1:A:129:ARG:NH1	4:A:601:HOH:O	2.04	0.90
1:A:202:THR:HG22	1:A:204:VAL:H	1.42	0.84
1:A:111:ASN:OD1	1:A:113:GLN:HB2	1.79	0.82
1:A:198:SER:O	1:A:202:THR:HB	1.79	0.81
1:B:311:MET:HE1	1:B:375:ILE:HD13	1.68	0.75
2:C:3:VAL:N	2:C:26:SER:HG	1.84	0.75
1:B:260[A]:GLN:CD	1:B:260[A]:GLN:H	1.94	0.74
1:A:311:MET:HE1	1:A:375:ILE:HD13	1.70	0.72
1:B:258:SER:HB2	1:B:260[A]:GLN:OE1	1.94	0.67
1:B:34:GLU:HG3	1:B:35:ASN:HB3	1.77	0.67
1:B:129:ARG:NH1	4:B:601:HOH:O	2.30	0.65
2:C:72:ARG:HD3	2:C:74:ASN:OD1	1.96	0.65
1:B:258:SER:CB	1:B:260[A]:GLN:OE1	2.45	0.64
1:B:398:LYS:HZ1	1:B:409:SER:HG	1.49	0.60
1:A:308:ILE:HA	1:A:311:MET:HE3	1.84	0.58
1:B:308:ILE:HA	1:B:311:MET:HE3	1.86	0.58
1:B:34:GLU:CG	1:B:35:ASN:HB3	2.35	0.57
2:C:73:ASP:OD2	2:C:76:LYS:HD3	2.04	0.56
1:B:398:LYS:NZ	1:B:409:SER:OG	2.36	0.55
1:B:282:VAL:HG11	1:B:291:MET:HG2	1.88	0.54
1:B:111:ASN:HB3	1:B:113:GLN:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:HG2	1:B:35:ASN:N	2.22	0.54
1:B:218:ILE:HD11	1:B:256:PRO:HG2	1.90	0.54
1:A:282:VAL:HG11	1:A:291:MET:HG2	1.90	0.53
1:B:398:LYS:CE	1:B:398:LYS:HA	2.39	0.53
1:A:42:ARG:HG3	1:A:43:TYR:CE2	2.43	0.53
1:A:156:LEU:C	1:A:156:LEU:HD23	2.34	0.53
2:C:72:ARG:CD	2:C:74:ASN:OD1	2.56	0.52
1:B:156:LEU:C	1:B:156:LEU:HD23	2.35	0.52
1:B:34:GLU:HG3	1:B:35:ASN:CB	2.41	0.51
1:B:34:GLU:CG	1:B:35:ASN:N	2.74	0.51
1:A:240:THR:HG22	1:A:241:THR:N	2.27	0.49
1:A:111:ASN:CG	1:A:113:GLN:HG2	2.37	0.49
1:A:239:ASN:OD1	1:A:241:THR:HG22	2.11	0.49
1:A:202:THR:HG23	1:A:204:VAL:HG23	1.95	0.49
1:B:273:ILE:HG23	1:B:298:LEU:HD23	1.95	0.48
1:B:218:ILE:HD12	1:B:219:ASP:HB2	1.95	0.48
1:B:258:SER:OG	1:B:260[A]:GLN:OE1	2.23	0.48
1:A:279:TYR:HH	1:A:295:ARG:HH11	1.60	0.47
1:A:273:ILE:HG23	1:A:298:LEU:HD23	1.96	0.47
1:A:42:ARG:HG3	1:A:43:TYR:CD2	2.50	0.47
1:B:218:ILE:O	1:B:219:ASP:C	2.58	0.47
1:B:240:THR:HG22	1:B:241:THR:N	2.29	0.47
1:A:410:PRO:O	1:A:413:THR:HG23	2.16	0.46
2:C:40:GLN:NE2	4:C:201:HOH:O	2.38	0.44
2:C:19:LEU:HB2	2:C:83:MET:HE3	2.00	0.43
2:C:38:TYR:OH	2:C:99:LEU:HD22	2.18	0.43
1:B:410:PRO:O	1:B:413:THR:HG23	2.18	0.42
2:C:83:MET:HB3	2:C:86:LEU:HD21	2.00	0.42
1:A:235:GLN:HA	1:A:235:GLN:OE1	2.19	0.42
1:B:240:THR:O	1:B:242:ARG:N	2.52	0.42
1:A:318:LEU:C	1:A:318:LEU:HD23	2.45	0.42
1:A:111:ASN:OD1	1:A:111:ASN:N	2.45	0.42
1:B:216:GLN:NE2	1:B:218:ILE:HG22	2.35	0.41
1:B:398:LYS:HA	1:B:398:LYS:HD3	1.82	0.41
1:A:82:ALA:HB1	1:A:318:LEU:HD21	2.03	0.41
2:D:83:MET:HB3	2:D:86:LEU:HD21	2.01	0.41
1:A:292:GLU:HA	1:A:293:PRO:C	2.44	0.40
1:B:287:GLY:O	1:B:288:GLY:O	2.39	0.40
2:D:38:TYR:OH	2:D:99:LEU:HD22	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	411/466 (88%)	396 (96%)	13 (3%)	2 (0%)	24	29
1	B	417/466 (90%)	399 (96%)	13 (3%)	5 (1%)	10	10
2	C	111/120 (92%)	110 (99%)	1 (1%)	0	100	100
2	D	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
All	All	1052/1172 (90%)	1017 (97%)	28 (3%)	7 (1%)	18	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	GLY
1	B	218	ILE
1	B	219	ASP
1	B	288	GLY
1	B	241	THR
1	A	242	ARG
1	B	289	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	343/381 (90%)	332 (97%)	11 (3%)	34	49
1	B	347/381 (91%)	333 (96%)	14 (4%)	28	40
2	C	92/99 (93%)	87 (95%)	5 (5%)	20	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	94/99 (95%)	91 (97%)	3 (3%)	34	49
All	All	876/960 (91%)	843 (96%)	33 (4%)	29	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	46	LEU
1	A	200	LYS
1	A	202	THR
1	A	227	ILE
1	A	240	THR
1	A	243	VAL
1	A	294	THR
1	A	298	LEU
1	A	334	VAL
1	A	383	THR
1	B	44	SER
1	B	46	LEU
1	B	178	ASN
1	B	199	LYS
1	B	200	LYS
1	B	206	ASP
1	B	218	ILE
1	B	227	ILE
1	B	230	LYS
1	B	240	THR
1	B	243	VAL
1	B	298	LEU
1	B	334	VAL
1	B	398	LYS
2	C	14	GLN
2	C	29	ILE
2	C	96	CYS
2	C	99	LEU
2	C	103	ARG
2	D	29	ILE
2	D	96	CYS
2	D	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	157	ASN
1	A	161	GLN
1	A	196	ASN
1	A	274	ASN
1	A	316	GLN
1	A	321	GLN
1	A	337	ASN
1	A	361	GLN
1	B	196	ASN
1	B	216	GLN
1	B	274	ASN
1	B	316	GLN
1	B	321	GLN
1	B	373	GLN
2	C	40	GLN
2	C	77	ASN
2	C	82	GLN
2	D	40	GLN
2	D	82	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 ⓘ

10 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	E	1	3	15,15,15	0.74	0	21,21,21	2.33	8 (38%)
3	GAL	E	2	3	11,11,12	0.96	0	15,15,17	1.33	2 (13%)
3	FUC	E	3	3	10,10,11	0.82	0	14,14,16	1.51	4 (28%)
3	A2G	E	4	3	14,14,15	0.78	0	17,19,21	1.40	4 (23%)
3	FUC	E	5	3	10,10,11	0.79	0	14,14,16	1.52	3 (21%)
3	NAG	F	1	3	15,15,15	0.65	0	21,21,21	1.00	1 (4%)
3	GAL	F	2	3	11,11,12	1.39	2 (18%)	15,15,17	2.60	6 (40%)
3	FUC	F	3	3	10,10,11	0.87	0	14,14,16	0.81	0
3	A2G	F	4	3	14,14,15	0.67	0	17,19,21	2.09	6 (35%)
3	FUC	F	5	3	10,10,11	0.70	0	14,14,16	1.21	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	E	1	3	-	0/6/26/26	0/1/1/1
3	GAL	E	2	3	-	0/2/19/22	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
3	A2G	E	4	3	-	0/6/23/26	0/1/1/1
3	FUC	E	5	3	-	-	0/1/1/1
3	NAG	F	1	3	-	0/6/26/26	0/1/1/1
3	GAL	F	2	3	-	2/2/19/22	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
3	A2G	F	4	3	-	3/6/23/26	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	GAL	O5-C1	-2.50	1.39	1.43
3	F	2	GAL	C2-C3	2.26	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-C2-N2	6.21	117.92	110.73
3	F	2	GAL	C1-O5-C5	5.49	119.55	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-C2-C3	-5.27	103.35	110.54
3	F	4	A2G	O5-C1-C2	-4.89	103.73	111.29
3	F	2	GAL	C1-C2-C3	4.69	116.47	109.64
3	F	2	GAL	O5-C5-C6	-3.98	99.92	107.66
3	F	4	A2G	O3-C3-C2	3.66	117.01	109.40
3	F	2	GAL	C3-C4-C5	3.34	116.28	110.23
3	E	1	NAG	O5-C1-C2	-3.32	106.18	109.52
3	F	1	NAG	O7-C7-N2	2.82	126.96	121.98
3	F	4	A2G	C1-O5-C5	2.76	115.88	112.19
3	E	1	NAG	C3-C4-C5	2.66	115.05	110.23
3	E	5	FUC	C2-C3-C4	-2.58	106.32	110.86
3	E	2	GAL	O5-C5-C6	2.58	112.69	107.66
3	F	2	GAL	O5-C5-C4	2.58	117.11	110.83
3	E	2	GAL	C1-C2-C3	2.52	113.31	109.64
3	E	3	FUC	O4-C4-C3	-2.52	104.44	110.38
3	E	5	FUC	O3-C3-C4	2.50	116.27	110.38
3	E	1	NAG	O1-C1-C2	2.47	114.35	109.22
3	E	3	FUC	O4-C4-C5	2.45	115.15	109.74
3	F	4	A2G	C4-C3-C2	-2.43	107.45	111.02
3	E	4	A2G	O6-C6-C5	-2.39	103.20	111.33
3	E	4	A2G	O5-C5-C4	2.28	116.37	110.83
3	E	4	A2G	C1-C2-N2	-2.27	106.85	110.43
3	F	2	GAL	O4-C4-C3	-2.24	105.09	110.38
3	F	4	A2G	O5-C5-C4	2.16	116.08	110.83
3	F	4	A2G	O7-C7-N2	2.15	125.79	121.98
3	E	4	A2G	C1-O5-C5	2.07	114.96	112.19
3	E	3	FUC	C6-C5-C4	2.07	116.86	113.08
3	E	1	NAG	O5-C5-C4	-2.04	106.02	109.70
3	E	1	NAG	C6-C5-C4	2.04	118.03	113.02
3	E	3	FUC	C1-C2-C3	2.04	112.61	109.64
3	E	1	NAG	O7-C7-C8	-2.02	118.45	122.05
3	E	5	FUC	O5-C5-C6	2.02	111.78	107.40
3	F	5	FUC	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	GAL	O5-C5-C6-O6
3	F	2	GAL	C4-C5-C6-O6
3	F	4	A2G	C1-C2-N2-C7
3	F	4	A2G	C3-C2-N2-C7

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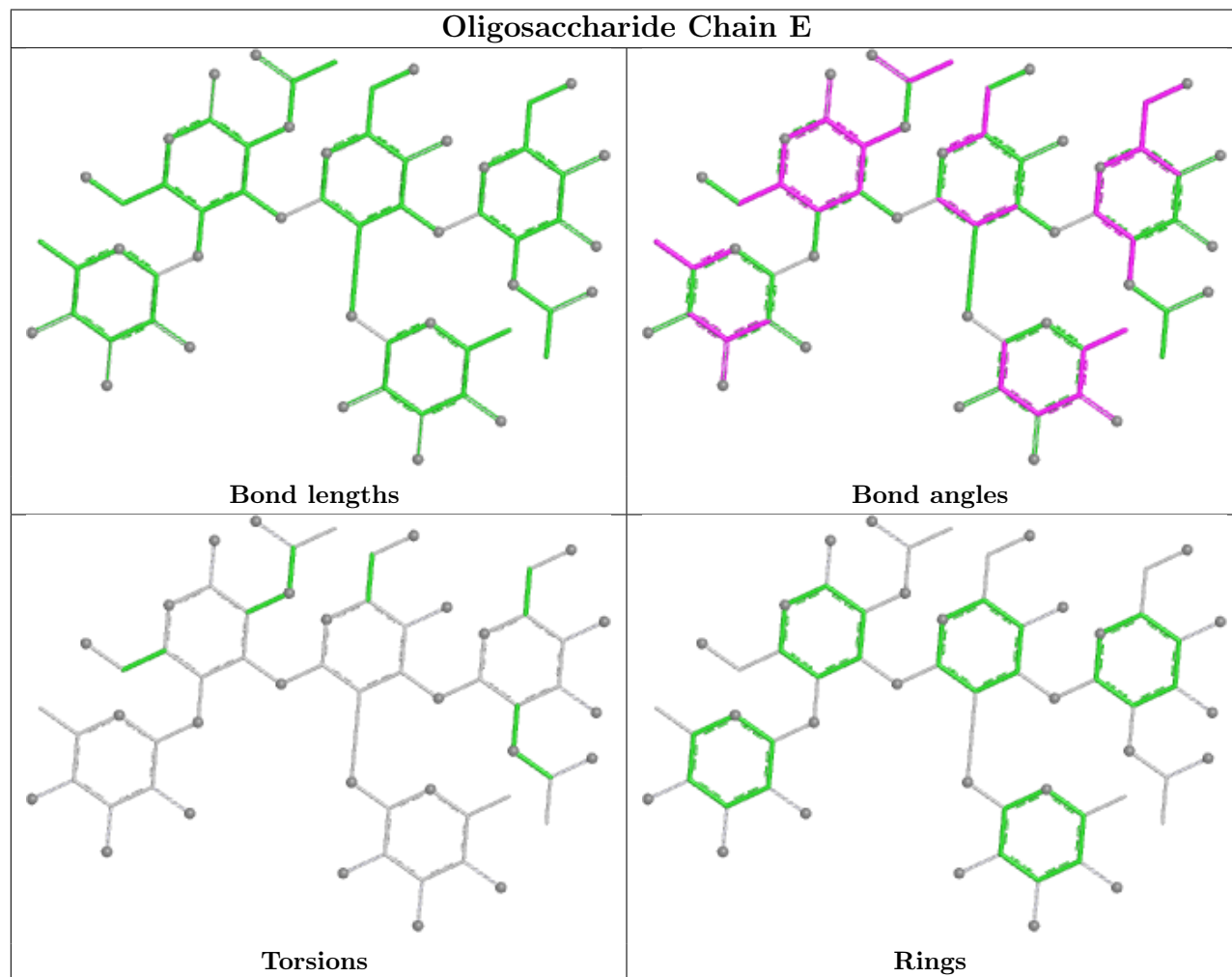
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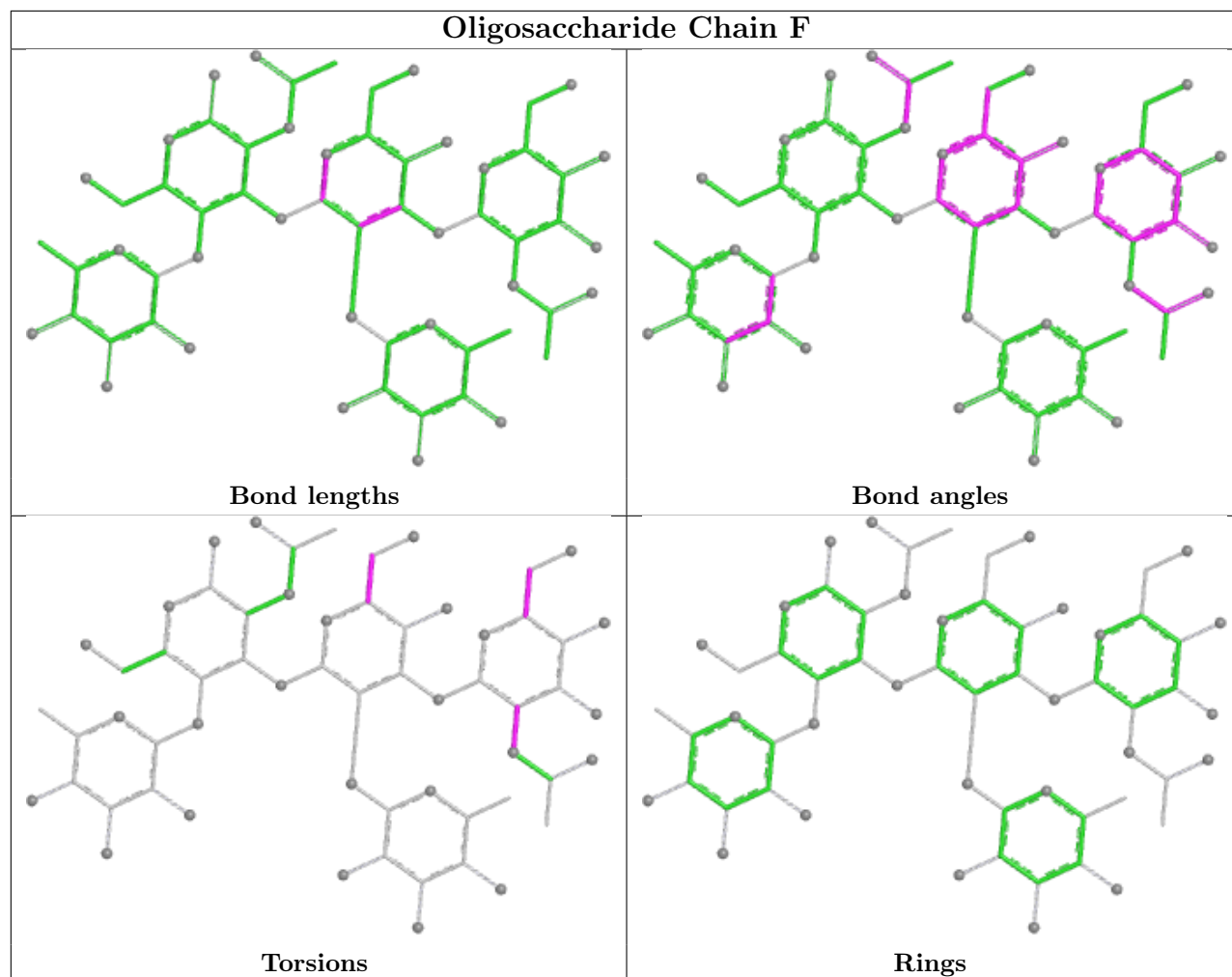
Mol	Chain	Res	Type	Atoms
3	F	4	A2G	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	417/466 (89%)	-0.02	17 (4%) 41 43	36, 53, 98, 126	0
1	B	420/466 (90%)	0.05	12 (2%) 53 55	26, 56, 103, 121	1 (0%)
2	C	113/120 (94%)	-0.18	1 (0%) 81 82	39, 53, 72, 102	0
2	D	115/120 (95%)	-0.26	2 (1%) 69 70	33, 45, 66, 105	0
All	All	1065/1172 (90%)	-0.04	32 (3%) 52 54	26, 53, 99, 126	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	VAL	6.4
2	D	3	VAL	3.8
1	B	218	ILE	3.8
1	A	340	LYS	3.6
1	A	398	LYS	3.6
2	D	117	HIS	3.3
1	B	207	GLN	3.2
1	A	217	THR	3.0
1	A	35	ASN	2.8
1	B	197	CYS	2.8
1	A	335	GLY	2.7
1	A	285	LYS	2.7
1	B	293	PRO	2.7
1	A	41	THR	2.7
1	A	283	THR	2.6
1	B	220	GLY	2.6
1	A	289	PRO	2.5
1	A	221	LYS	2.4
1	A	294	THR	2.4
1	B	200	LYS	2.4
1	B	329	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	38	LYS	2.3
1	A	295	ARG	2.3
1	A	293	PRO	2.3
1	A	220	GLY	2.2
1	B	408	GLY	2.2
1	B	398	LYS	2.2
1	A	240	THR	2.1
1	A	288	GLY	2.1
1	B	241	THR	2.1
1	B	34	GLU	2.0
1	B	221	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](#)

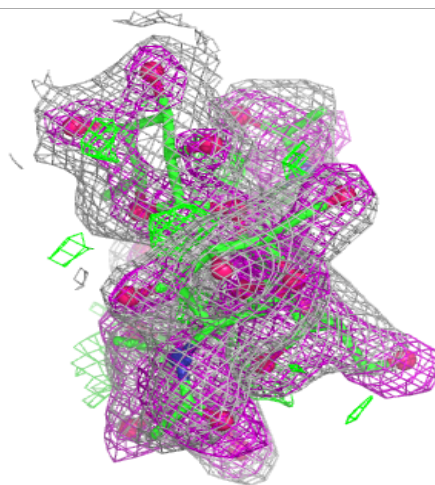
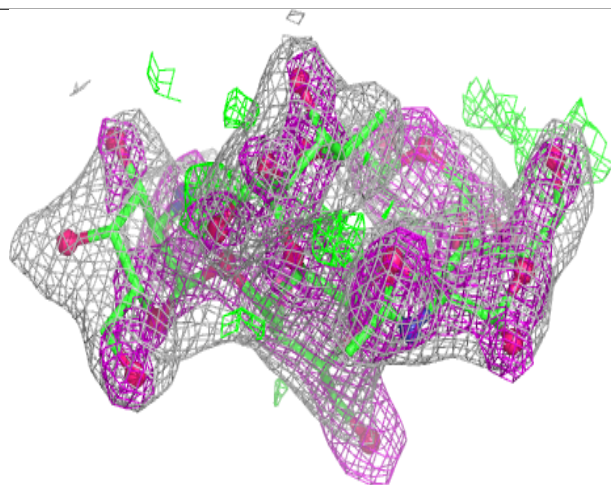
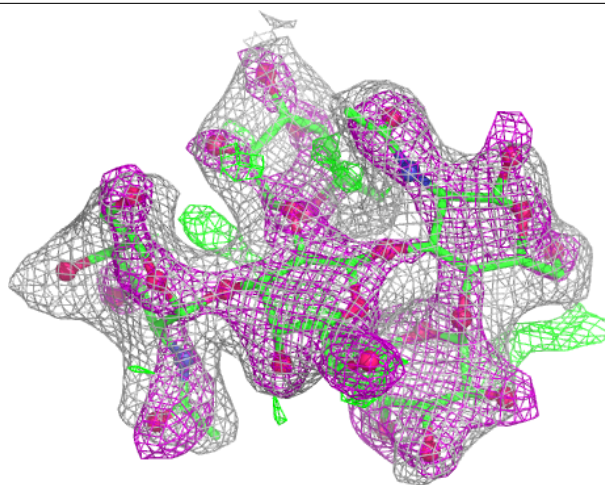
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

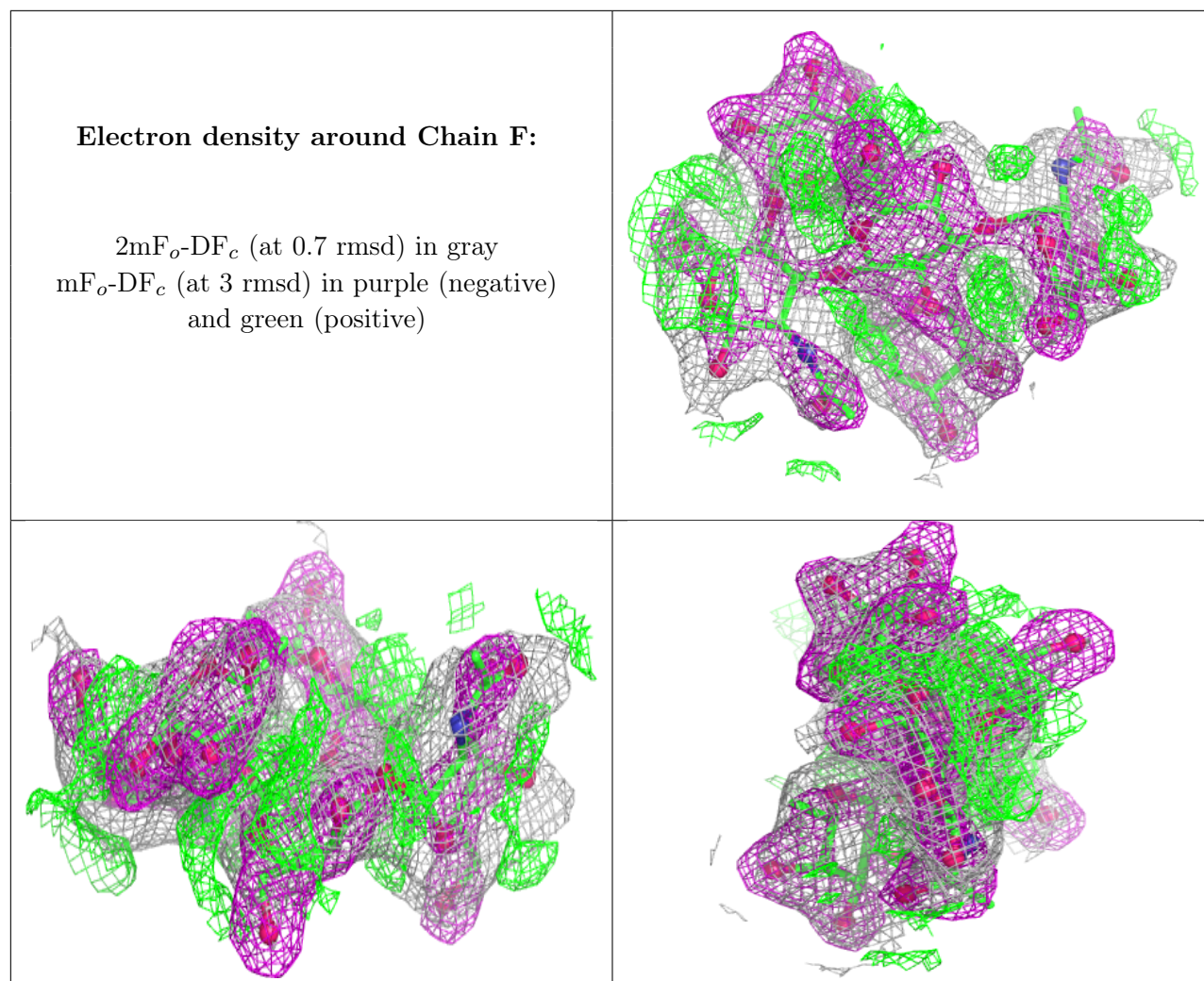
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A2G	F	4	14/15	0.64	0.18	44,50,69,72	0
3	NAG	F	1	15/15	0.68	0.16	44,50,53,54	0
3	GAL	F	2	11/12	0.69	0.15	38,41,44,48	0
3	FUC	F	5	10/11	0.70	0.17	43,44,46,46	0
3	A2G	E	4	14/15	0.79	0.13	37,46,52,54	0
3	FUC	E	5	10/11	0.81	0.14	43,49,51,51	0
3	FUC	F	3	10/11	0.81	0.14	39,42,44,44	0
3	GAL	E	2	11/12	0.82	0.13	33,42,47,51	0
3	NAG	E	1	15/15	0.83	0.13	43,49,53,58	0
3	FUC	E	3	10/11	0.86	0.11	30,35,37,39	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 E:

$2mF_o-DF_c$ (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.