wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 09:35 PM BST

PDB ID	:	3WN5
Title	:	Crystal structure of asymmetrically engineered Fc variant in complex with FcgRIIIa
Authors	:	Kadono, S.; Mimoto, F.; Katada, H.; Igawa, T.; Kamikawa, T.; Hattori, K.
Deposited on	:	2013-12-05
Resolution	:	2.78 Å(reported)

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

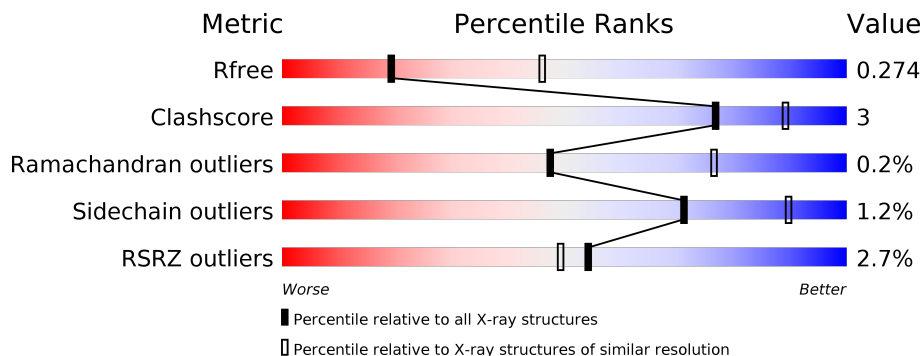|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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.
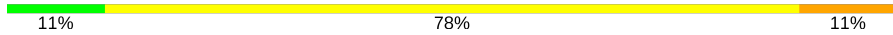
Metric	Percentile Ranks	Value
Rfree		0.274
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		1.2%
RSRZ outliers		2.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
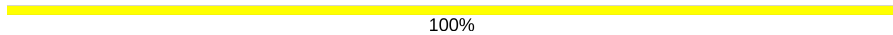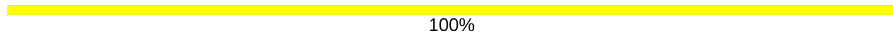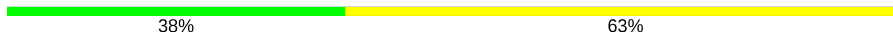
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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 <=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	230	2% 85% 7% 8%
1	D	230	% 86% 6% 8%
2	B	230	2% 78% 12% • 9%
2	E	230	5% 83% 8% 9%
3	C	197	2% 80% 6% 14%
3	F	197	2% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	G	9	44% 33% 22%
4	H	9	11% 78% 11%
4	L	9	56% 44%
5	I	5	60% 40%
6	J	2	100%
6	M	2	100%
7	K	8	38% 63%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9947 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-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total 1664	C 1057	N 277	O 323	S 7	0	0	0
1	D	212	Total 1646	C 1046	N 274	O 319	S 7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	CYS	engineered mutation	UNP P01857
A	270	GLU	ASP	engineered mutation	UNP P01857
A	326	ASP	LYS	engineered mutation	UNP P01857
A	330	LYS	ALA	engineered mutation	UNP P01857
A	334	GLU	LYS	engineered mutation	UNP P01857
A	356	CYS	ASP	engineered mutation	UNP P01857
A	366	SER	THR	engineered mutation	UNP P01857
A	368	ALA	LEU	engineered mutation	UNP P01857
A	407	VAL	TYR	engineered mutation	UNP P01857
D	220	SER	CYS	engineered mutation	UNP P01857
D	270	GLU	ASP	engineered mutation	UNP P01857
D	326	ASP	LYS	engineered mutation	UNP P01857
D	330	LYS	ALA	engineered mutation	UNP P01857
D	334	GLU	LYS	engineered mutation	UNP P01857
D	356	CYS	ASP	engineered mutation	UNP P01857
D	366	SER	THR	engineered mutation	UNP P01857
D	368	ALA	LEU	engineered mutation	UNP P01857
D	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total 1664	C 1065	N 271	O 320	S 8	0	0	0

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Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	210	1644	1056	267	313	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	SER	CYS	engineered mutation	UNP P01857
B	234	TYR	LEU	engineered mutation	UNP P01857
B	235	TYR	LEU	engineered mutation	UNP P01857
B	236	TRP	GLY	engineered mutation	UNP P01857
B	239	MET	SER	engineered mutation	UNP P01857
B	268	ASP	HIS	engineered mutation	UNP P01857
B	298	ALA	SER	engineered mutation	UNP P01857
B	327	ASP	ALA	engineered mutation	UNP P01857
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	TRP	THR	engineered mutation	UNP P01857
E	220	SER	CYS	engineered mutation	UNP P01857
E	234	TYR	LEU	engineered mutation	UNP P01857
E	235	TYR	LEU	engineered mutation	UNP P01857
E	236	TRP	GLY	engineered mutation	UNP P01857
E	239	MET	SER	engineered mutation	UNP P01857
E	268	ASP	HIS	engineered mutation	UNP P01857
E	298	ALA	SER	engineered mutation	UNP P01857
E	327	ASP	ALA	engineered mutation	UNP P01857
E	349	CYS	TYR	engineered mutation	UNP P01857
E	366	TRP	THR	engineered mutation	UNP P01857

- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	169	1358	867	232	255	4	0	0	0
3	F	170	1354	862	230	258	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLN	ASN	engineered mutation	UNP P08637
C	71	GLN	ASN	engineered mutation	UNP P08637
C	155	VAL	PHE	SEE REMARK 999	UNP P08637
C	166	GLN	ASN	engeneered mutation	UNP P08637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	188	HIS	-	expression tag	UNP P08637
C	189	HIS	-	expression tag	UNP P08637
C	190	HIS	-	expression tag	UNP P08637
C	191	HIS	-	expression tag	UNP P08637
C	192	HIS	-	expression tag	UNP P08637
C	193	HIS	-	expression tag	UNP P08637
F	35	GLN	ASN	engineered mutation	UNP P08637
F	71	GLN	ASN	engineered mutation	UNP P08637
F	155	VAL	PHE	SEE REMARK 999	UNP P08637
F	166	GLN	ASN	engineered mutation	UNP P08637
F	188	HIS	-	expression tag	UNP P08637
F	189	HIS	-	expression tag	UNP P08637
F	190	HIS	-	expression tag	UNP P08637
F	191	HIS	-	expression tag	UNP P08637
F	192	HIS	-	expression tag	UNP P08637
F	193	HIS	-	expression tag	UNP P08637

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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.
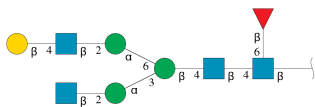
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	9	Total 110	C 62	N 4	O 44	0	0	0
4	H	9	Total 110	C 62	N 4	O 44	0	0	0
4	L	9	Total 110	C 62	N 4	O 44	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.
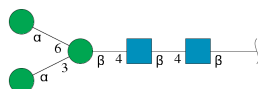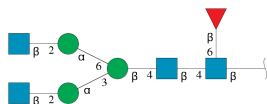
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp ha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-man nopyranose-(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
7	K	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 8 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	I	0	0
			1	1		
8	E	4	Total	I	0	0
			4	4		
8	B	3	Total	I	0	0
			3	3		
8	C	2	Total	I	0	0
			2	2		
8	A	2	Total	I	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	4	Total I		0	0
			4	4		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
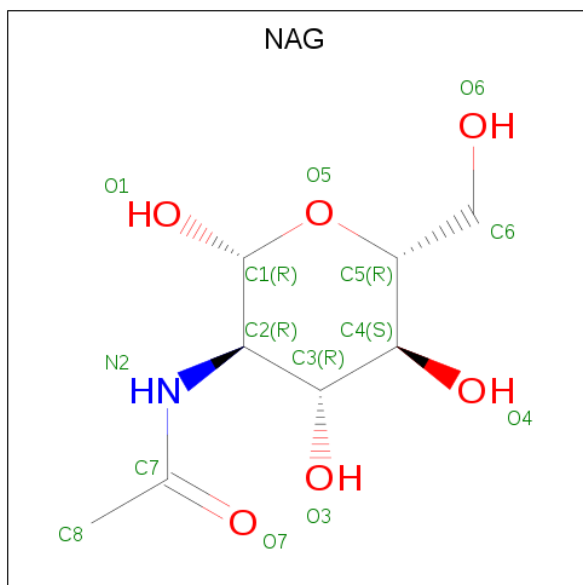
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	7	Total O		0	0
			7	7		
10	B	11	Total O		0	0
			11	11		
10	C	6	Total O		0	0
			6	6		
10	D	4	Total O		0	0
			4	4		
10	E	3	Total O		0	0
			3	3		
10	F	10	Total O		0	0
			10	10		

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.
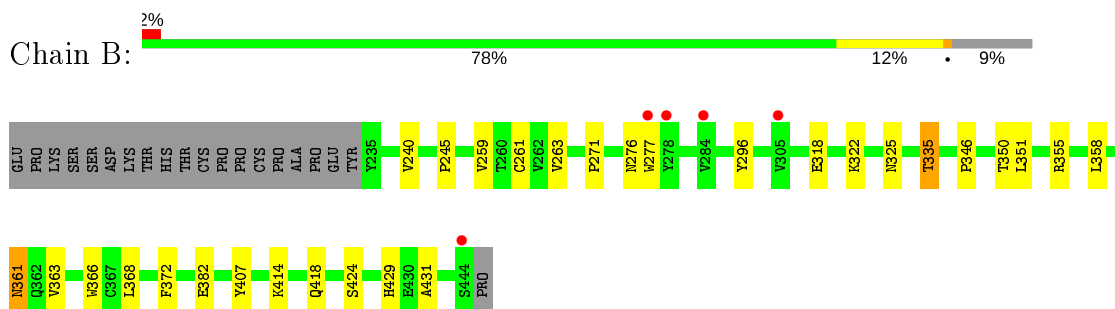
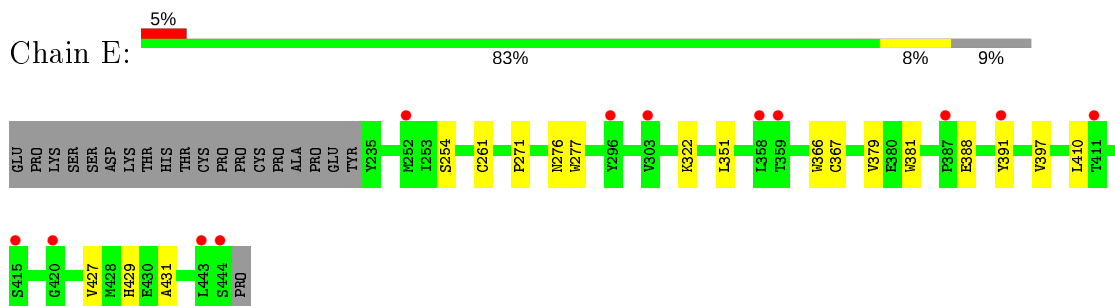- Molecule 1: Ig gamma-1 chain C region
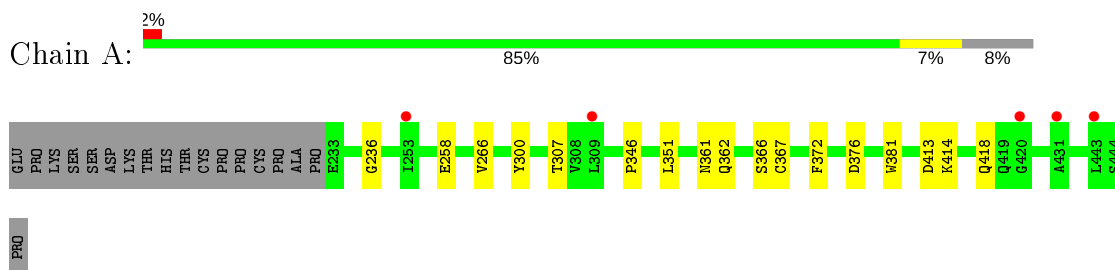
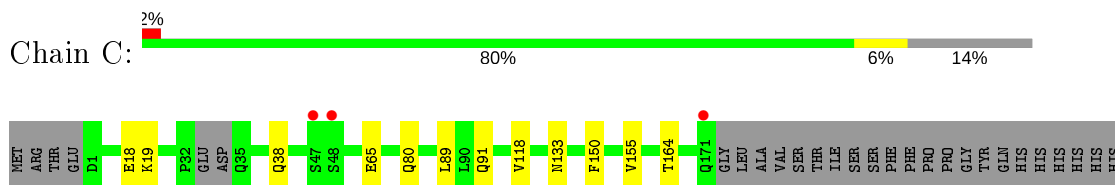

- Molecule 1: Ig gamma-1 chain C region
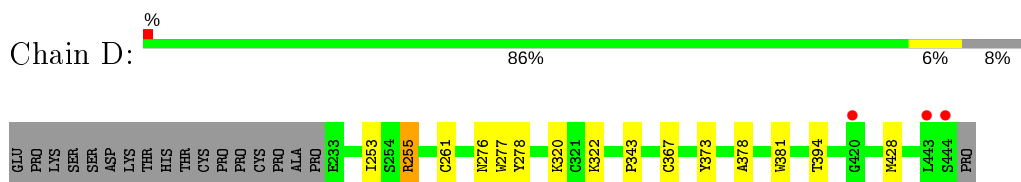
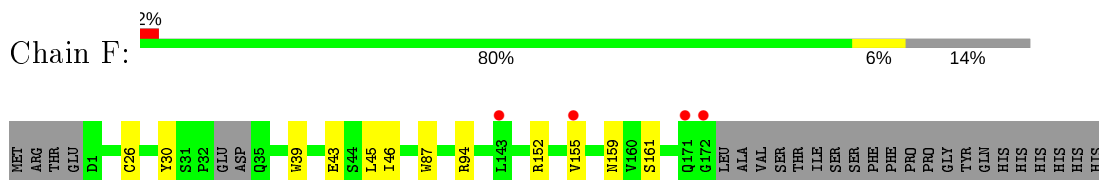- Molecule 2: Ig gamma-1 chain C region

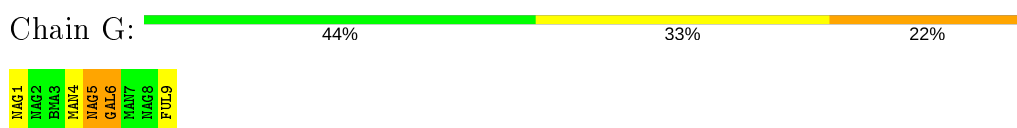- Molecule 2: Ig gamma-1 chain C region

• Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C:

• Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain F:

• Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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

Chain G:

• Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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

Chain H:

• Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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

Chain L:

• Molecule 5: alpha-D-mannopyranose-(1-3)-[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

Chain I:

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain J: 100%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain M: 100%

NAG1 NAG2

• Molecule 7: 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-mannopyra
nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetami
do-2-deoxy-beta-D-glucopyranose

Chain K: 38% 63%

NAG1 NAG2 BMA3 MAN4 NAG5 MAN6 NAG7 FUL8
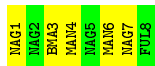
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.03Å 72.49Å 163.48Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.78 44.51 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.78) 98.1 (44.51-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.274 0.236 , 0.274	Depositor DCC
R_{free} test set	2192 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å²)	54.5	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 44.0	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l 0.016 for -k,-h,-l 0.020 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GAL, FUL, IOD, 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	0.28	0/1709	0.46	0/2334
1	D	0.28	0/1691	0.46	0/2313
2	B	0.28	0/1713	0.46	0/2343
2	E	0.28	0/1693	0.44	0/2318
3	C	0.30	0/1395	0.49	0/1897
3	F	0.29	0/1391	0.48	0/1895
All	All	0.28	0/9592	0.46	0/13100

There are no bond length outliers.

There are no bond angle outliers.

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	1664	0	1594	8	0
1	D	1646	0	1567	11	0
2	B	1664	0	1580	16	0
2	E	1644	0	1547	11	0
3	C	1358	0	1299	7	0
3	F	1354	0	1273	4	0
4	G	110	0	94	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	110	0	94	2	0
4	L	110	0	94	0	0
5	I	61	0	52	0	0
6	J	28	0	25	0	0
6	M	28	0	25	0	0
7	K	99	0	85	0	0
8	A	2	0	0	0	0
8	B	3	0	0	1	0
8	C	2	0	0	0	0
8	D	1	0	0	0	0
8	E	4	0	0	1	0
8	F	4	0	0	1	0
9	F	14	0	13	0	0
10	A	7	0	0	0	0
10	B	11	0	0	0	0
10	C	6	0	0	0	0
10	D	4	0	0	0	0
10	E	3	0	0	0	0
10	F	10	0	0	0	0
All	All	9947	0	9342	57	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 3.

The worst 5 of 57 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:D:255:ARG:HG2	1:D:255:ARG:HH11	1.47	0.80
1:D:255:ARG:CG	1:D:255:ARG:HH11	2.04	0.71
2:B:296:TYR:H	4:H:9:FUL:H61	1.57	0.69
3:F:152:ARG:HB3	3:F:161:SER:HB3	1.75	0.68
2:E:351:LEU:HB2	2:E:366:TRP:HB2	1.81	0.61

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	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
1	D	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
2	B	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	29	58
2	E	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	29	58
3	C	165/197 (84%)	162 (98%)	3 (2%)	0	100	100
3	F	166/197 (84%)	162 (98%)	4 (2%)	0	100	100
All	All	1167/1314 (89%)	1130 (97%)	35 (3%)	2 (0%)	47	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	PRO
2	E	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	190/214 (89%)	188 (99%)	2 (1%)	73	90
1	D	187/214 (87%)	186 (100%)	1 (0%)	88	95
2	B	188/215 (87%)	184 (98%)	4 (2%)	53	81
2	E	181/215 (84%)	181 (100%)	0	100	100
3	C	150/178 (84%)	149 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
3	F	148/178 (83%)	143 (97%)	5 (3%)		37	68
All	All	1044/1214 (86%)	1031 (99%)	13 (1%)		71	90

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	363	VAL
3	C	38	GLN
3	F	46	ILE
2	B	361	ASN
3	F	45	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	171	GLN
1	D	315	ASN
2	E	429	HIS
3	C	71	GLN
3	C	80	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates (i)

44 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	G	1	1,4	14,14,15	0.47	0	17,19,21	1.29	3 (17%)
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	0.81	0
4	BMA	G	3	4	11,11,12	0.45	0	15,15,17	0.76	0
4	MAN	G	4	4	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
4	NAG	G	5	4	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
4	GAL	G	6	4	11,11,12	0.59	0	15,15,17	1.22	1 (6%)
4	MAN	G	7	4	11,11,12	0.57	0	15,15,17	0.90	0
4	NAG	G	8	4	14,14,15	0.46	0	17,19,21	0.76	0
4	FUL	G	9	4	10,10,11	0.64	0	14,14,16	1.48	3 (21%)
4	NAG	H	1	2,4	14,14,15	0.59	0	17,19,21	0.95	1 (5%)
4	NAG	H	2	4	14,14,15	0.51	0	17,19,21	0.89	0
4	BMA	H	3	4	11,11,12	0.56	0	15,15,17	1.19	2 (13%)
4	MAN	H	4	4	11,11,12	0.55	0	15,15,17	0.84	1 (6%)
4	NAG	H	5	4	14,14,15	0.59	0	17,19,21	1.22	1 (5%)
4	GAL	H	6	4	11,11,12	0.59	0	15,15,17	0.79	0
4	MAN	H	7	4	11,11,12	0.50	0	15,15,17	1.67	3 (20%)
4	NAG	H	8	4	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
4	FUL	H	9	4	10,10,11	0.43	0	14,14,16	0.89	1 (7%)
5	NAG	I	1	3,5	14,14,15	0.48	0	17,19,21	1.89	2 (11%)
5	NAG	I	2	5	14,14,15	0.49	0	17,19,21	0.79	0
5	BMA	I	3	5	11,11,12	0.44	0	15,15,17	0.77	0
5	MAN	I	4	5	11,11,12	0.60	0	15,15,17	0.97	0
5	MAN	I	5	5	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
6	NAG	J	1	3,6	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
6	NAG	J	2	6	14,14,15	0.45	0	17,19,21	0.94	1 (5%)
7	NAG	K	1	1,7	14,14,15	0.53	0	17,19,21	1.12	2 (11%)
7	NAG	K	2	7	14,14,15	0.54	0	17,19,21	0.70	0
7	BMA	K	3	7	11,11,12	0.43	0	15,15,17	1.14	2 (13%)
7	MAN	K	4	7	11,11,12	0.52	0	15,15,17	0.85	1 (6%)
7	NAG	K	5	7	14,14,15	0.49	0	17,19,21	0.73	0
7	MAN	K	6	7	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
7	NAG	K	7	7	14,14,15	0.50	0	17,19,21	0.82	1 (5%)
7	FUL	K	8	7	10,10,11	0.45	0	14,14,16	0.59	0
4	NAG	L	1	2,4	14,14,15	0.44	0	17,19,21	1.35	1 (5%)
4	NAG	L	2	4	14,14,15	0.47	0	17,19,21	0.83	0
4	BMA	L	3	4	11,11,12	0.46	0	15,15,17	0.79	0
4	MAN	L	4	4	11,11,12	0.57	0	15,15,17	0.92	1 (6%)
4	NAG	L	5	4	14,14,15	0.54	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GAL	L	6	4	11,11,12	0.64	0	15,15,17	0.73	0
4	MAN	L	7	4	11,11,12	0.48	0	15,15,17	1.19	1 (6%)
4	NAG	L	8	4	14,14,15	0.58	0	17,19,21	1.09	1 (5%)
4	FUL	L	9	4	10,10,11	0.49	0	14,14,16	0.64	0
6	NAG	M	1	3,6	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
6	NAG	M	2	6	14,14,15	0.48	0	17,19,21	0.93	1 (5%)

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	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	NAG	G	5	4	-	2/6/23/26	0/1/1/1
4	GAL	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
4	NAG	G	8	4	-	0/6/23/26	0/1/1/1
4	FUL	G	9	4	-	-	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	NAG	H	5	4	-	0/6/23/26	0/1/1/1
4	GAL	H	6	4	-	0/2/19/22	0/1/1/1
4	MAN	H	7	4	-	0/2/19/22	0/1/1/1
4	NAG	H	8	4	-	0/6/23/26	0/1/1/1
4	FUL	H	9	4	-	-	0/1/1/1
5	NAG	I	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
6	NAG	J	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	NAG	K	5	7	-	0/6/23/26	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
7	NAG	K	7	7	-	0/6/23/26	0/1/1/1
7	FUL	K	8	7	-	-	0/1/1/1
4	NAG	L	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1
4	NAG	L	5	4	-	2/6/23/26	0/1/1/1
4	GAL	L	6	4	-	2/2/19/22	0/1/1/1
4	MAN	L	7	4	-	0/2/19/22	0/1/1/1
4	NAG	L	8	4	-	1/6/23/26	0/1/1/1
4	FUL	L	9	4	-	-	0/1/1/1
6	NAG	M	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	NAG	C1-O5-C5	5.68	119.89	112.19
4	L	1	NAG	C1-O5-C5	4.09	117.73	112.19
4	H	5	NAG	C4-C3-C2	3.67	116.40	111.02
4	G	6	GAL	C1-O5-C5	3.50	116.94	112.19
4	G	9	FUL	C3-C4-C5	3.48	115.19	109.77

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	L	6	GAL	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
4	G	6	GAL	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	9	FUL	2	0
4	G	5	NAG	1	0
4	G	6	GAL	1	0
4	H	2	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.
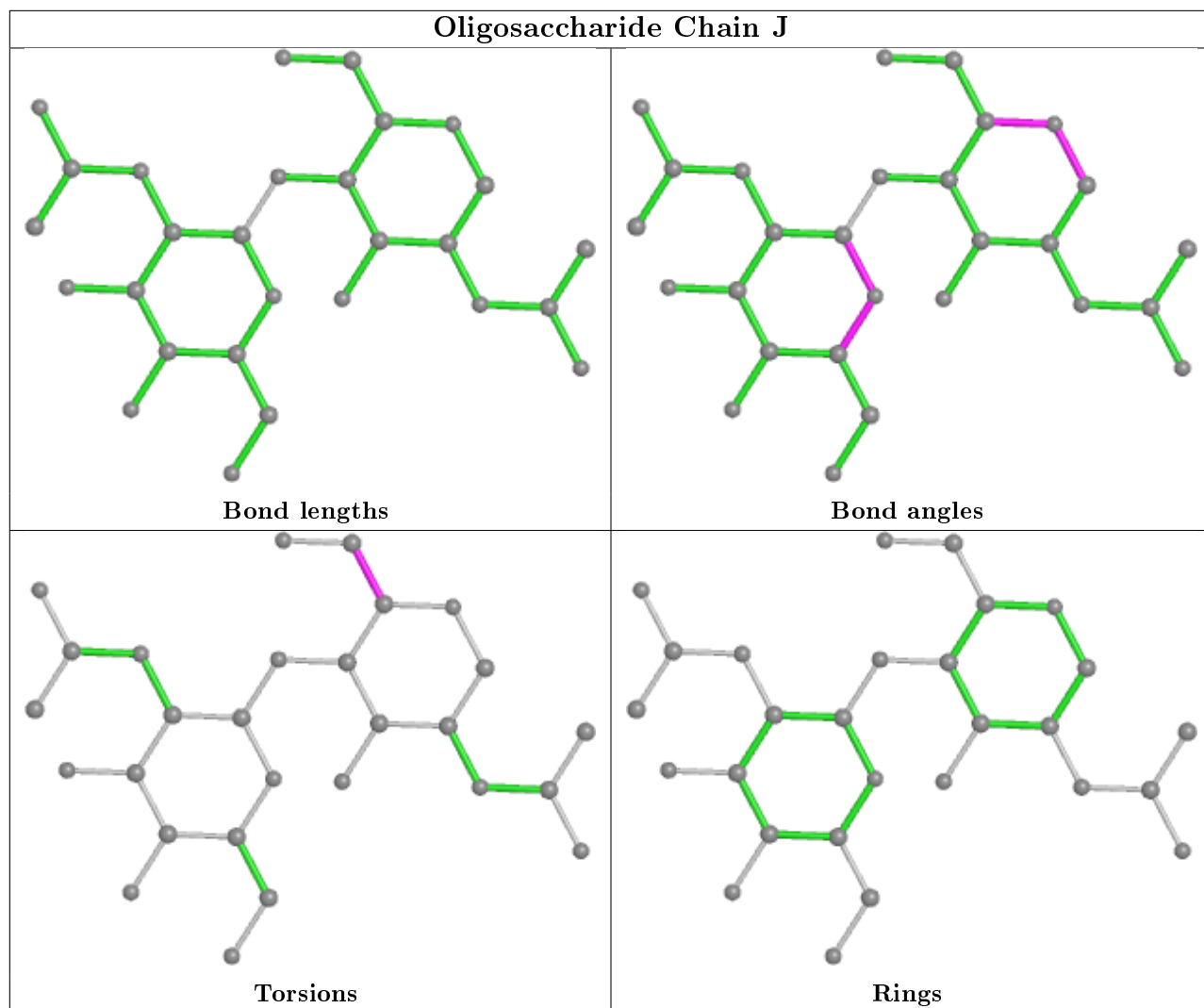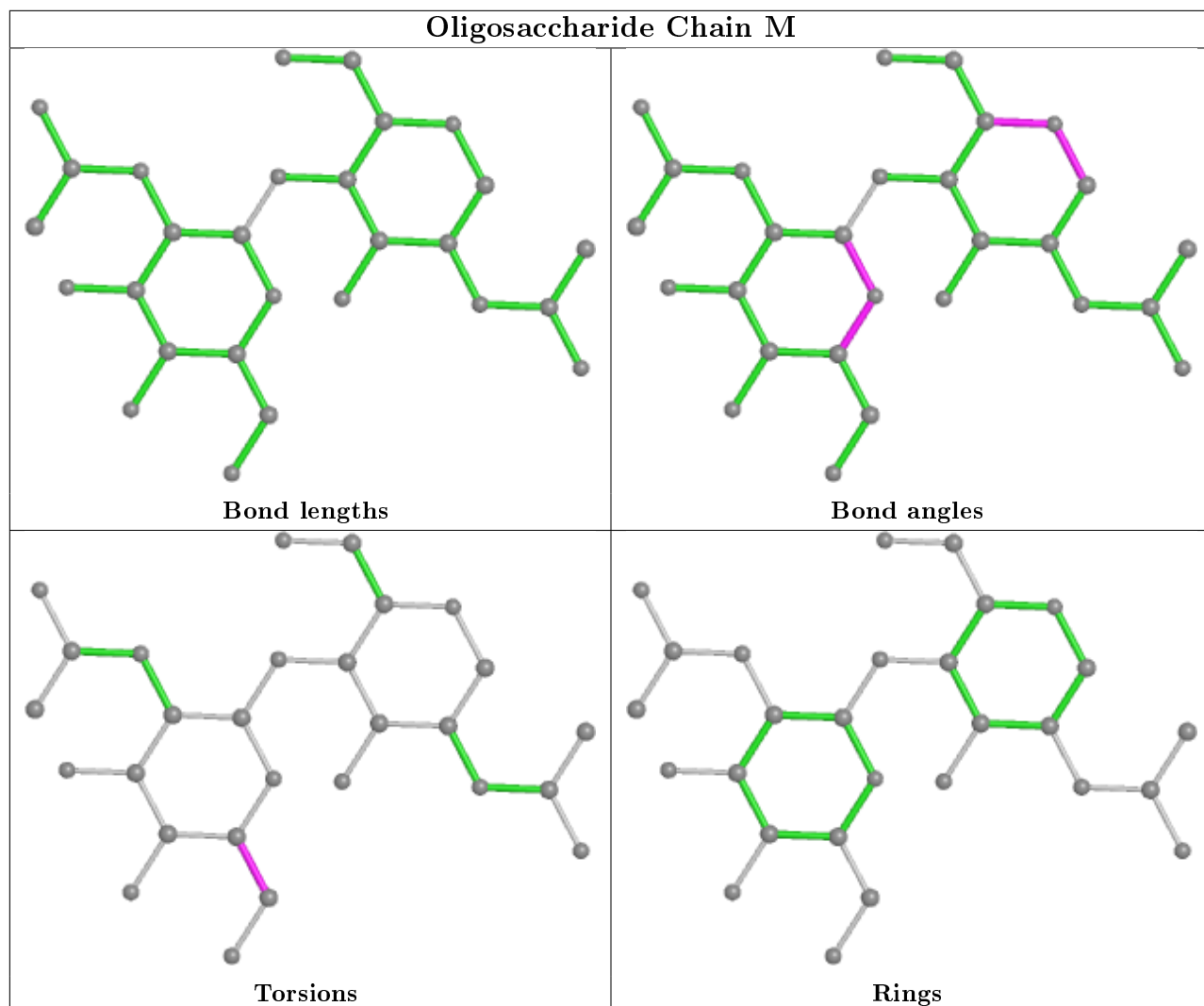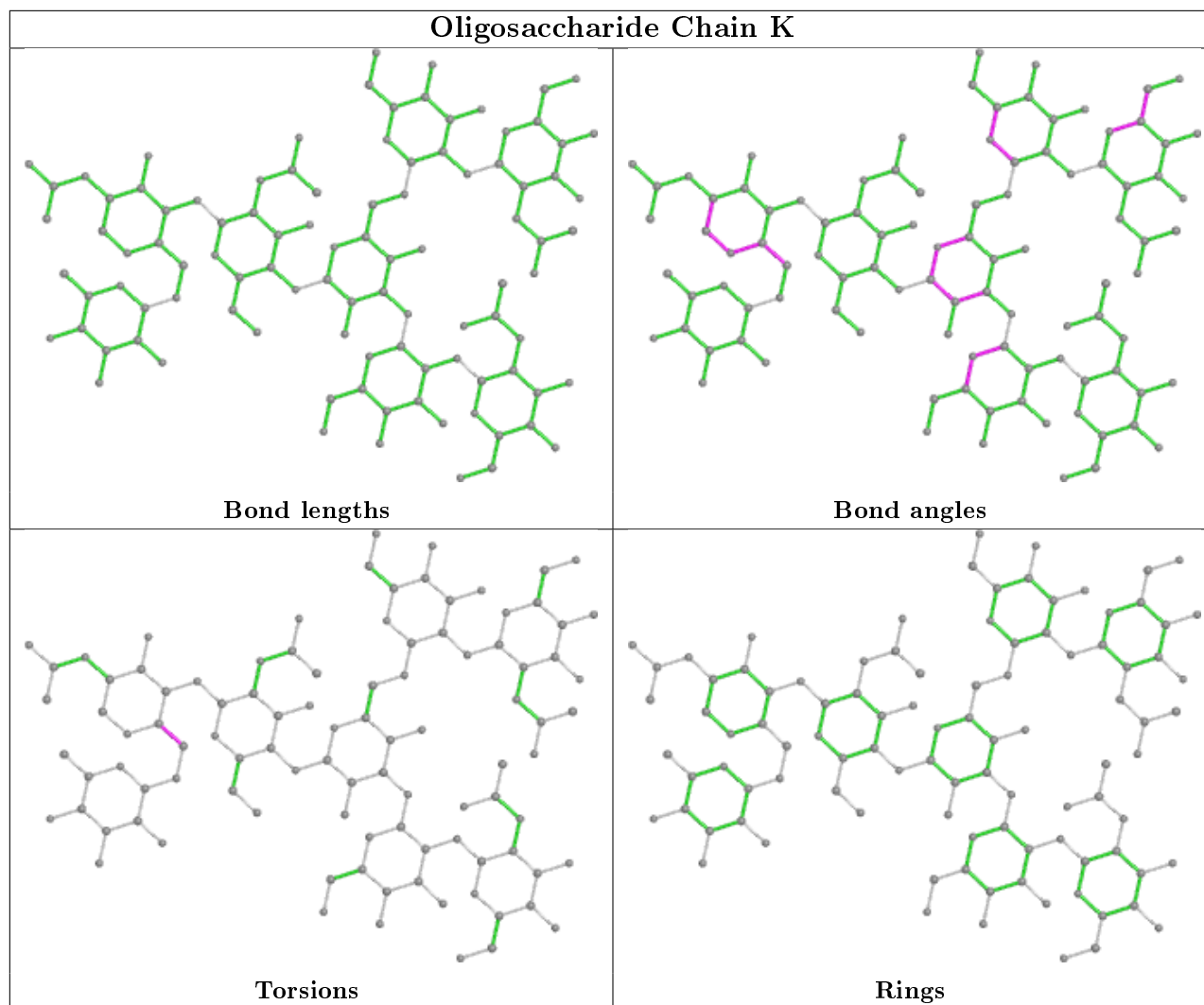

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 for Mogul analysis.

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
9	NAG	F	201	3	14,14,15	0.50	0	17,19,21	0.80	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
9	NAG	F	201	3	-	2/6/23/26	0/1/1/1

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
9	F	201	NAG	C4-C5-C6-O6
9	F	201	NAG	O5-C5-C6-O6

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 (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	212/230 (92%)	0.36	5 (2%)	59	54	38, 52, 68, 79	0
1	D	212/230 (92%)	0.26	3 (1%)	75	73	37, 57, 84, 98	0
2	B	210/230 (91%)	0.36	5 (2%)	59	54	31, 48, 77, 94	0
2	E	210/230 (91%)	0.59	12 (5%)	23	18	44, 70, 111, 121	0
3	C	169/197 (85%)	0.22	3 (1%)	68	65	30, 44, 73, 98	0
3	F	170/197 (86%)	0.29	4 (2%)	59	54	30, 45, 68, 94	0
All	All	1183/1314 (90%)	0.35	32 (2%)	54	49	30, 53, 85, 121	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	47	SER	5.8
1	D	420	GLY	3.9
1	D	443	LEU	3.9
2	E	443	LEU	3.7
3	C	48	SER	3.5

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.
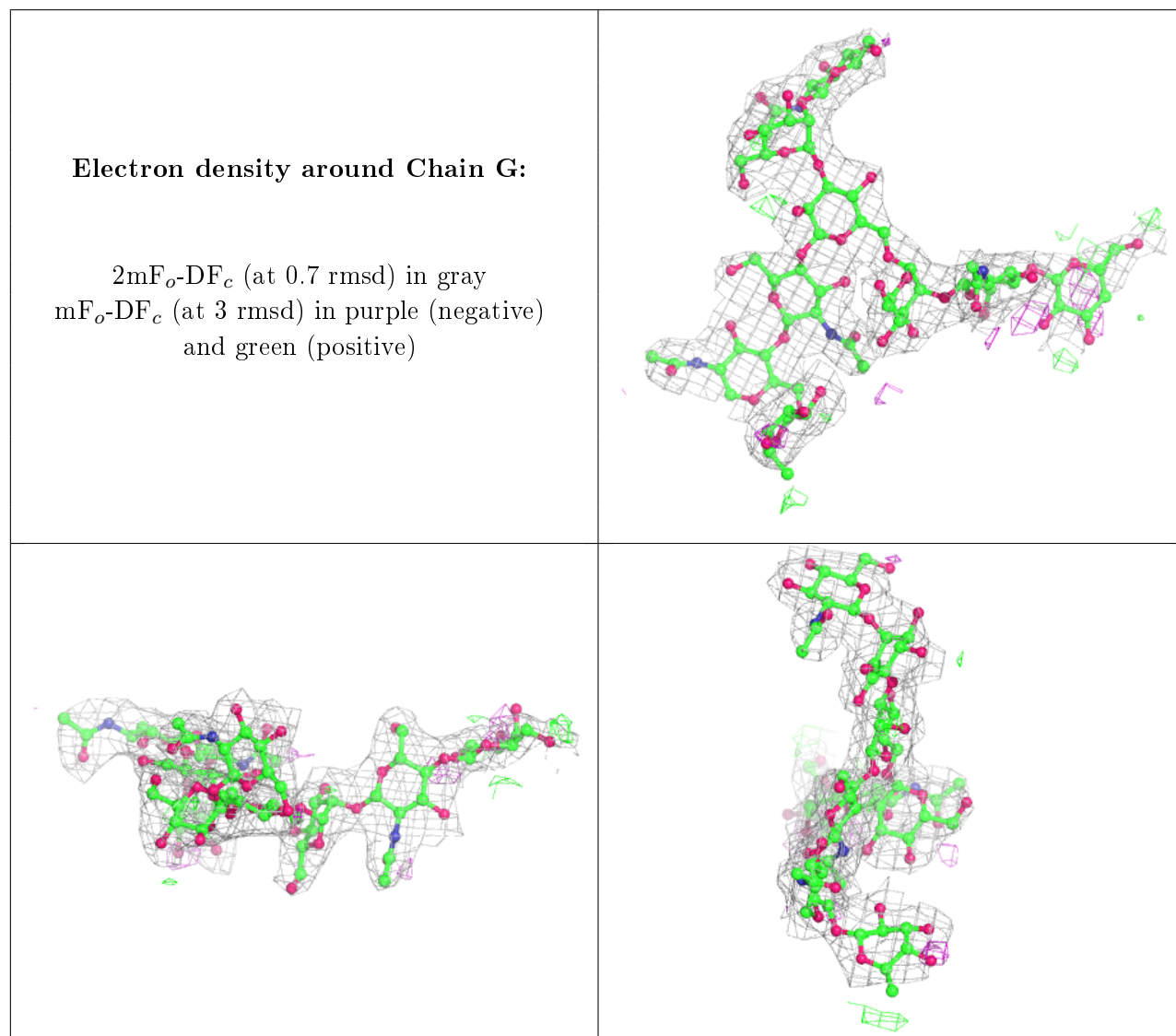
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	L	8	14/15	0.66	0.34	96,100,107,108	0
4	GAL	G	6	11/12	0.70	0.39	77,83,85,86	0
5	MAN	I	5	11/12	0.71	0.23	84,86,90,93	0
4	NAG	H	8	14/15	0.75	0.25	88,91,93,93	0
4	FUL	L	9	10/11	0.80	0.24	75,78,79,79	0
7	NAG	K	5	14/15	0.83	0.23	71,74,75,76	0
4	FUL	H	9	10/11	0.83	0.23	63,65,66,67	0
6	NAG	M	2	14/15	0.84	0.30	65,69,71,71	0
6	NAG	J	2	14/15	0.86	0.19	65,68,71,72	0
5	MAN	I	4	11/12	0.86	0.26	82,84,86,87	0
4	FUL	G	9	10/11	0.87	0.24	46,47,48,51	0
4	MAN	H	7	11/12	0.88	0.17	68,72,75,83	0
7	FUL	K	8	10/11	0.88	0.19	59,60,61,62	0
4	NAG	L	1	14/15	0.89	0.18	61,64,68,72	0
4	GAL	L	6	11/12	0.89	0.21	64,66,67,67	0
4	NAG	L	5	14/15	0.91	0.15	56,59,61,62	0
4	GAL	H	6	11/12	0.91	0.22	73,74,76,78	0
5	BMA	I	3	11/12	0.91	0.13	71,74,78,80	0
7	NAG	K	7	14/15	0.91	0.20	54,56,58,58	0
4	NAG	G	8	14/15	0.91	0.20	52,53,56,59	0
4	MAN	L	7	11/12	0.91	0.16	76,80,82,89	0
4	NAG	H	5	14/15	0.92	0.18	67,68,70,72	0
7	MAN	K	4	11/12	0.92	0.14	62,64,65,68	0
7	NAG	K	1	14/15	0.93	0.18	49,51,54,59	0
4	NAG	H	2	14/15	0.93	0.17	50,54,56,57	0
4	MAN	G	7	11/12	0.93	0.17	51,53,55,55	0
4	BMA	H	3	11/12	0.93	0.17	57,59,61,67	0
5	NAG	I	1	14/15	0.94	0.20	47,49,53,54	0
4	MAN	G	4	11/12	0.94	0.18	53,54,55,56	0
6	NAG	M	1	14/15	0.94	0.17	46,49,53,58	0
4	NAG	G	5	14/15	0.94	0.21	55,58,62,68	0
4	BMA	L	3	11/12	0.94	0.15	60,63,65,71	0
4	MAN	L	4	11/12	0.94	0.12	55,58,59,60	0
4	MAN	H	4	11/12	0.95	0.16	62,63,64,65	0
4	NAG	G	2	14/15	0.96	0.18	42,43,44,44	0
5	NAG	I	2	14/15	0.96	0.14	51,57,61,67	0
4	NAG	G	1	14/15	0.96	0.12	43,44,45,46	0
7	NAG	K	2	14/15	0.96	0.19	47,50,53,53	0
4	NAG	H	1	14/15	0.96	0.17	45,50,56,61	0
6	NAG	J	1	14/15	0.96	0.20	57,60,63,65	0
4	BMA	G	3	11/12	0.97	0.18	44,46,50,51	0
7	BMA	K	3	11/12	0.97	0.14	49,52,54,58	0
7	MAN	K	6	11/12	0.97	0.15	47,48,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	L	2	14/15	0.97	0.14	55,60,61,63	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.
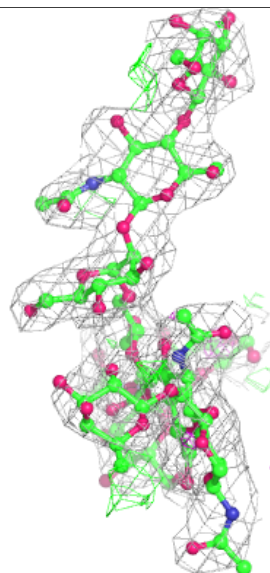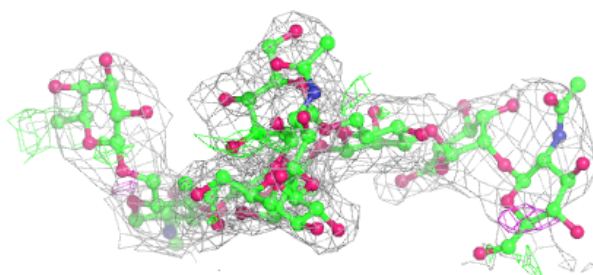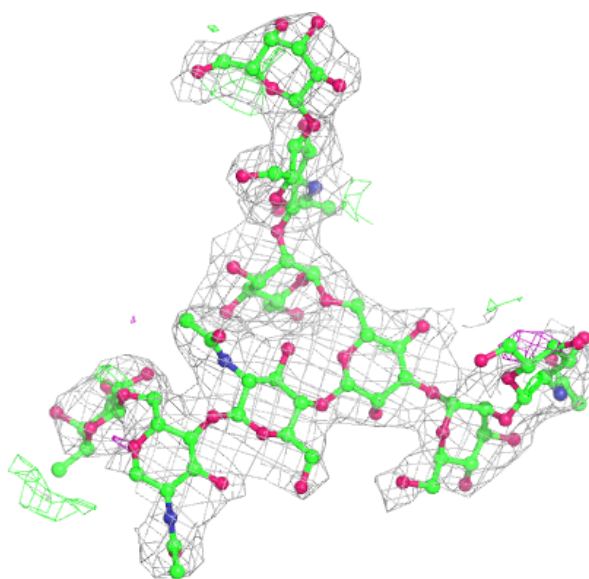

Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
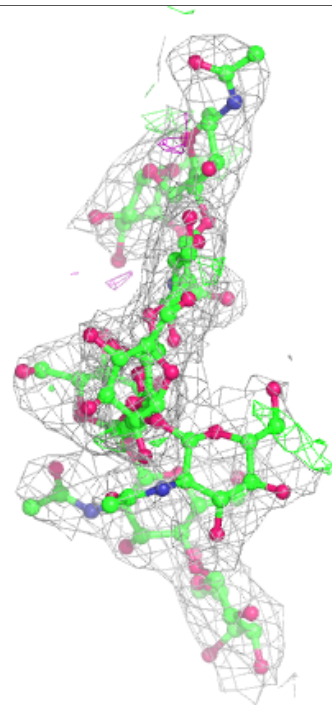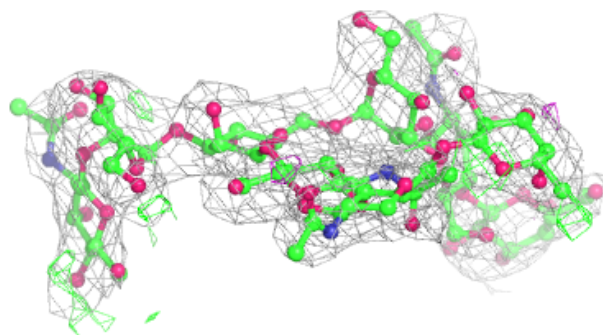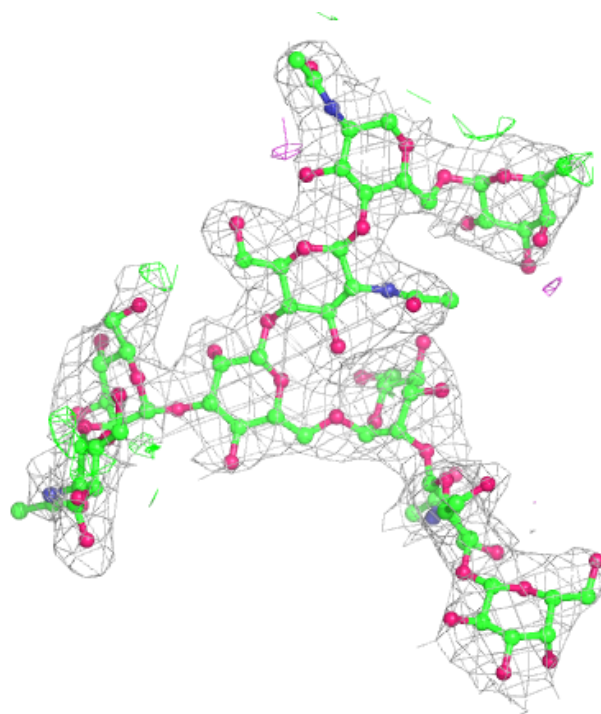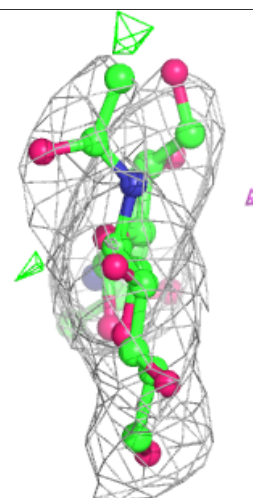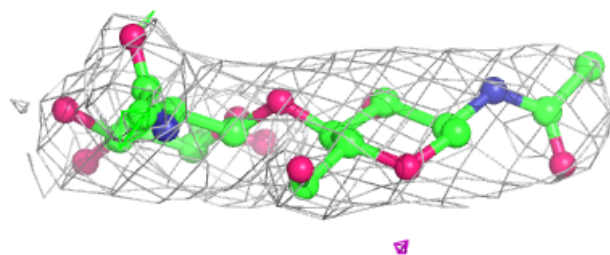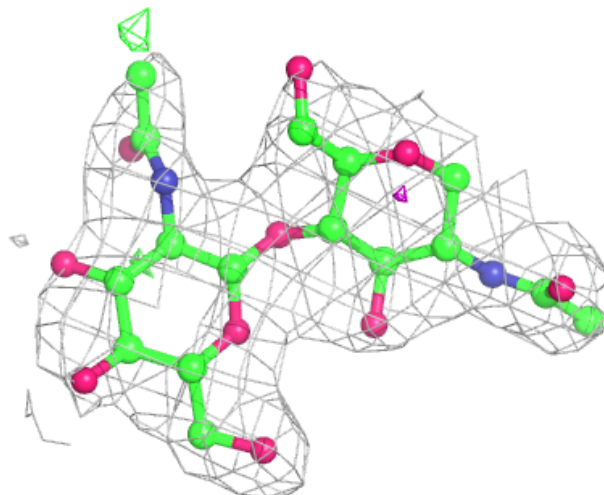
Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
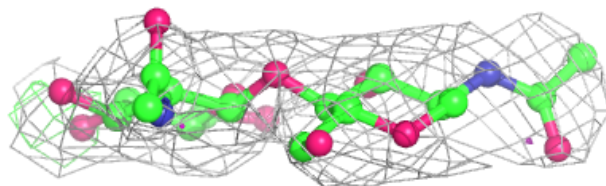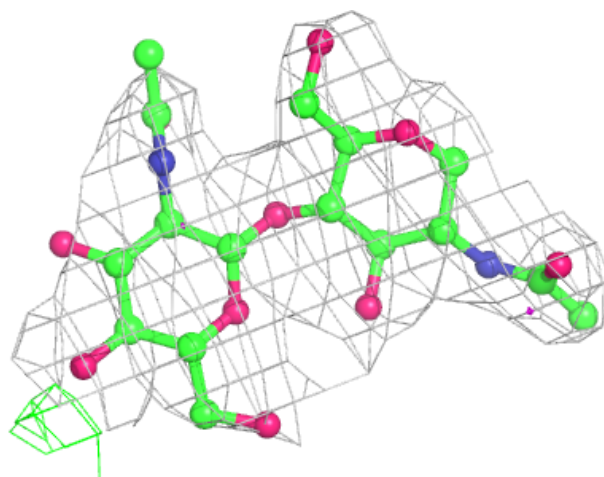and green (positive)
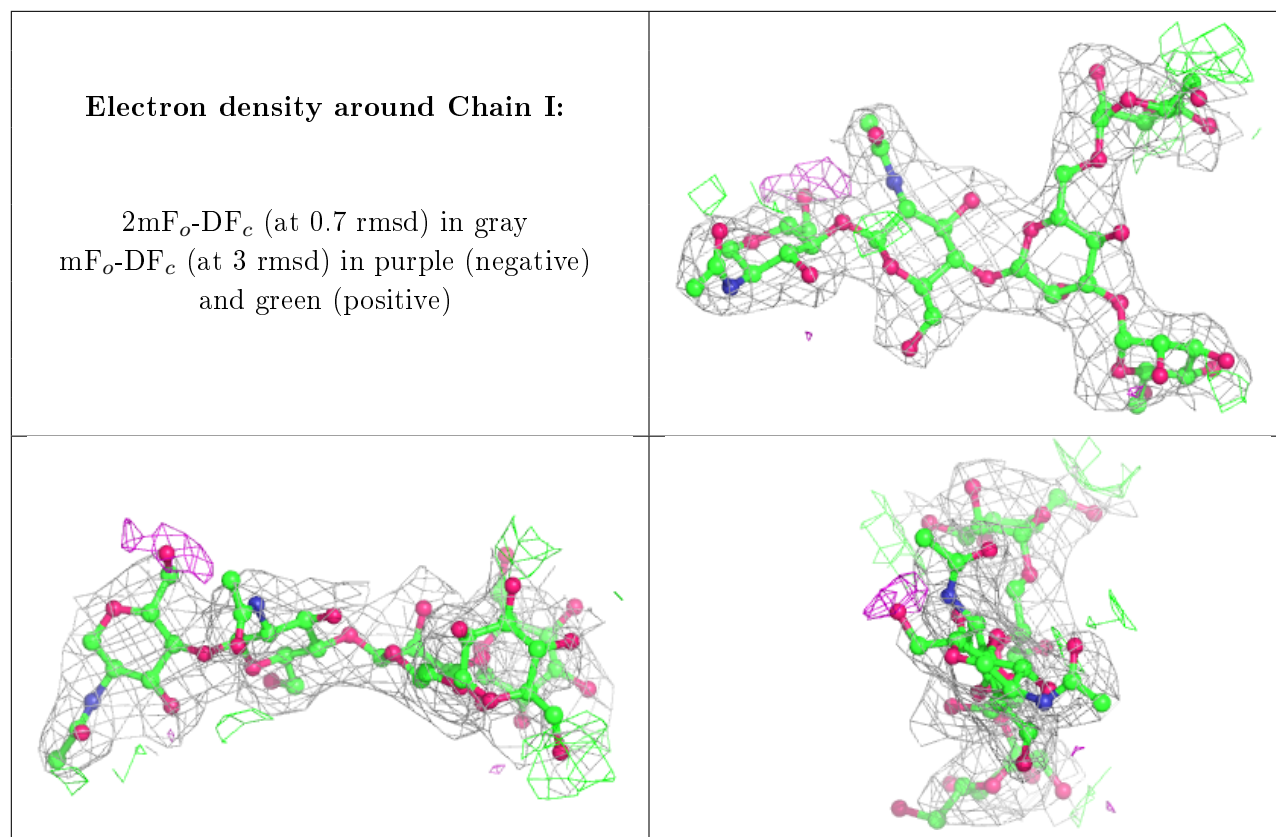
Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
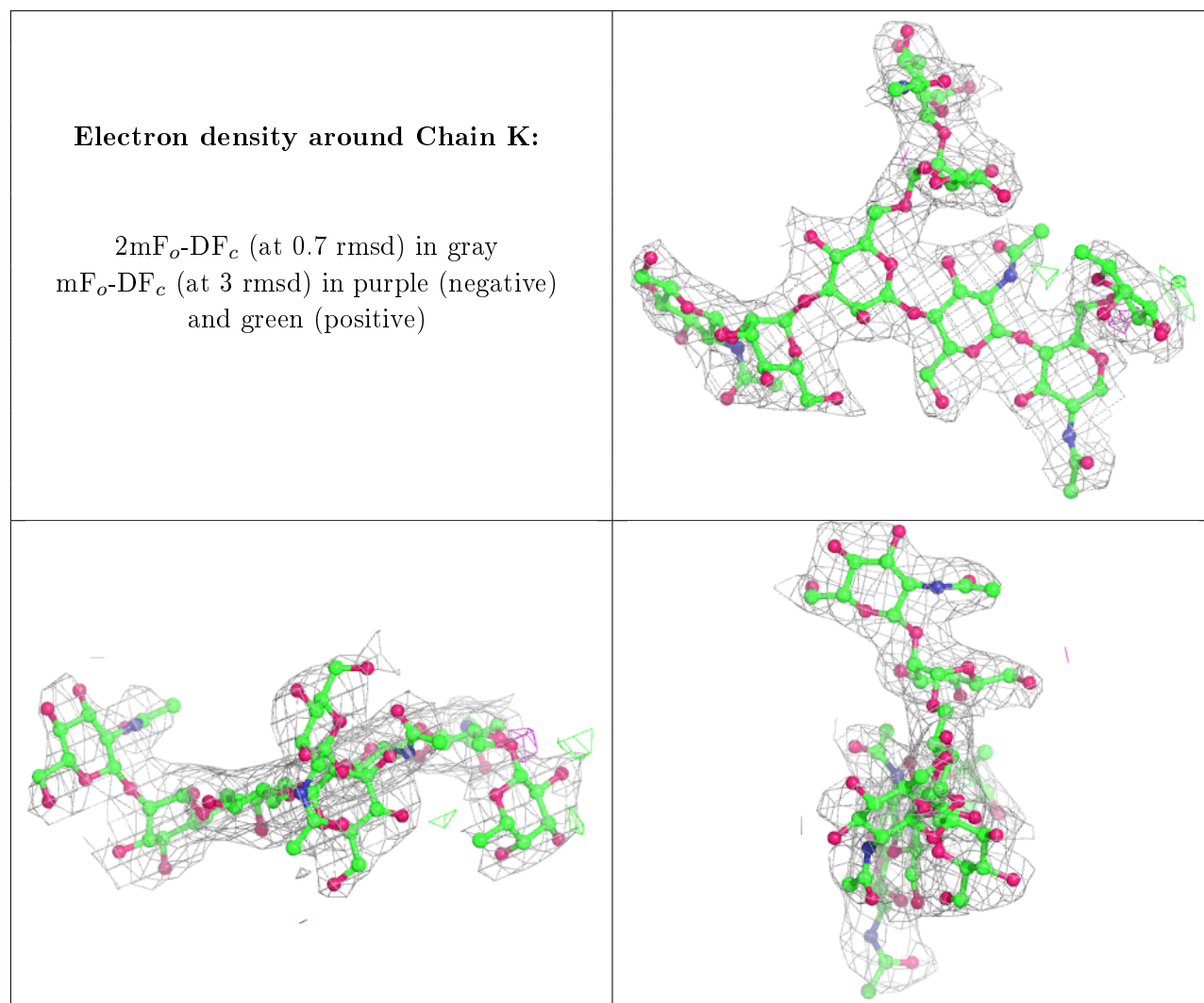and green (positive)

Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
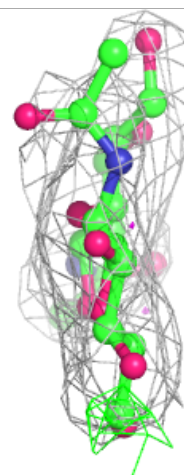
6.4 Ligands (i)

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(Å^2)	Q<0.9
9	NAG	F	201	14/15	0.84	0.27	64,74,77,78	0
8	IOD	A	1010	1/1	0.89	0.14	71,71,71,71	1
8	IOD	D	1009	1/1	0.91	0.12	86,86,86,86	1
8	IOD	A	1011	1/1	0.91	0.10	75,75,75,75	1
8	IOD	B	1012	1/1	0.93	0.11	80,80,80,80	1
8	IOD	F	207	1/1	0.95	0.10	81,81,81,81	1
8	IOD	E	1013	1/1	0.96	0.07	99,99,99,99	0
8	IOD	F	206	1/1	0.97	0.09	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	IOD	E	1011	1/1	0.97	0.09	85,85,85,85	0
8	IOD	C	209	1/1	0.98	0.09	91,91,91,91	0
8	IOD	E	1012	1/1	0.98	0.06	93,93,93,93	0
8	IOD	F	205	1/1	0.99	0.09	68,68,68,68	0
8	IOD	B	1010	1/1	0.99	0.13	49,49,49,49	0
8	IOD	B	1011	1/1	0.99	0.07	83,83,83,83	0
8	IOD	E	1010	1/1	0.99	0.08	102,102,102,102	0
8	IOD	C	208	1/1	1.00	0.16	36,36,36,36	0
8	IOD	F	204	1/1	1.00	0.17	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.