



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:55 AM UTC

PDB ID : 6IFJ / pdb_00006ifj
Title : Structure of bispecific Fc
Authors : Qian, X.; Lescar, J.; Sasisekahrán, R.
Deposited on : 2018-09-20
Resolution : 2.40 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

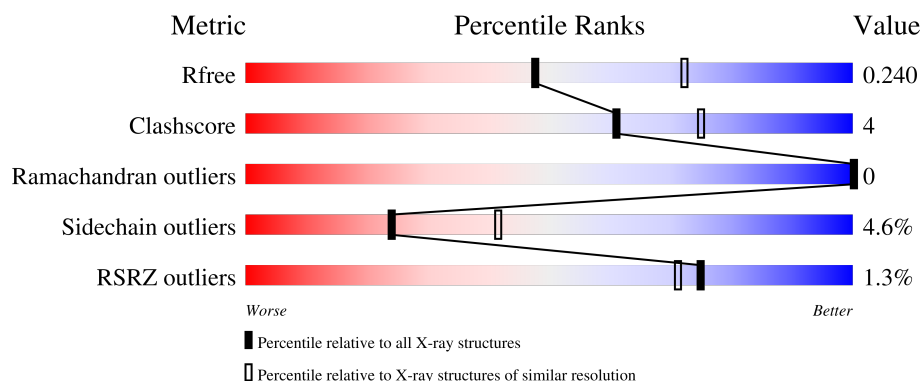
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	8% 75% 14% 10%
2	B	232	79% 10% 9%
3	C	13	77% 23%
3	D	13	8% 77% 23%
4	E	7	14% 86%

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Mol	Chain	Length	Quality of chain
4	F	7	 71% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4125 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	209	Total	C	N	O	S	0	0	0
			1670	1062	284	318	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	LYS	GLU	engineered mutation	UNP P0DOX5
A	409	ARG	LYS	engineered mutation	UNP P0DOX5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	2	0
			1691	1074	283	328	6			

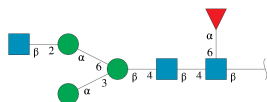
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	370	GLU	LYS	engineered mutation	UNP P0DOX5

- Molecule 3 is a protein called 13-mer peptide.

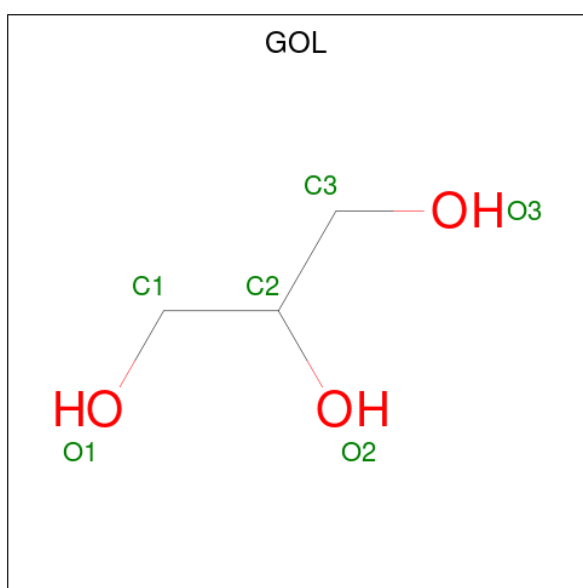
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	S	0	0	0
			107	69	17	19	2			
3	D	13	Total	C	N	O	S	0	0	0
			107	69	17	19	2			

- Molecule 4 is an oligosaccharide called 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
4	E	7	Total	C	N	O	0	0	0
			85	48	3	34			
4	F	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

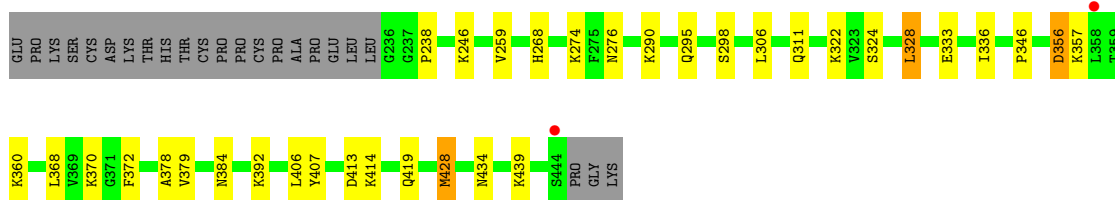


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

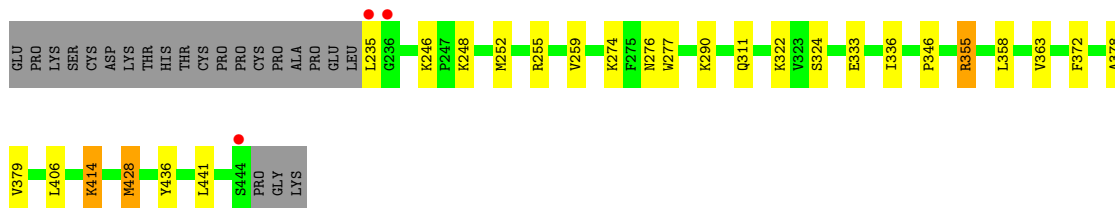
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total 171	O 171	0	0
6	B	163	Total 163	O 163	0	0
6	C	10	Total 10	O 10	0	0
6	D	6	Total 6	O 6	0	0

- Molecule 1: Immunoglobulin gamma-1 heavy chain

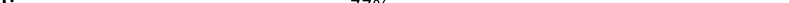


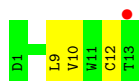
Chain B:  79% 10% 9% 2%



Chain C: 77% 23%



Chain D:  8% 77% 23%

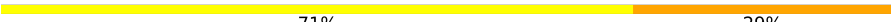


nose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  14% 86%

NAG1	NAG2	BNA3	MAN4	NAG5	MAN6	FUC7
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● Molecule 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

Chain F:  71% 29%

NAG1	NAG2	BNA3	MAN4	NAG5	MAN6	FUC7
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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	60.66Å 67.26Å 78.73Å 90.00° 106.23° 90.00°	Depositor
Resolution (Å)	37.18 – 2.40 37.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.18-2.40) 99.8 (37.18-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.171 , 0.231 0.176 , 0.240	Depositor DCC
R_{free} test set	1228 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.8	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	0.95	EDS
Total number of atoms	4125	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% 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: BMA, FUC, GOL, MAN, NAG

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	0.90	1/1716 (0.1%)	1.18	4/2337 (0.2%)
2	B	0.88	1/1737 (0.1%)	1.16	0/2367
3	C	0.72	0/111	1.03	0/151
3	D	0.73	0/111	1.01	0/151
All	All	0.88	2/3675 (0.1%)	1.16	4/5006 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	428	MET	SD-CE	-6.00	1.64	1.79
1	A	428	MET	SD-CE	-5.52	1.65	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	HIS	CA-C-N	5.58	128.22	120.29
1	A	268	HIS	C-N-CA	5.58	128.22	120.29
1	A	356	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	413	ASP	CA-CB-CG	5.08	117.68	112.60

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	1670	0	1640	15	0
2	B	1691	0	1646	12	0
3	C	107	0	93	2	0
3	D	107	0	93	2	0
4	E	85	0	73	1	0
4	F	85	0	73	2	0
5	A	18	0	24	3	0
5	B	12	0	16	0	0
6	A	171	0	0	0	0
6	B	163	0	0	0	0
6	C	10	0	0	0	0
6	D	6	0	0	0	0
All	All	4125	0	3658	31	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 (31) 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)
4:F:1:NAG:H61	4:F:7:FUC:H5	1.43	0.98
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.59	0.84
2:B:252:MET:HE3	2:B:255:ARG:HG3	1.61	0.79
4:F:1:NAG:H61	4:F:7:FUC:C5	2.20	0.70
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.84	0.58
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.88	0.56
2:B:274:LYS:HB3	2:B:324:SER:HB2	1.87	0.55
2:B:276:ASN:HB2	2:B:322:LYS:HB3	1.89	0.54
2:B:322:LYS:HG3	2:B:333:GLU:HG2	1.90	0.53
2:B:363:VAL:HG13	2:B:414:LYS:HG3	1.92	0.51
1:A:322:LYS:HG3	1:A:333:GLU:HG2	1.93	0.51
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.92	0.51
1:A:392:LYS:HA	5:A:510:GOL:H32	1.92	0.50
1:A:259:VAL:HG23	1:A:306:LEU:HB3	1.93	0.50
2:B:346:PRO:HB3	2:B:372:PHE:HB3	1.93	0.48
1:A:379:VAL:HG21	1:A:406:LEU:HD11	1.97	0.47
2:B:379:VAL:HG21	2:B:406:LEU:HD11	1.97	0.45
2:B:378:ALA:HB3	2:B:428:MET:HB2	1.98	0.44
2:B:248:LYS:HG2	2:B:252:MET:HE2	2.00	0.43
2:B:355:ARG:HA	2:B:358:LEU:HD12	1.99	0.43
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.54	0.42
1:A:378:ALA:HB3	1:A:428:MET:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LEU:HD11	3:C:12:CYS:SG	2.59	0.42
1:A:360:LYS:O	1:A:414:LYS:HD3	2.19	0.42
2:B:436:TYR:HB2	3:D:10:VAL:HG11	2.02	0.42
1:A:295:GLN:HE21	4:E:1:NAG:H62	1.84	0.41
1:A:439:LYS:HE3	5:A:509:GOL:O2	2.21	0.41
1:A:392:LYS:HD3	5:A:510:GOL:H11	2.01	0.41
3:D:9:LEU:HD11	3:D:12:CYS:SG	2.60	0.41
2:B:259:VAL:HG12	2:B:277:TRP:CH2	2.55	0.41
1:A:434:ASN:ND2	3:C:13:THR:HG23	2.36	0.41

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	207/232 (89%)	205 (99%)	2 (1%)	0	100	100
2	B	210/232 (90%)	208 (99%)	2 (1%)	0	100	100
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
3	D	11/13 (85%)	11 (100%)	0	0	100	100
All	All	439/490 (90%)	434 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	194/215 (90%)	183 (94%)	11 (6%)	18	33
2	B	197/215 (92%)	189 (96%)	8 (4%)	27	46
3	C	11/11 (100%)	11 (100%)	0	100	100
3	D	11/11 (100%)	11 (100%)	0	100	100
All	All	413/452 (91%)	394 (95%)	19 (5%)	24	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	290	LYS
1	A	298	SER
1	A	311	GLN
1	A	328	LEU
1	A	336	ILE
1	A	356	ASP
1	A	357	LYS
1	A	370	LYS
1	A	384	ASN
1	A	419	GLN
2	B	235	LEU
2	B	246	LYS
2	B	290	LYS
2	B	311	GLN
2	B	336	ILE
2	B	355	ARG
2	B	414	LYS
2	B	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	325	ASN
1	A	384	ASN
1	A	389	ASN
1	A	434	ASN
1	A	438	GLN
2	B	310	HIS
2	B	325	ASN

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Mol	Chain	Res	Type
2	B	389	ASN
2	B	438	GLN
3	C	5	HIS
3	D	5	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	5	4	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
4	NAG	F	1	4,2	14,14,15	0.39	0	17,19,21	2.05	3 (17%)
4	FUC	F	7	4	10,10,11	0.67	0	14,14,16	1.42	3 (21%)
4	MAN	E	4	4	11,11,12	0.46	0	15,15,17	1.03	1 (6%)
4	FUC	E	7	4	10,10,11	0.53	0	14,14,16	0.76	0
4	MAN	F	4	4	11,11,12	0.37	0	15,15,17	0.95	1 (6%)
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.98	1 (5%)
4	MAN	E	6	4	11,11,12	0.38	0	15,15,17	0.92	1 (6%)
4	NAG	F	5	4	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
4	MAN	F	6	4	11,11,12	0.36	0	15,15,17	0.93	1 (6%)
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.29	0	17,19,21	0.57	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	NAG	E	5	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	FUC	F	7	4	-	-	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	FUC	E	7	4	-	-	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	NAG	F	5	4	-	2/6/23/26	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	6.96	121.51	112.19
4	F	7	FUC	C1-C2-C3	3.71	115.05	109.64
4	E	4	MAN	C1-O5-C5	3.46	116.82	112.19
4	F	4	MAN	C1-O5-C5	3.33	116.65	112.19
4	E	5	NAG	C1-O5-C5	3.32	116.64	112.19
4	F	6	MAN	C1-O5-C5	3.30	116.61	112.19
4	E	6	MAN	C1-O5-C5	3.23	116.52	112.19
4	F	5	NAG	C1-O5-C5	2.62	115.69	112.19
4	F	7	FUC	C6-C5-C4	2.56	117.76	113.08
4	E	2	NAG	O5-C1-C2	-2.53	107.37	111.29
4	F	1	NAG	C3-C4-C5	2.40	114.58	110.23
4	F	1	NAG	C6-C5-C4	-2.33	107.29	113.02
4	F	7	FUC	C3-C4-C5	-2.04	106.71	109.81
4	F	2	NAG	O5-C1-C2	-2.01	108.17	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	5	NAG	O5-C5-C6-O6
4	F	5	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	E	5	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	5	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	2	0
4	F	7	FUC	2	0
4	E	1	NAG	1	0

5.5 Carbohydrates [i](#)

14 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	$\# Z > 2$
4	NAG	E	1	1,4	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.98	1 (5%)
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	1.05	1 (6%)
4	MAN	E	4	4	11,11,12	0.46	0	15,15,17	1.03	1 (6%)
4	NAG	E	5	4	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
4	MAN	E	6	4	11,11,12	0.38	0	15,15,17	0.92	1 (6%)
4	FUC	E	7	4	10,10,11	0.53	0	14,14,16	0.76	0
4	NAG	F	1	4,2	14,14,15	0.39	0	17,19,21	2.05	3 (17%)
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
4	BMA	F	3	4	11,11,12	0.28	0	15,15,17	0.94	1 (6%)
4	MAN	F	4	4	11,11,12	0.37	0	15,15,17	0.95	1 (6%)
4	NAG	F	5	4	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
4	MAN	F	6	4	11,11,12	0.36	0	15,15,17	0.93	1 (6%)
4	FUC	F	7	4	10,10,11	0.67	0	14,14,16	1.42	3 (21%)

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	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	NAG	E	5	4	-	2/6/23/26	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	FUC	E	7	4	-	-	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NAG	F	5	4	-	2/6/23/26	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	FUC	F	7	4	-	-	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	6.96	121.51	112.19
4	F	7	FUC	C1-C2-C3	3.71	115.05	109.64
4	E	4	MAN	C1-O5-C5	3.46	116.82	112.19
4	F	4	MAN	C1-O5-C5	3.33	116.65	112.19
4	E	5	NAG	C1-O5-C5	3.32	116.64	112.19
4	F	6	MAN	C1-O5-C5	3.30	116.61	112.19
4	E	6	MAN	C1-O5-C5	3.23	116.52	112.19
4	E	3	BMA	C1-O5-C5	3.02	116.24	112.19
4	F	3	BMA	C1-O5-C5	2.78	115.92	112.19
4	F	5	NAG	C1-O5-C5	2.62	115.69	112.19
4	F	7	FUC	C6-C5-C4	2.56	117.76	113.08
4	E	2	NAG	O5-C1-C2	-2.53	107.37	111.29
4	F	1	NAG	C3-C4-C5	2.40	114.58	110.23
4	F	1	NAG	C6-C5-C4	-2.33	107.29	113.02
4	F	7	FUC	C3-C4-C5	-2.04	106.71	109.81
4	F	2	NAG	O5-C1-C2	-2.01	108.17	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

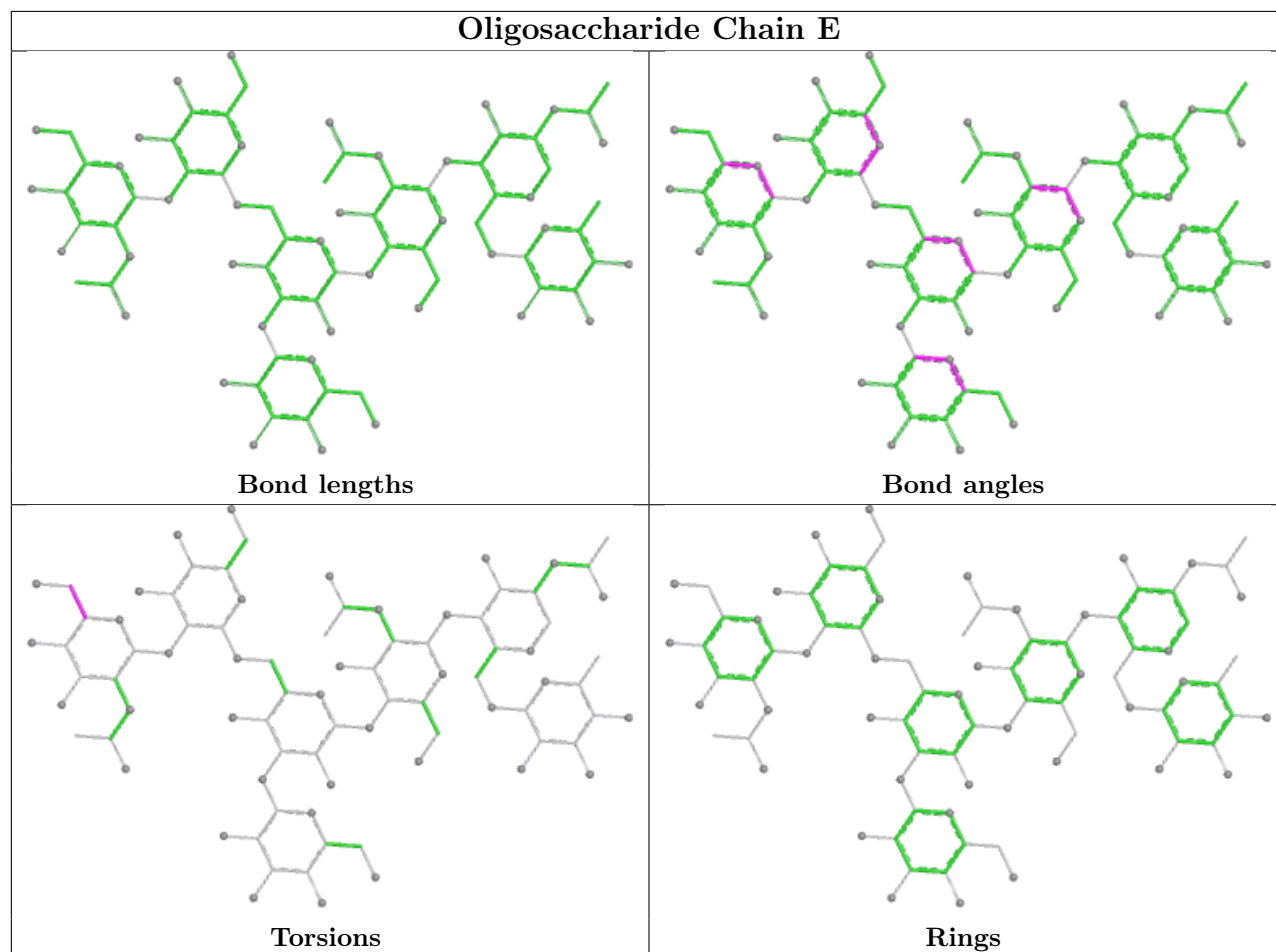
Mol	Chain	Res	Type	Atoms
4	F	5	NAG	O5-C5-C6-O6
4	F	5	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	E	5	NAG	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6

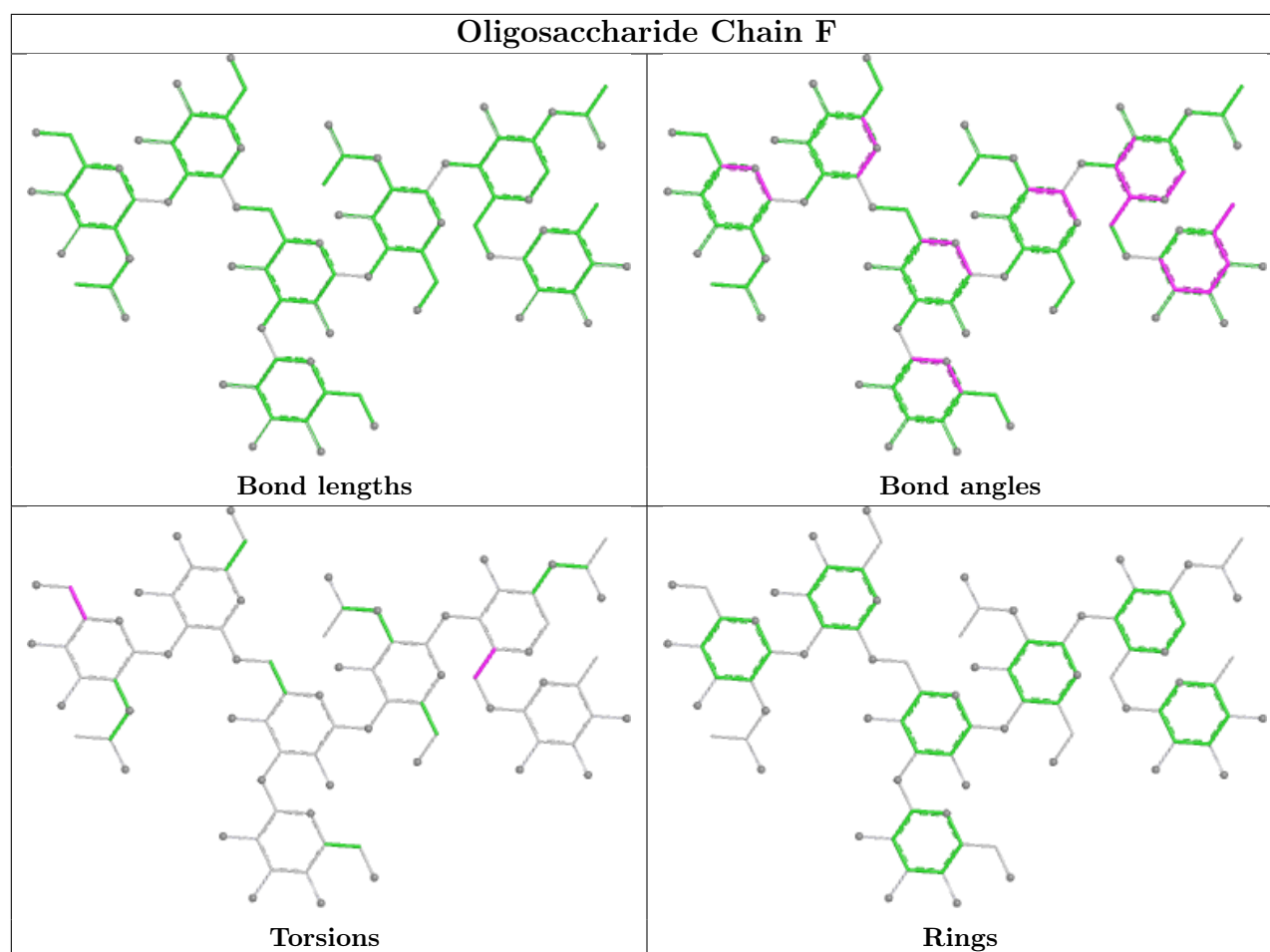
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	2	0
4	F	7	FUC	2	0
4	E	1	NAG	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](#)

5 ligands 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	$\# Z > 2$
5	GOL	B	501	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	B	509	-	5,5,5	0.06	0	5,5,5	0.35	0
5	GOL	A	509	-	5,5,5	0.12	0	5,5,5	0.18	0
5	GOL	A	510	-	5,5,5	0.18	0	5,5,5	0.38	0
5	GOL	A	508	-	5,5,5	0.15	0	5,5,5	0.26	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
5	GOL	B	501	-	-	2/4/4/4	-
5	GOL	B	509	-	-	2/4/4/4	-
5	GOL	A	509	-	-	2/4/4/4	-
5	GOL	A	510	-	-	2/4/4/4	-
5	GOL	A	508	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	O1-C1-C2-C3
5	A	509	GOL	C1-C2-C3-O3
5	A	510	GOL	O1-C1-C2-C3
5	B	509	GOL	O1-C1-C2-C3
5	B	509	GOL	O1-C1-C2-O2
5	A	508	GOL	C1-C2-C3-O3
5	B	501	GOL	O1-C1-C2-C3
5	A	508	GOL	O1-C1-C2-O2
5	A	509	GOL	O2-C2-C3-O3
5	A	510	GOL	O1-C1-C2-O2
5	B	501	GOL	O1-C1-C2-O2
5	A	508	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	GOL	1	0
5	A	510	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	209/232 (90%)	-0.46	2 (0%) 79 76	23, 39, 59, 91	0
2	B	210/232 (90%)	-0.42	3 (1%) 73 69	15, 41, 61, 89	2 (0%)
3	C	13/13 (100%)	0.02	0 100 100	37, 52, 66, 71	0
3	D	13/13 (100%)	0.56	1 (7%) 19 16	51, 64, 81, 85	0
All	All	445/490 (90%)	-0.40	6 (1%) 75 71	15, 40, 65, 91	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	235	LEU	3.2
3	D	13	THR	3.0
2	B	236	GLY	2.9
2	B	444	SER	2.8
1	A	358	LEU	2.6
1	A	444	SER	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	F	6	11/12	0.68	0.12	76,79,83,86	0
4	MAN	E	6	11/12	0.75	0.12	66,69,70,72	0
4	FUC	F	7	10/11	0.88	0.15	53,59,64,67	0
4	MAN	F	4	11/12	0.90	0.09	56,61,65,67	0
4	FUC	E	7	10/11	0.92	0.10	52,62,64,65	0
4	NAG	E	5	14/15	0.93	0.08	51,57,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	E	4	11/12	0.93	0.08	47,51,57,57	0
4	NAG	F	5	14/15	0.94	0.10	50,54,55,57	0
4	NAG	E	2	14/15	0.95	0.06	35,45,51,51	0
4	NAG	F	1	14/15	0.95	0.07	47,52,55,55	0
4	NAG	E	1	14/15	0.95	0.07	44,49,56,56	0
4	NAG	F	2	14/15	0.96	0.07	41,45,50,51	0

6.3 Carbohydrates

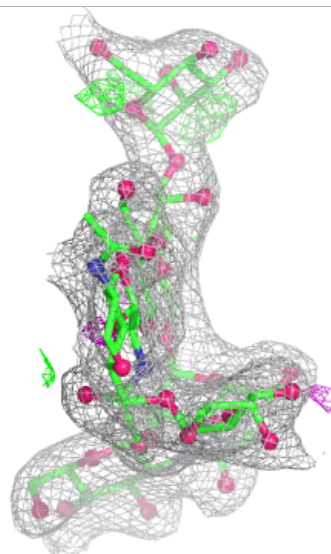
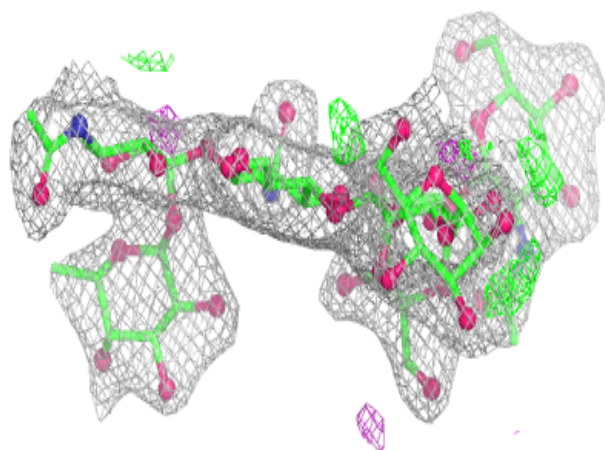
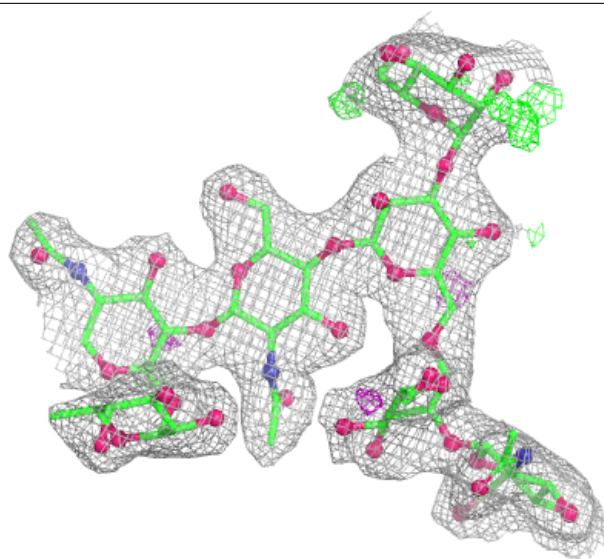
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

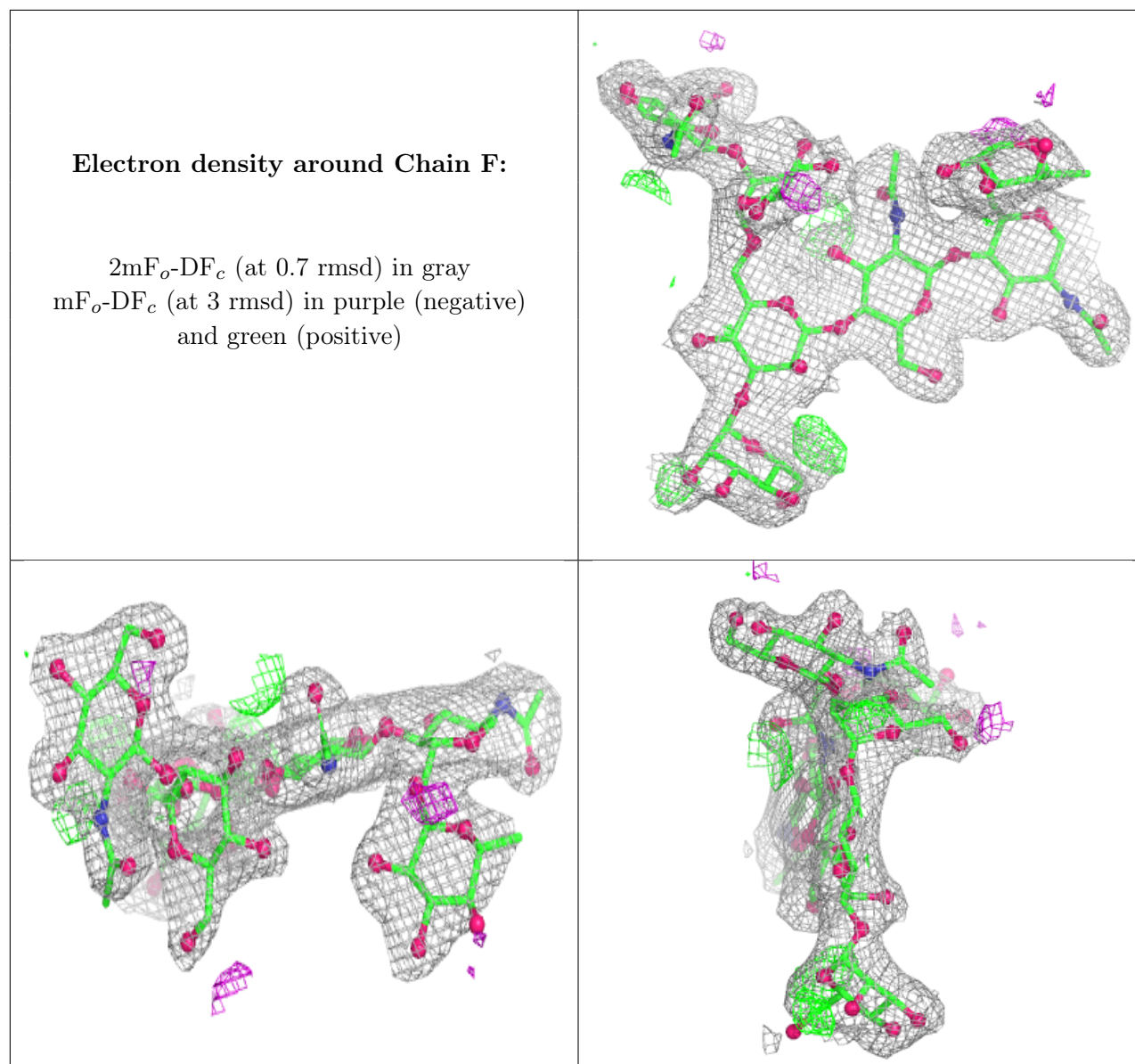
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	F	6	11/12	0.68	0.12	76,79,83,86	0
4	MAN	E	6	11/12	0.75	0.12	66,69,70,72	0
4	FUC	F	7	10/11	0.88	0.15	53,59,64,67	0
4	MAN	F	4	11/12	0.90	0.09	56,61,65,67	0
4	BMA	E	3	11/12	0.91	0.08	42,50,56,60	0
4	FUC	E	7	10/11	0.92	0.10	52,62,64,65	0
4	MAN	E	4	11/12	0.93	0.08	47,51,57,57	0
4	NAG	E	5	14/15	0.93	0.08	51,57,61,62	0
4	BMA	F	3	11/12	0.93	0.09	47,52,59,69	0
4	NAG	F	5	14/15	0.94	0.10	50,54,55,57	0
4	NAG	F	1	14/15	0.95	0.07	47,52,55,55	0
4	NAG	E	2	14/15	0.95	0.06	35,45,51,51	0
4	NAG	E	1	14/15	0.95	0.07	44,49,56,56	0
4	NAG	F	2	14/15	0.96	0.07	41,45,50,51	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 ⓘ

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
5	GOL	B	509	6/6	0.83	0.15	62,72,74,74	0
5	GOL	A	509	6/6	0.85	0.14	57,60,61,61	0
5	GOL	A	510	6/6	0.87	0.15	56,60,60,62	0
5	GOL	B	501	6/6	0.89	0.13	67,70,73,75	0
5	GOL	A	508	6/6	0.93	0.11	27,50,57,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.