wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 01:19 PM EDT

PDB ID	:	4JM2
Title	:	Crystal Structure of PGT 135 Fab in Complex with gp120 Core Protein from HIV-1 Strain JR-FL Bound to CD4 and 17b Fab
Authors	:	Kong, L.; Wilson, I.A.
Deposited on	:	2013-03-13
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

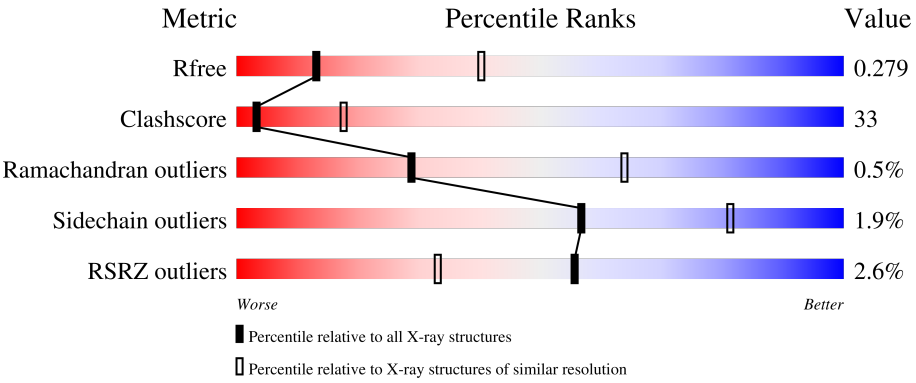
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	236	51% 43%
2	B	214	4% 54% 45%
3	C	214	4% 55% 45%
4	D	229	2% 53% 41%
5	E	321	55% 41%

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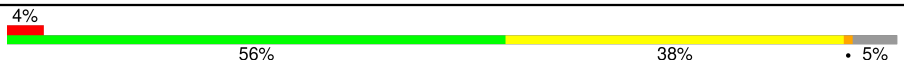
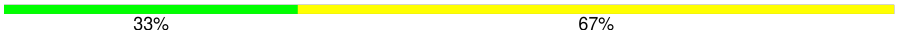
Mol	Chain	Length	Quality of chain
6	F	185	
7	G	8	
8	H	10	
9	I	3	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10907 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 PGT 135 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1744	1106	308	323	7	0	0	0

- Molecule 2 is a protein called PGT 135 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1672	1050	279	336	7	0	0	0

- Molecule 3 is a protein called 17b Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1646	1028	282	331	5	0	0	0

- Molecule 4 is a protein called 17b Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	220	1668	1056	279	328	5	0	0	0

- Molecule 5 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	315	2467	1539	437	470	21	0	0	0

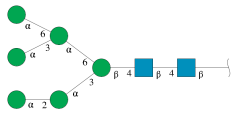
- Molecule 6 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	175	1363	851	239	269	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

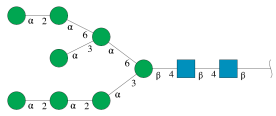
Chain	Residue	Modelled	Actual	Comment	Reference
F	184	ASN	-	expression tag	UNP P01730
F	185	THR	-	expression tag	UNP P01730

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



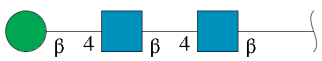
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	G	8	94	52	2	40	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



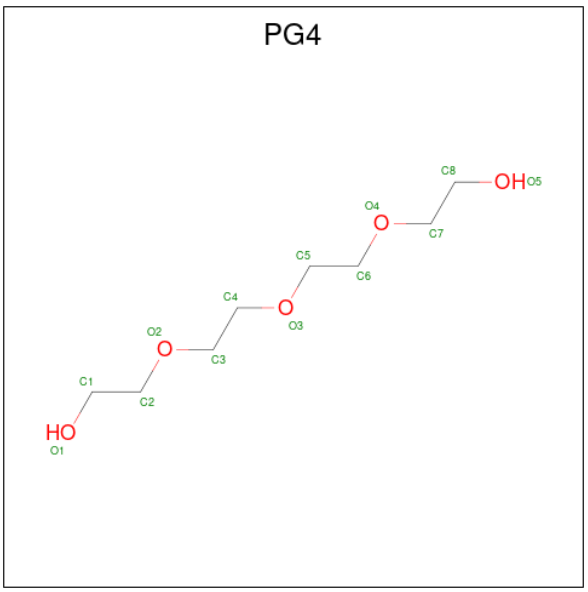
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	H	10	116	64	2	50	0	0	0

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



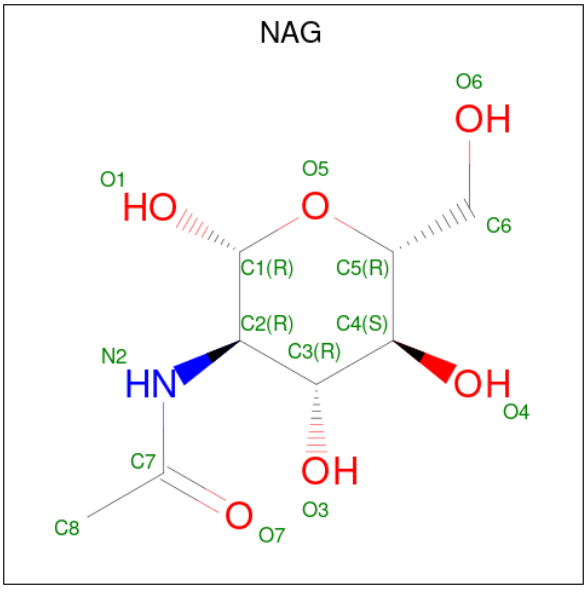
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	3	39	22	2	15	0	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 13 8 5	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O 1 1	0	0

3 Residue-property plots (i)

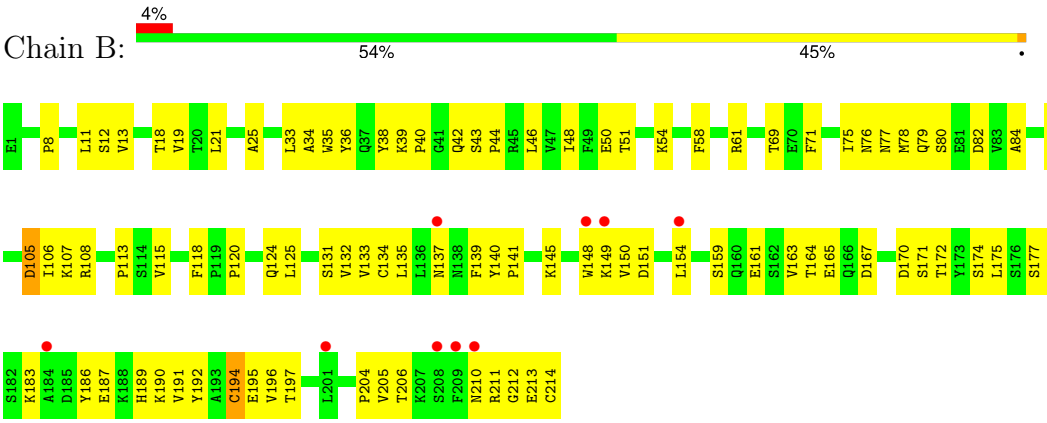
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PGT 135 Heavy chain

Chain A:

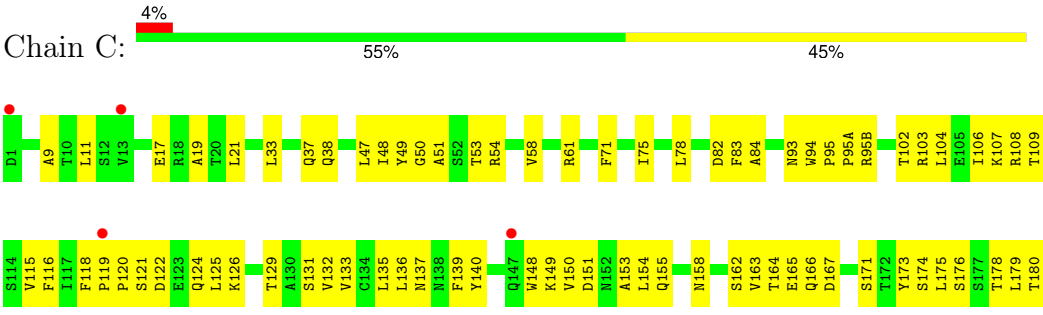
• Molecule 2: PGT 135 Light chain

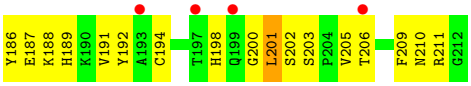
Chain B:



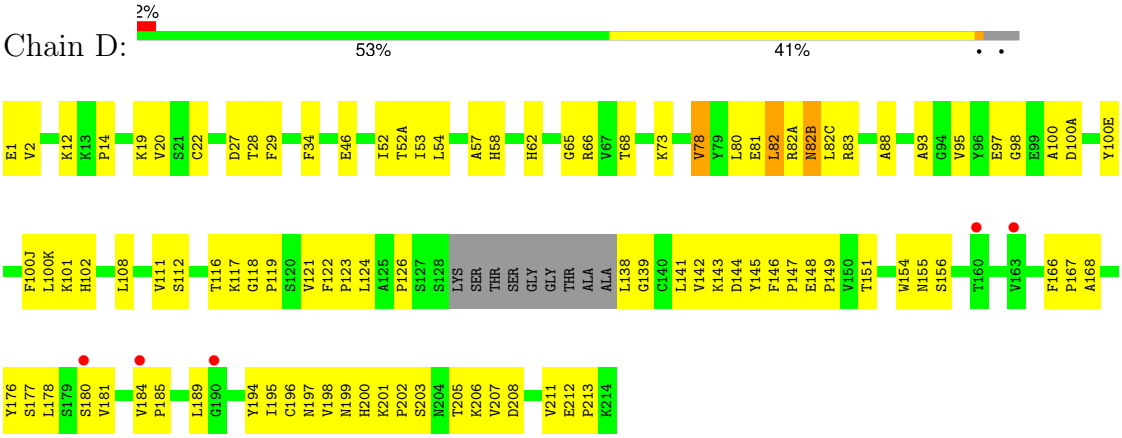
• Molecule 3: 17b Light chain

Chain C:

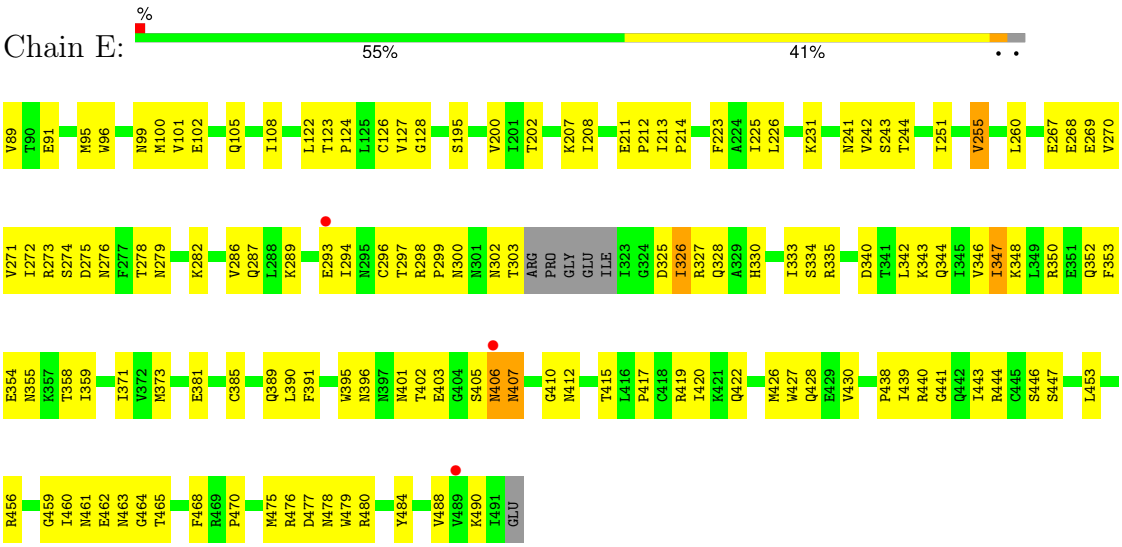




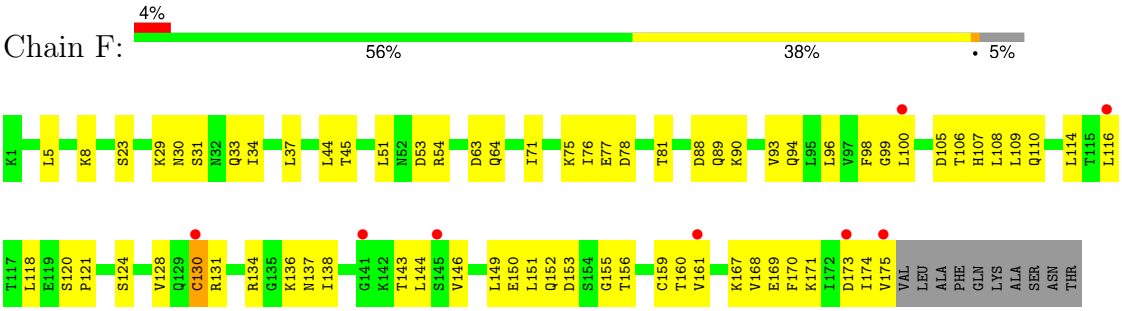
• Molecule 4: 17b Heavy chain



• Molecule 5: gp120



• Molecule 6: T-cell surface glycoprotein CD4



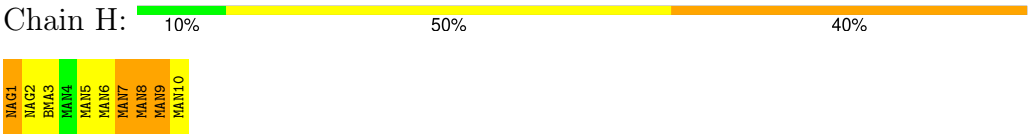
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain G:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran
ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-
(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl
ucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	218.41Å 92.15Å 88.19Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	43.58 – 3.10 43.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.58-3.10) 99.7 (43.58-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.238 , 0.285 0.243 , 0.279	Depositor DCC
R_{free} test set	1567 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	104.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 89.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10907	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA, PG4

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	0.43	0/1795	0.67	0/2447
2	B	0.45	0/1709	0.70	0/2323
3	C	0.41	0/1683	0.63	0/2288
4	D	0.51	0/1707	0.69	0/2325
5	E	0.48	0/2514	0.70	1/3404 (0.0%)
6	F	0.37	0/1382	0.62	0/1863
All	All	0.45	0/10790	0.67	1/14650 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	406	ASN	N-CA-C	-5.47	96.23	111.00

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	1744	0	1700	126	0
2	B	1672	0	1619	115	0
3	C	1646	0	1595	124	0
4	D	1668	0	1637	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2467	0	2412	159	0
6	F	1363	0	1389	92	0
7	G	94	0	79	7	0
8	H	116	0	97	4	0
9	I	39	0	34	0	0
10	C	13	0	18	0	0
11	E	84	0	78	10	0
12	A	1	0	0	0	0
All	All	10907	0	10658	710	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 33.

The worst 5 of 710 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)
5:E:268:GLU:CG	5:E:269:GLU:H	1.32	1.34
4:D:82(C):LEU:O	4:D:111:VAL:HG11	1.35	1.26
1:A:33:GLU:HG3	1:A:34:TRP:N	1.37	1.12
5:E:268:GLU:HG2	5:E:269:GLU:N	1.61	1.11
3:C:151:ASP:OD1	3:C:191:VAL:HG12	1.50	1.10

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	223/236 (94%)	201 (90%)	20 (9%)	2 (1%)	17 52
2	B	212/214 (99%)	199 (94%)	13 (6%)	0	100 100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	216/229 (94%)	213 (99%)	2 (1%)	1 (0%)	29 64
5	E	311/321 (97%)	291 (94%)	16 (5%)	4 (1%)	12 42
6	F	173/185 (94%)	165 (95%)	8 (5%)	0	100 100
All	All	1347/1399 (96%)	1273 (94%)	67 (5%)	7 (0%)	29 64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	326	ILE
5	E	407	ASN
1	A	62	SER
5	E	299	PRO
4	D	82(B)	ASN

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	193/201 (96%)	184 (95%)	9 (5%)	26 59
2	B	190/190 (100%)	187 (98%)	3 (2%)	62 84
3	C	184/184 (100%)	182 (99%)	2 (1%)	73 89
4	D	188/193 (97%)	184 (98%)	4 (2%)	53 79
5	E	282/287 (98%)	279 (99%)	3 (1%)	73 89
6	F	159/167 (95%)	157 (99%)	2 (1%)	69 87
All	All	1196/1222 (98%)	1173 (98%)	23 (2%)	57 81

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	78	VAL
4	D	208	ASP
4	D	117	LYS
5	E	255	VAL

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Mol	Chain	Res	Type
1	A	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	249	HIS
5	E	463	ASN
5	E	302	ASN
6	F	40	GLN
2	B	189	HIS

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)

21 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	$\#\|Z\| > 2$
7	NAG	G	1	5,7	14,14,15	1.07	1 (7%)	17,19,21	1.87	4 (23%)
7	NAG	G	2	7	14,14,15	1.32	2 (14%)	17,19,21	3.04	6 (35%)
7	BMA	G	3	7	11,11,12	1.47	1 (9%)	15,15,17	3.22	9 (60%)
7	MAN	G	4	7	11,11,12	1.54	3 (27%)	15,15,17	1.54	2 (13%)
7	MAN	G	5	7	11,11,12	1.53	3 (27%)	15,15,17	1.57	1 (6%)
7	MAN	G	6	7	11,11,12	1.01	0	15,15,17	2.39	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	G	7	7	11,11,12	1.25	1 (9%)	15,15,17	1.00	1 (6%)
7	MAN	G	8	7	11,11,12	0.69	0	15,15,17	1.57	2 (13%)
8	NAG	H	1	8,5	14,14,15	0.54	0	17,19,21	1.10	1 (5%)
8	MAN	H	10	8	11,11,12	0.65	0	15,15,17	0.70	0
8	NAG	H	2	8	14,14,15	1.00	1 (7%)	17,19,21	3.16	8 (47%)
8	BMA	H	3	8	11,11,12	1.45	2 (18%)	15,15,17	0.84	1 (6%)
8	MAN	H	4	8	11,11,12	0.59	0	15,15,17	0.71	0
8	MAN	H	5	8	11,11,12	0.69	0	15,15,17	1.46	3 (20%)
8	MAN	H	6	8	11,11,12	0.70	0	15,15,17	1.10	1 (6%)
8	MAN	H	7	8	11,11,12	1.53	3 (27%)	15,15,17	1.20	2 (13%)
8	MAN	H	8	8	11,11,12	1.51	3 (27%)	15,15,17	1.35	1 (6%)
8	MAN	H	9	8	11,11,12	1.29	1 (9%)	15,15,17	2.35	4 (26%)
9	NAG	I	1	9,5	14,14,15	1.42	3 (21%)	17,19,21	1.13	1 (5%)
9	NAG	I	2	9	14,14,15	0.53	0	17,19,21	1.17	2 (11%)
9	BMA	I	3	9	11,11,12	0.64	0	15,15,17	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
7	NAG	G	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1
7	MAN	G	6	7	-	0/2/19/22	0/1/1/1
7	MAN	G	7	7	-	0/2/19/22	0/1/1/1
7	MAN	G	8	7	-	0/2/19/22	0/1/1/1
8	NAG	H	1	8,5	-	1/6/23/26	0/1/1/1
8	MAN	H	10	8	-	0/2/19/22	0/1/1/1
8	NAG	H	2	8	-	2/6/23/26	0/1/1/1
8	BMA	H	3	8	-	0/2/19/22	0/1/1/1
8	MAN	H	4	8	-	0/2/19/22	0/1/1/1
8	MAN	H	5	8	-	2/2/19/22	0/1/1/1
8	MAN	H	6	8	-	0/2/19/22	0/1/1/1
8	MAN	H	7	8	-	0/2/19/22	0/1/1/1
8	MAN	H	8	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	H	9	8	-	2/2/19/22	0/1/1/1
9	NAG	I	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	7	MAN	O5-C1	-3.69	1.37	1.43
7	G	3	BMA	O5-C5	-3.15	1.37	1.43
8	H	9	MAN	O5-C1	3.10	1.48	1.43
8	H	7	MAN	O5-C1	3.06	1.48	1.43
7	G	5	MAN	O5-C1	2.97	1.48	1.43

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	2	NAG	C2-N2-C7	-8.31	111.77	122.90
8	H	2	NAG	O5-C1-C2	-7.46	99.75	111.29
8	H	9	MAN	C1-O5-C5	-7.37	102.31	112.19
7	G	3	BMA	C1-O5-C5	-6.93	102.90	112.19
7	G	2	NAG	O5-C5-C6	6.17	119.68	107.66

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	2	NAG	O5-C5-C6-O6
8	H	5	MAN	C4-C5-C6-O6
8	H	9	MAN	O5-C5-C6-O6
8	H	5	MAN	O5-C5-C6-O6
8	H	9	MAN	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	NAG	3	0
7	G	3	BMA	2	0
7	G	7	MAN	1	0
8	H	9	MAN	1	0

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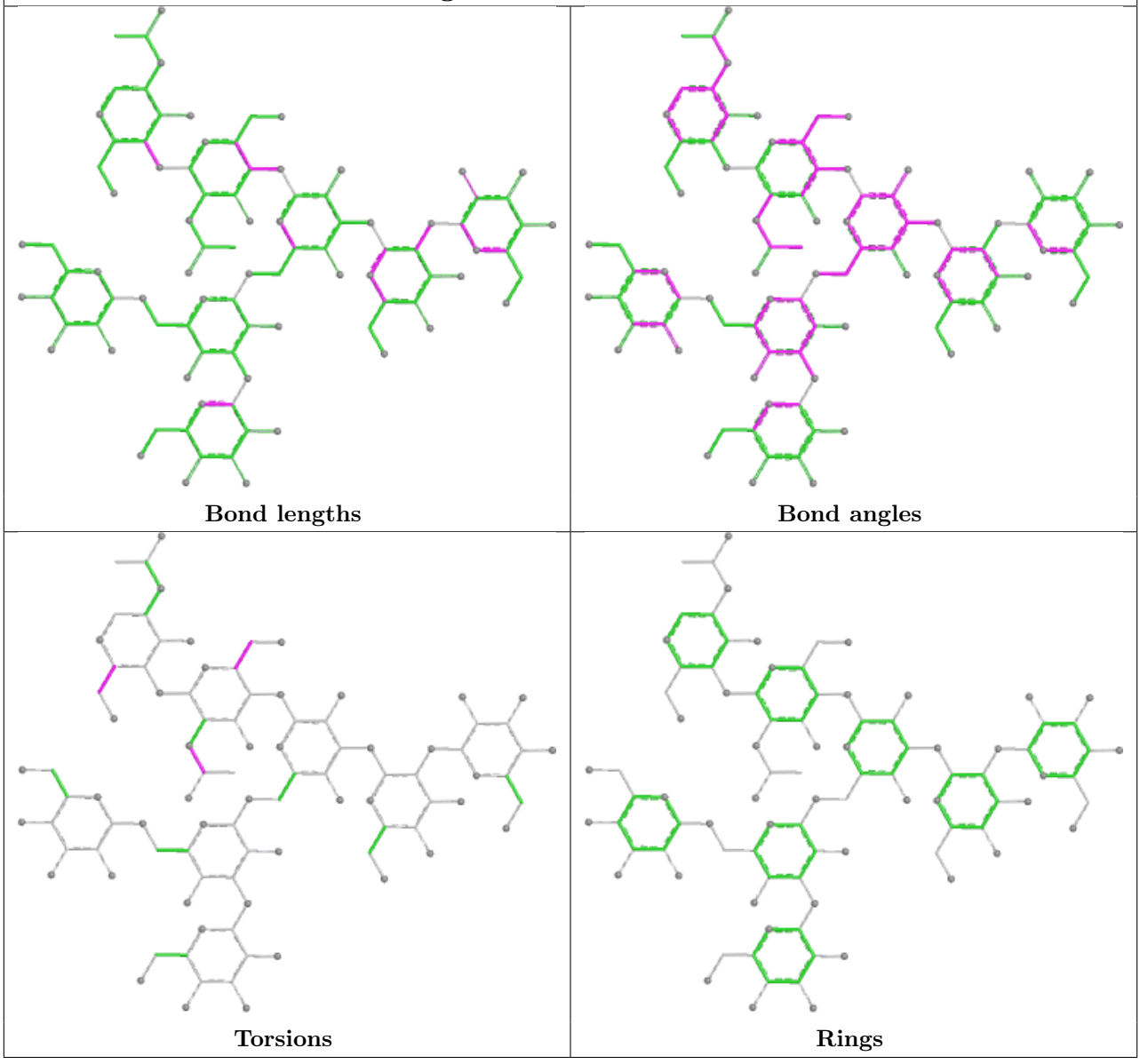
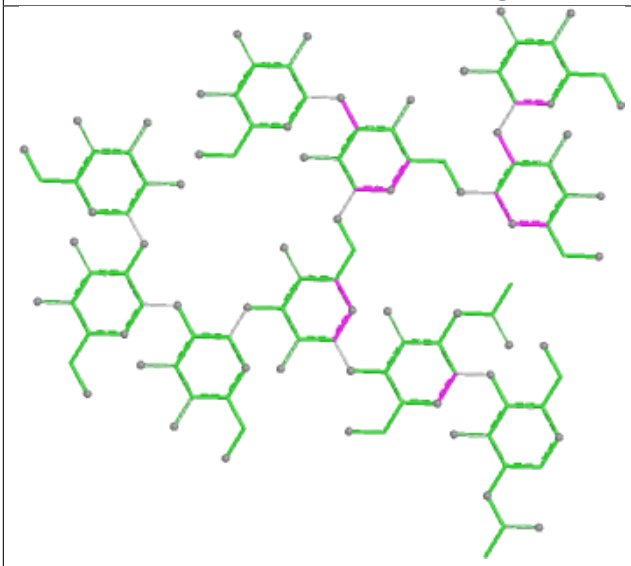
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	8	MAN	2	0
8	H	10	MAN	1	0
8	H	1	NAG	1	0
7	G	4	MAN	2	0
7	G	8	MAN	1	0
8	H	7	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

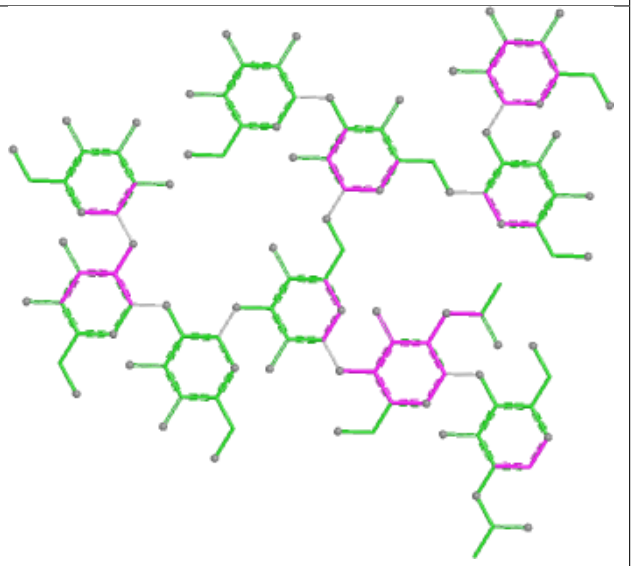
Oligosaccharide Chain G



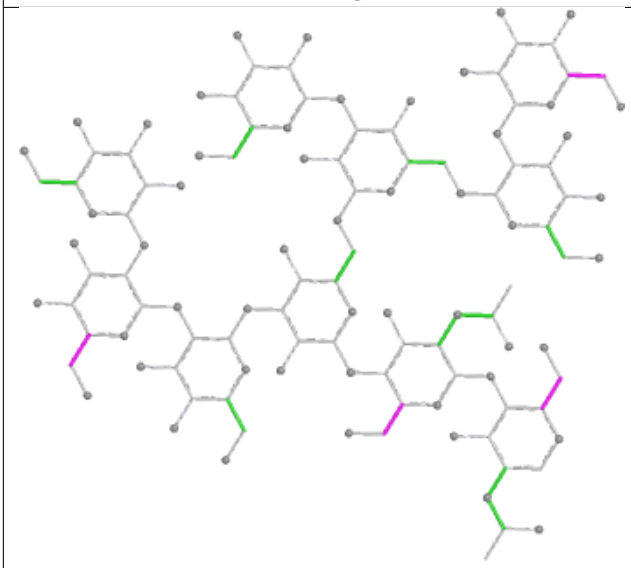
Oligosaccharide Chain H



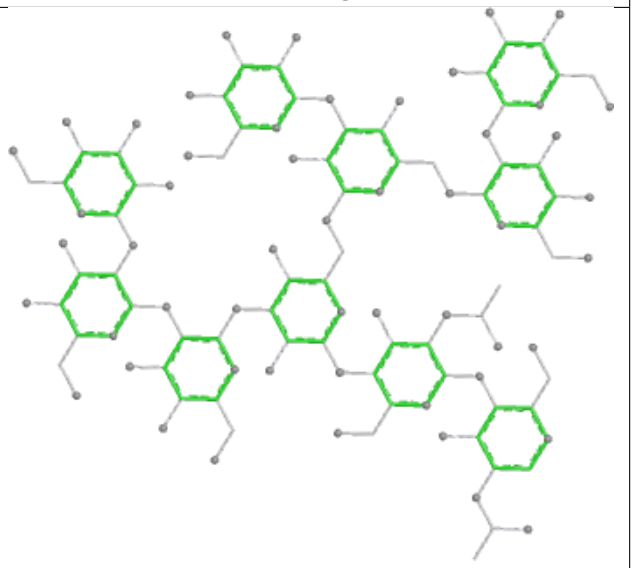
Bond lengths



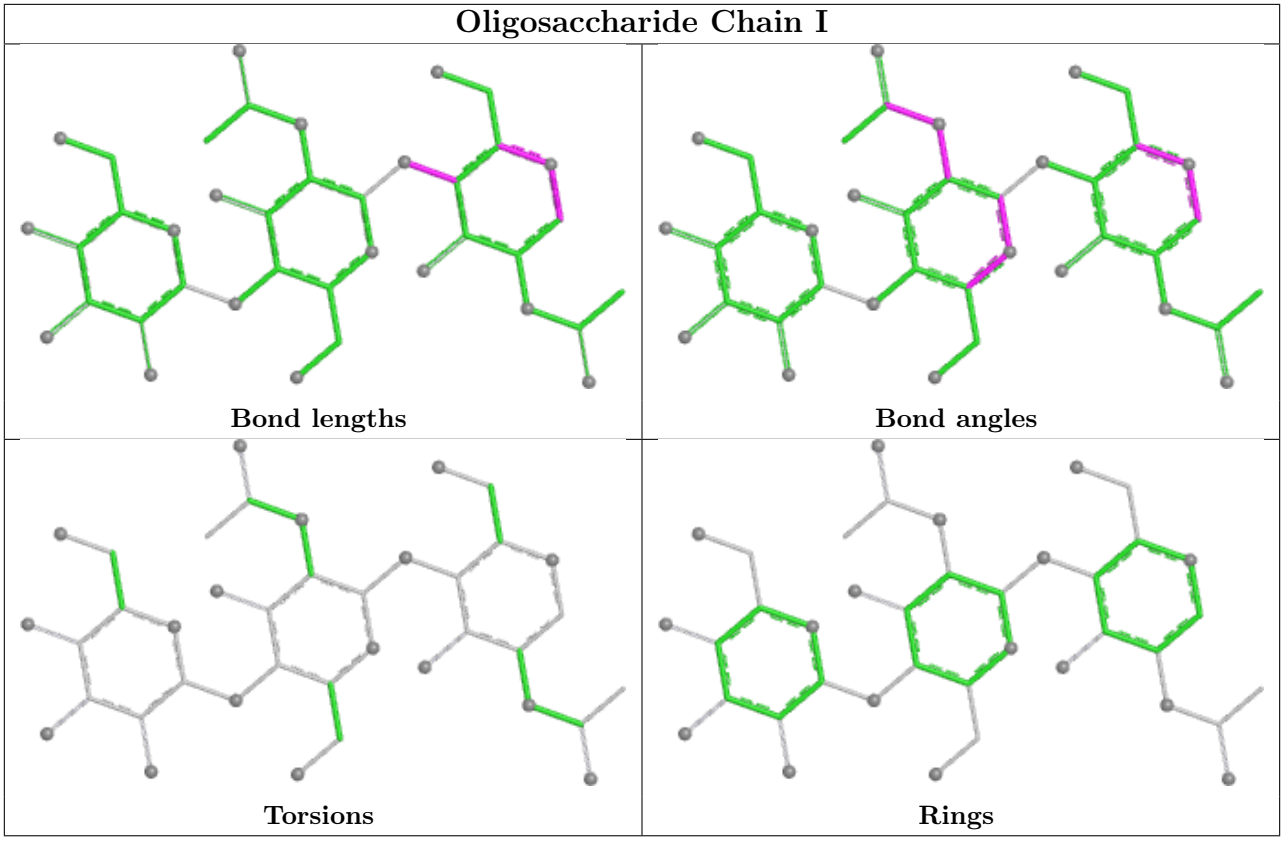
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
11	NAG	E	524	5	14,14,15	0.51	0	17,19,21	1.31	2 (11%)
11	NAG	E	526	5	14,14,15	0.64	0	17,19,21	0.70	0
11	NAG	E	522	5	14,14,15	0.54	0	17,19,21	0.78	0
10	PG4	C	301	-	12,12,12	0.68	0	11,11,11	0.81	0
11	NAG	E	523	5	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
11	NAG	E	525	5	14,14,15	0.55	0	17,19,21	0.70	0
11	NAG	E	527	5	14,14,15	0.62	0	17,19,21	0.55	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
11	NAG	E	524	5	-	1/6/23/26	0/1/1/1
11	NAG	E	526	5	-	3/6/23/26	0/1/1/1
11	NAG	E	522	5	-	2/6/23/26	0/1/1/1
10	PG4	C	301	-	-	4/10/10/10	-
11	NAG	E	523	5	-	4/6/23/26	0/1/1/1
11	NAG	E	525	5	-	4/6/23/26	0/1/1/1
11	NAG	E	527	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	524	NAG	C2-N2-C7	-2.85	119.08	122.90
11	E	523	NAG	C1-O5-C5	2.81	115.95	112.19
11	E	524	NAG	O5-C1-C2	-2.56	107.33	111.29

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	522	NAG	C8-C7-N2-C2
11	E	522	NAG	O7-C7-N2-C2
11	E	525	NAG	O7-C7-N2-C2
11	E	526	NAG	C8-C7-N2-C2
11	E	526	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	524	NAG	3	0
11	E	526	NAG	4	0
11	E	525	NAG	2	0
11	E	527	NAG	1	0

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, 95^{th} 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	227/236 (96%)	0.03	3 (1%)	77	59	75, 122, 168, 178	0
2	B	214/214 (100%)	0.21	9 (4%)	36	18	72, 121, 182, 197	0
3	C	214/214 (100%)	0.03	8 (3%)	41	21	81, 145, 187, 197	0
4	D	220/229 (96%)	0.05	5 (2%)	60	39	49, 96, 210, 242	0
5	E	315/321 (98%)	-0.02	3 (0%)	82	67	27, 110, 174, 204	0
6	F	175/185 (94%)	0.22	8 (4%)	32	16	79, 143, 214, 222	0
All	All	1365/1399 (97%)	0.07	36 (2%)	56	33	27, 122, 194, 242	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	SER	4.1
2	B	208	SER	3.8
6	F	145	SER	3.8
2	B	210	ASN	3.5
4	D	184	VAL	3.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

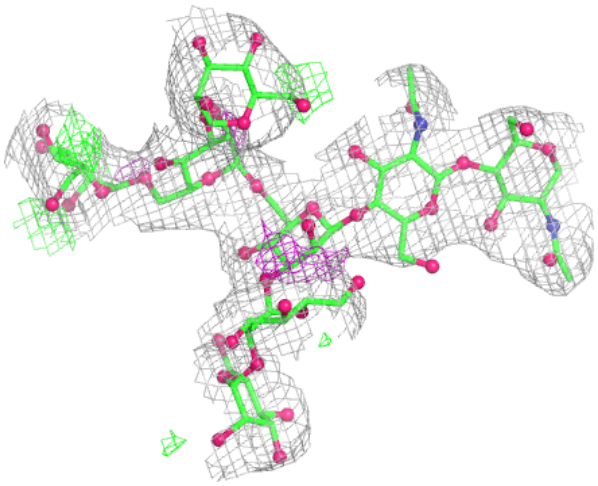
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

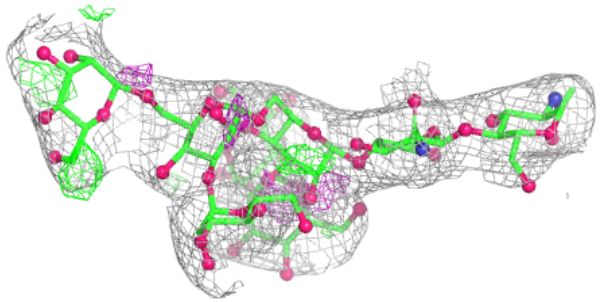
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BMA	I	3	11/12	0.76	0.14	131,140,144,146	0
7	MAN	G	8	11/12	0.80	0.23	94,97,103,110	0
8	MAN	H	9	11/12	0.82	0.19	135,140,144,152	0
7	MAN	G	5	11/12	0.85	0.21	148,152,157,159	0
7	MAN	G	4	11/12	0.86	0.21	121,125,134,144	0
8	MAN	H	6	11/12	0.86	0.25	100,107,114,114	0
7	MAN	G	6	11/12	0.88	0.18	85,91,95,101	0
9	NAG	I	1	14/15	0.89	0.23	104,113,123,136	0
9	NAG	I	2	14/15	0.89	0.19	116,125,135,139	0
8	MAN	H	10	11/12	0.89	0.26	87,88,90,93	0
8	MAN	H	7	11/12	0.90	0.18	89,93,101,107	0
8	MAN	H	4	11/12	0.92	0.20	86,88,97,97	0
7	BMA	G	3	11/12	0.92	0.14	88,94,105,110	0
8	NAG	H	1	14/15	0.93	0.20	87,96,99,101	0
8	NAG	H	2	14/15	0.93	0.17	94,102,105,118	0
8	MAN	H	8	11/12	0.93	0.26	116,121,127,128	0
7	MAN	G	7	11/12	0.93	0.20	86,92,103,104	0
8	MAN	H	5	11/12	0.94	0.21	80,86,94,100	0
7	NAG	G	2	14/15	0.95	0.21	77,87,100,110	0
8	BMA	H	3	11/12	0.95	0.17	83,89,96,96	0
7	NAG	G	1	14/15	0.97	0.19	75,86,100,106	0

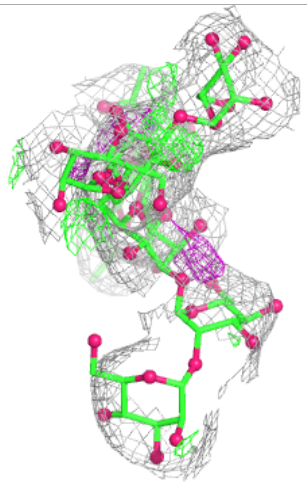
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

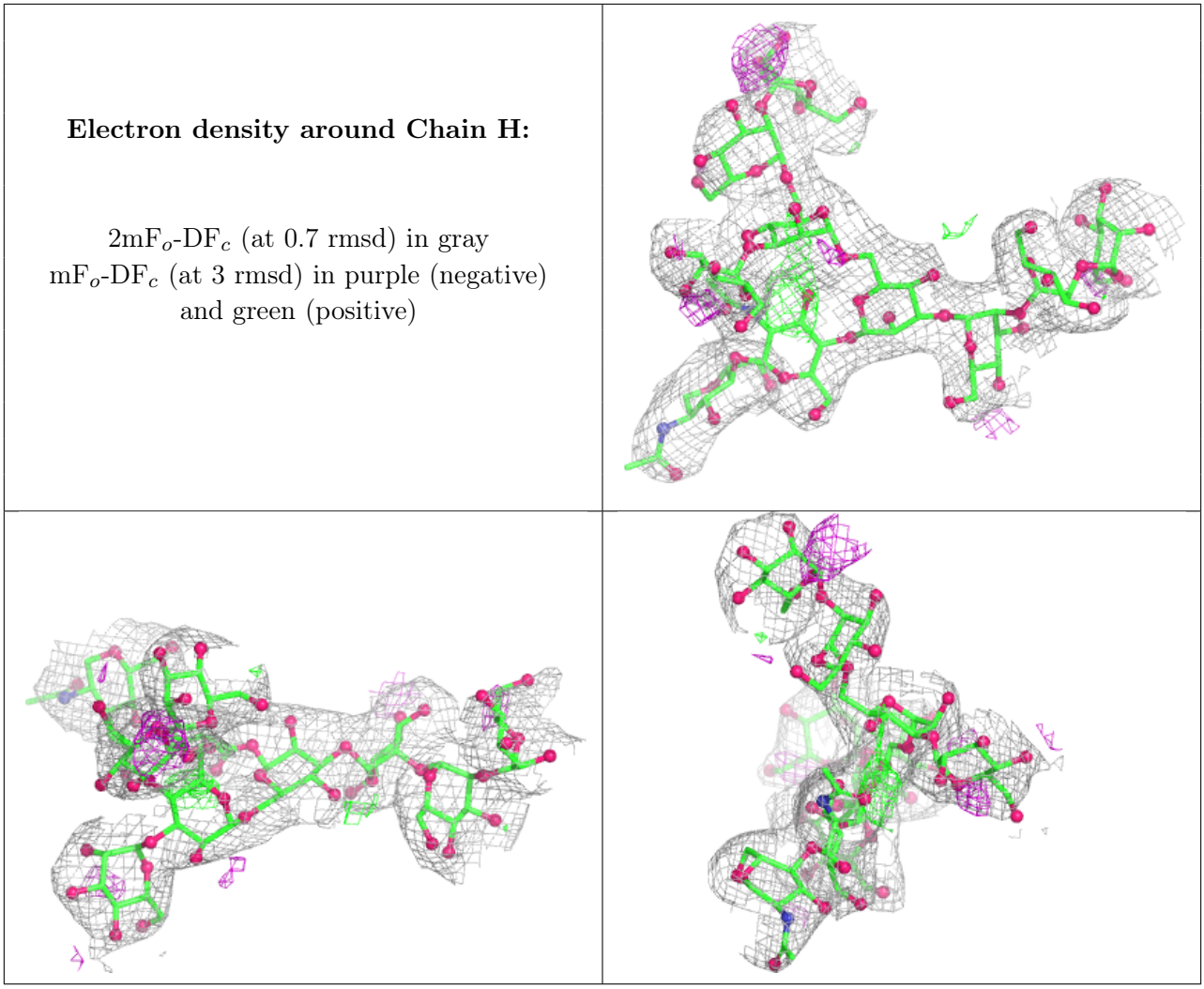






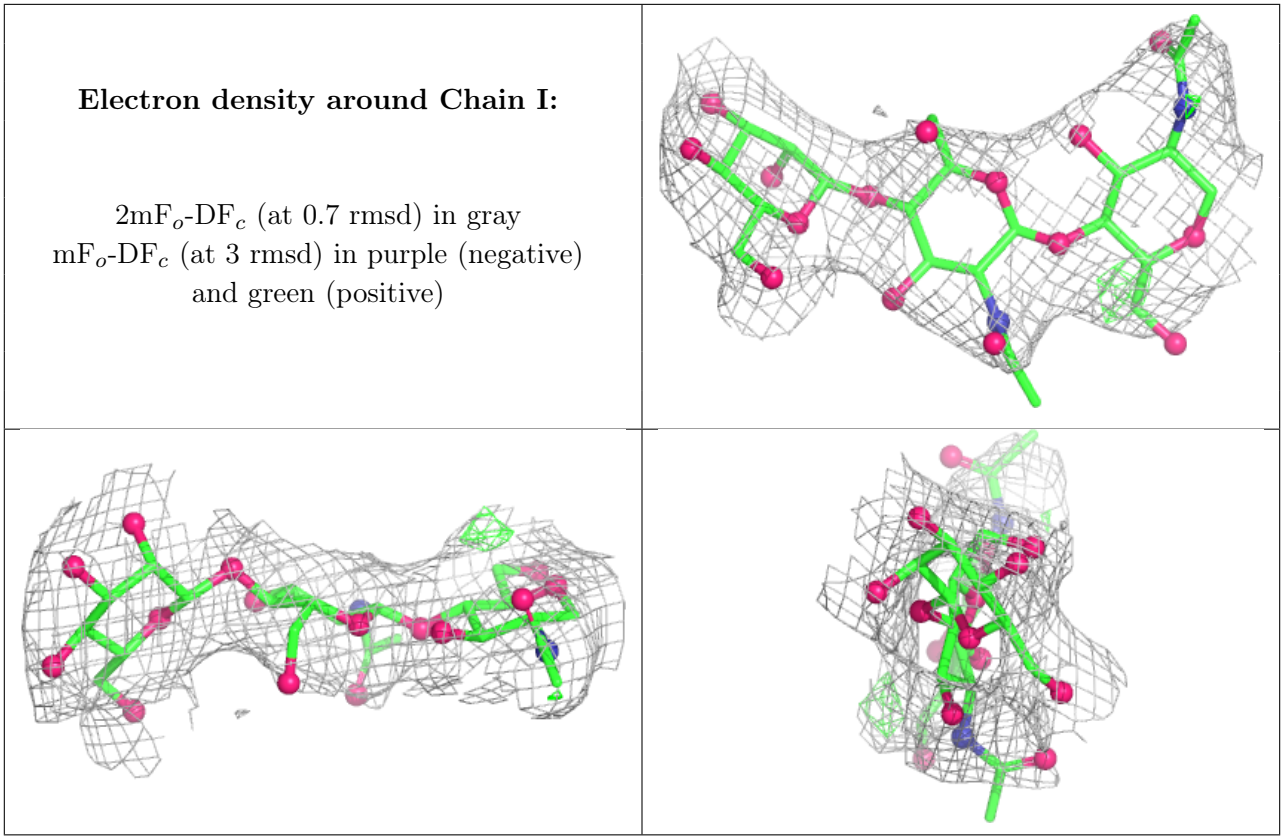
Electron density around Chain H:

$2mF_o$-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 I:

$2mF_o$-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, 95^{th} 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
11	NAG	E	525	14/15	0.58	0.37	148,154,164,165	0
10	PG4	C	301	13/13	0.73	0.26	85,107,121,123	0
11	NAG	E	524	14/15	0.82	0.25	120,142,156,156	0
11	NAG	E	526	14/15	0.86	0.16	114,126,132,132	0
11	NAG	E	522	14/15	0.92	0.20	100,107,112,115	0
11	NAG	E	527	14/15	0.92	0.18	115,135,142,144	0
11	NAG	E	523	14/15	0.94	0.22	86,91,97,100	0

6.5 Other polymers

There are no such residues in this entry.