Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 10:29 pm BST

PDB ID	:	5JPN / pdb_00005jpn
Title	:	Structure of human complement C4 rebuilt using iMDFF
Authors	:	Croll, T.I.; Andersen, G.R.
Deposited on	:	2016-05-03
Resolution	:	3.60 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 (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:

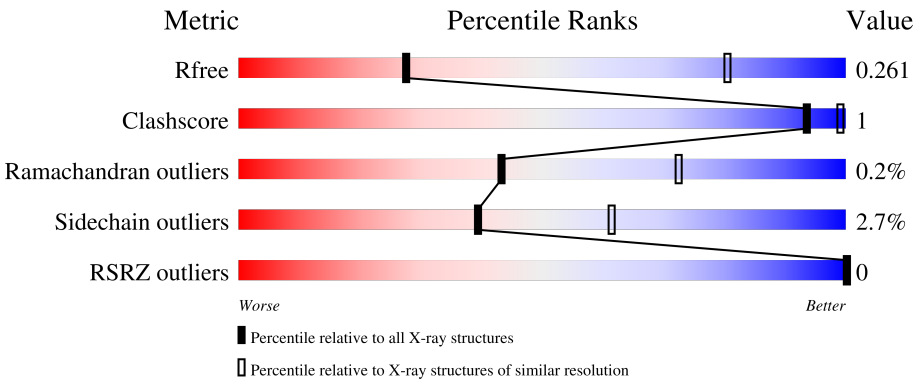
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	656	93% 6% •
2	B	767	87% • • 9%
3	C	290	92% 8%
4	D	3	100%
5	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
6	F	5	40% 60%
6	G	5	40% 60%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12891 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 Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	651	5012	3185	872	939	16	0	0	0

- Molecule 2 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	697	5361	3371	943	1023	24	0	0	0

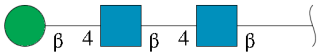
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	SER	THR	variant	UNP P0C0L4

- Molecule 3 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	290	2311	1451	411	432	17	0	0	0

- Molecule 4 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.

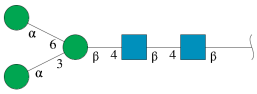


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

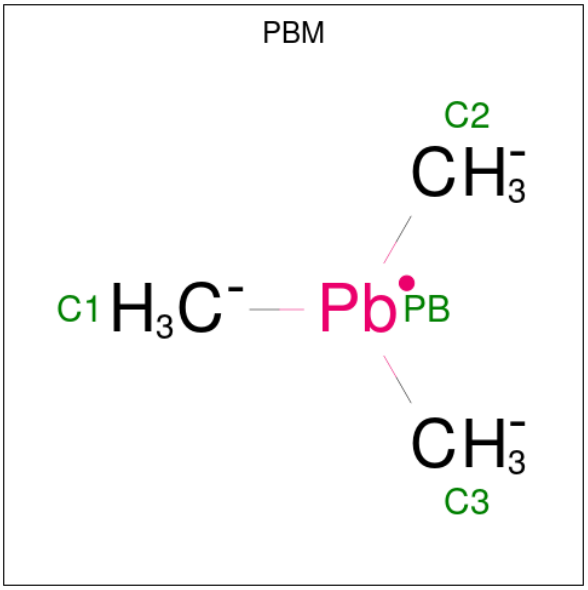
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0

- Molecule 6 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.



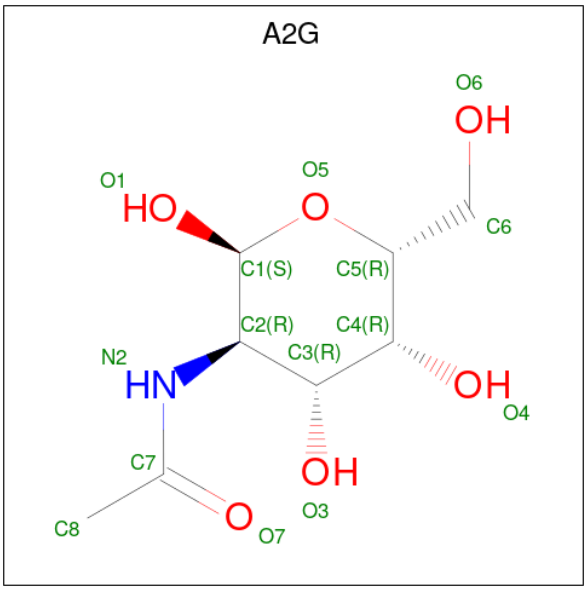
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	5	61	34	2	25	0	0	0
6	G	5	61	34	2	25	0	0	0

- Molecule 7 is TRIMETHYL LEAD ION (CCD ID: PBM) (formula: C_3H_9Pb).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Pb 1 1	0	0
7	B	1	Total Pb 1 1	0	0
7	B	1	Total Pb 1 1	0	0
7	C	1	Total Pb 1 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



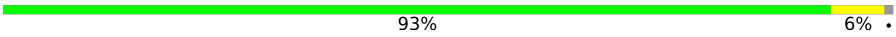
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O 14 8 1 5	0	0

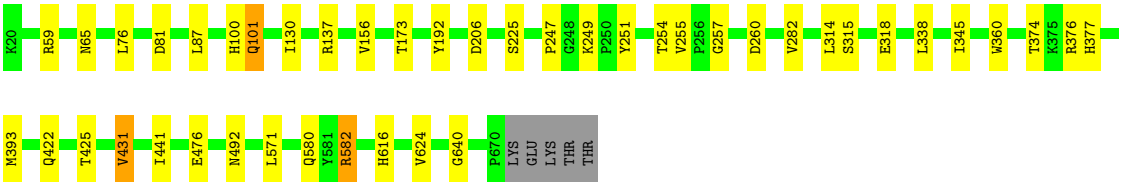
3 Residue-property plots (i)

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: Complement C4-A

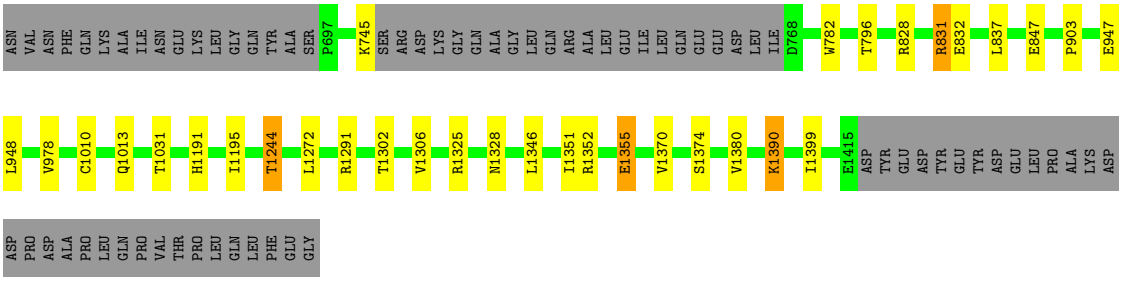
Chain A:





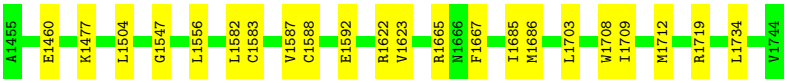
• Molecule 2: Complement C4-A

Chain B:



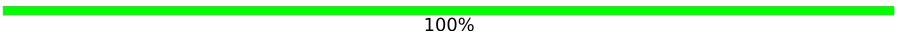
• Molecule 3: Complement C4-A

Chain C:



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

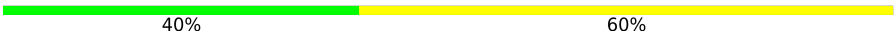
Chain D:



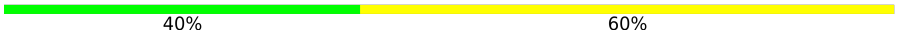
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 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

Chain F: 

• Molecule 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

Chain G: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.45Å 103.31Å 256.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 3.60 45.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.90-3.60) 99.6 (45.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.57Å)	Xtriage
Refinement program	PHENIX dev_2376	Depositor
R, R_{free}	0.215 , 0.263 0.216 , 0.261	Depositor DCC
R_{free} test set	1348 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	113.2	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 89.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12891	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PBM, NAG, A2G, MAN, BMA

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	0.11	0/5128	0.35	1/6961 (0.0%)
2	B	0.11	0/5472	0.32	0/7436
3	C	0.11	0/2359	0.35	0/3188
All	All	0.11	0/12959	0.34	1/17585 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	MET	CB-CA-C	-5.88	109.77	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	582	ARG	Peptide

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	5012	0	5025	17	0
2	B	5361	0	5310	13	0
3	C	2311	0	2253	8	0
4	D	39	0	34	0	0
5	E	28	0	25	0	0
6	F	61	0	52	0	0
6	G	61	0	52	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	B	14	0	12	0	0
All	All	12891	0	12763	37	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 1.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLU:HB3	1:A:492:ASN:HB2	1.71	0.72
1:A:100:HIS:CG	1:A:101:GLN:H	2.08	0.71
2:B:1325:ARG:HB3	2:B:1374:SER:HB2	1.89	0.55
1:A:81:ASP:OD1	1:A:81:ASP:N	2.39	0.53
3:C:1712:MET:HE2	3:C:1712:MET:HA	1.92	0.51
2:B:1013:GLN:OE1	2:B:1013:GLN:N	2.38	0.49
2:B:832:GLU:H	2:B:832:GLU:CD	2.20	0.49
3:C:1667:PHE:HB3	3:C:1703:LEU:HD21	1.94	0.49
2:B:1191:HIS:CE1	2:B:1195:ILE:HD11	2.47	0.49
1:A:100:HIS:CG	1:A:101:GLN:N	2.79	0.49
3:C:1685:ILE:HA	3:C:1708:TRP:O	2.13	0.48
2:B:978:VAL:HG12	2:B:1380:VAL:HG22	1.95	0.48
3:C:1547:GLY:HA3	3:C:1582:LEU:HD22	1.93	0.48
2:B:831:ARG:HA	2:B:831:ARG:HH11	1.79	0.48
3:C:1583:CYS:HB2	3:C:1587:VAL:HG23	1.97	0.46
1:A:137:ARG:HG3	1:A:225:SER:HA	1.97	0.46
2:B:847:GLU:O	2:B:903:PRO:HD2	2.16	0.46
2:B:1352:ARG:HA	2:B:1355:GLU:OE2	2.16	0.46
1:A:255:VAL:HG12	1:A:257:GLY:H	1.81	0.45
2:B:1399:ILE:HD12	3:C:1556:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:OD2	1:A:206:ASP:N	2.45	0.44
3:C:1685:ILE:HG22	3:C:1709:ILE:HG12	2.00	0.44
2:B:948:LEU:HD22	2:B:1370:VAL:HG21	2.00	0.44
2:B:947:GLU:OE2	2:B:1291:ARG:NH1	2.51	0.43
2:B:782:TRP:H	2:B:782:TRP:CD1	2.36	0.43
3:C:1623:VAL:HG21	3:C:1686:MET:HB2	2.01	0.43
1:A:338:LEU:N	1:A:360:TRP:O	2.48	0.43
1:A:425:THR:HG22	1:A:431:VAL:HG23	2.01	0.43
1:A:247:PRO:HB3	1:A:360:TRP:CZ2	2.54	0.42
1:A:249:LYS:C	1:A:251:TYR:H	2.26	0.42
1:A:377:HIS:CG	1:A:640:GLY:HA2	2.54	0.42
1:A:315:SER:HB2	1:A:318:GLU:HG3	2.02	0.42
2:B:1302:THR:O	2:B:1306:VAL:HG12	2.20	0.41
1:A:374:THR:O	1:A:376:ARG:NH1	2.47	0.40
1:A:59:ARG:HD2	1:A:65:ASN:HB3	2.03	0.40
1:A:173:THR:HG22	1:A:192:TYR:HA	2.03	0.40
1:A:582:ARG:HD2	1:A:582:ARG:HA	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	649/656 (99%)	618 (95%)	30 (5%)	1 (0%)	43 72
2	B	693/767 (90%)	661 (95%)	30 (4%)	2 (0%)	36 65
3	C	288/290 (99%)	272 (94%)	15 (5%)	1 (0%)	36 65
All	All	1630/1713 (95%)	1551 (95%)	75 (5%)	4 (0%)	43 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1390	LYS
1	A	101	GLN
3	C	1622	ARG
2	B	1244	THR

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	557/562 (99%)	541 (97%)	16 (3%)	37	60
2	B	581/641 (91%)	567 (98%)	14 (2%)	43	63
3	C	248/248 (100%)	240 (97%)	8 (3%)	34	58
All	All	1386/1451 (96%)	1348 (97%)	38 (3%)	39	61

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	87	LEU
1	A	130	ILE
1	A	156	VAL
1	A	254	THR
1	A	260	ASP
1	A	282	VAL
1	A	314	LEU
1	A	345	ILE
1	A	422	GLN
1	A	431	VAL
1	A	441	ILE
1	A	571	LEU
1	A	580	GLN
1	A	616	HIS
1	A	624	VAL
2	B	745	LYS
2	B	796	THR
2	B	828	ARG

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Mol	Chain	Res	Type
2	B	831	ARG
2	B	837	LEU
2	B	1010	CYS
2	B	1031	THR
2	B	1244	THR
2	B	1272	LEU
2	B	1328	ASN
2	B	1346	LEU
2	B	1351	ILE
2	B	1355	GLU
2	B	1390	LYS
3	C	1460	GLU
3	C	1477	LYS
3	C	1504	LEU
3	C	1588	CYS
3	C	1592	GLU
3	C	1665	ARG
3	C	1719	ARG
3	C	1734	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	320	GLN
1	A	430	GLN
2	B	836	HIS
2	B	940	HIS
2	B	1033	GLN
2	B	1092	GLN
2	B	1129	GLN
2	B	1296	GLN
2	B	1303	GLN
2	B	1320	HIS
3	C	1467	HIS
3	C	1652	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)

15 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	D	1	4,1	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	0.58	0
4	BMA	D	3	4	11,11,12	0.61	0	15,15,17	0.74	0
5	NAG	E	1	5,2	14,14,15	0.62	1 (7%)	17,19,21	0.68	0
5	NAG	E	2	5	14,14,15	0.30	0	17,19,21	0.45	0
6	NAG	F	1	6,2	14,14,15	0.29	0	17,19,21	0.53	0
6	NAG	F	2	6	14,14,15	0.39	0	17,19,21	0.56	0
6	BMA	F	3	6	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
6	MAN	F	4	6	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
6	MAN	F	5	6	11,11,12	0.79	0	15,15,17	0.84	1 (6%)
6	NAG	G	1	6,2	14,14,15	0.43	0	17,19,21	0.53	0
6	NAG	G	2	6	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
6	BMA	G	3	6	11,11,12	0.55	0	15,15,17	0.77	0
6	MAN	G	4	6	11,11,12	0.73	0	15,15,17	0.89	1 (6%)
6	MAN	G	5	6	11,11,12	0.72	0	15,15,17	0.89	1 (6%)

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	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	1/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	NAG	G	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	1/2/19/22	0/1/1/1
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-2.07	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	4	MAN	C1-O5-C5	2.27	115.26	112.19
6	F	5	MAN	O2-C2-C3	-2.26	105.61	110.14
6	G	4	MAN	O2-C2-C3	-2.25	105.64	110.14
6	G	5	MAN	O2-C2-C3	-2.23	105.67	110.14
6	F	4	MAN	O2-C2-C3	-2.18	105.77	110.14
6	G	2	NAG	C1-O5-C5	2.16	115.12	112.19
6	F	3	BMA	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

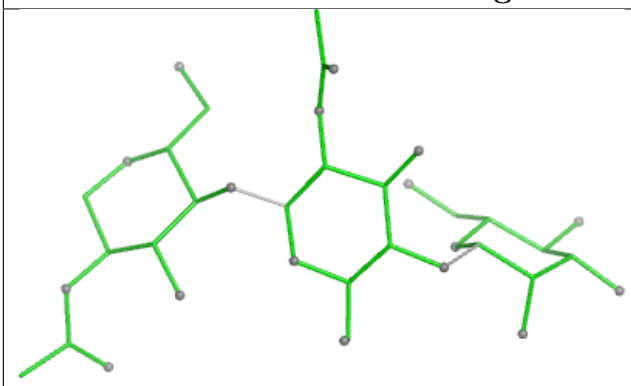
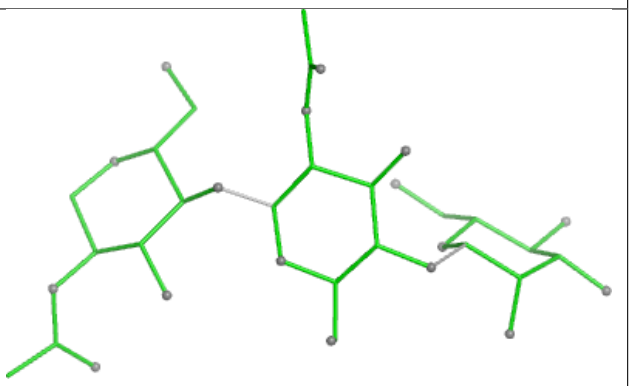
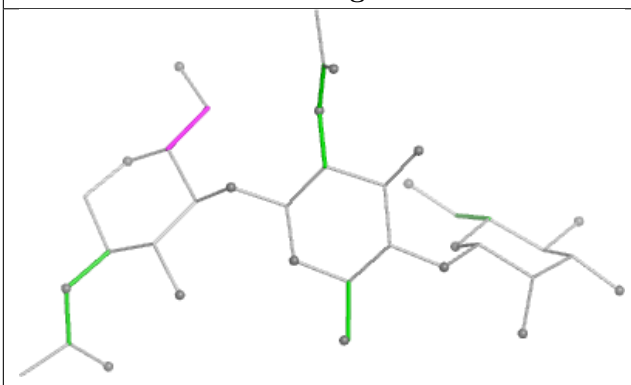
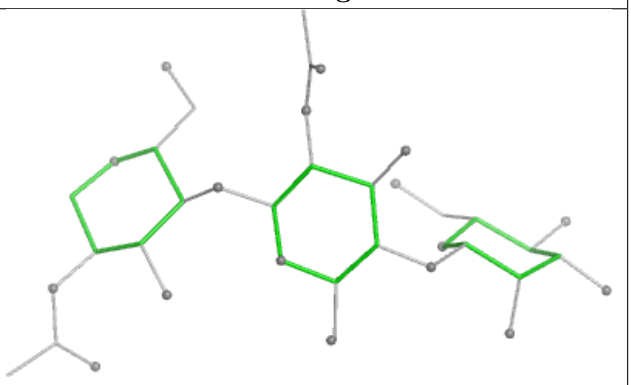
Mol	Chain	Res	Type	Atoms
6	F	4	MAN	O5-C5-C6-O6
6	G	4	MAN	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

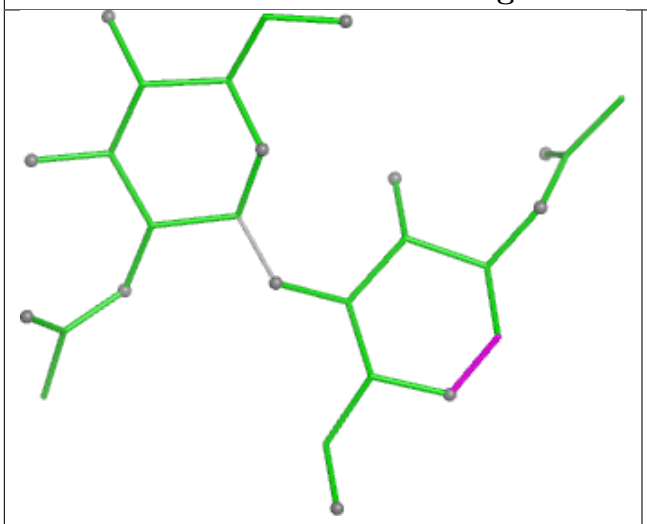
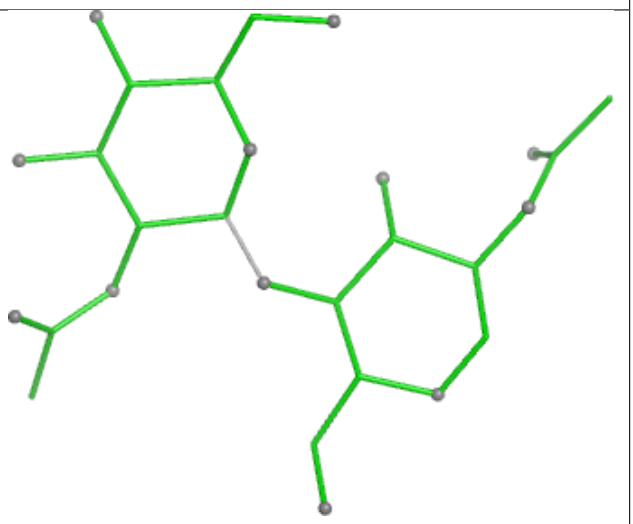
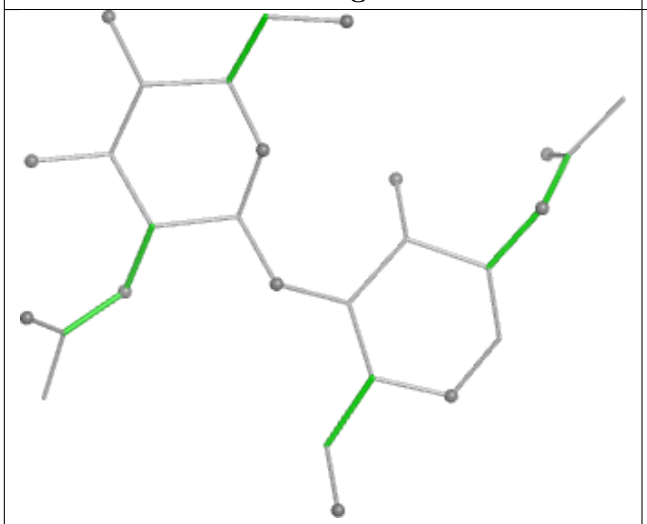
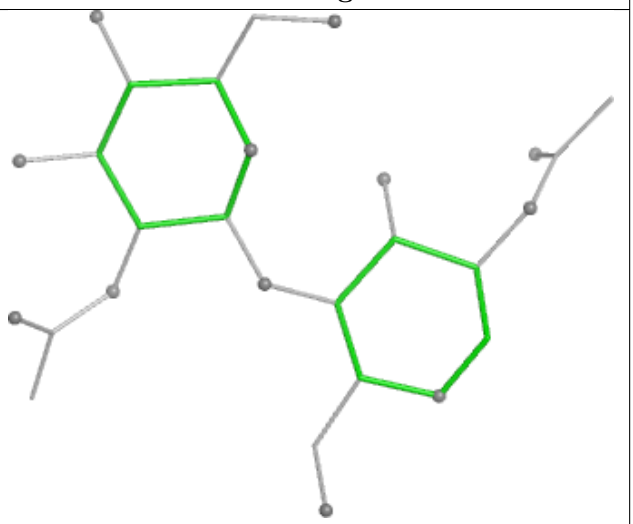
There are no ring outliers.

No monomer is involved in short contacts.

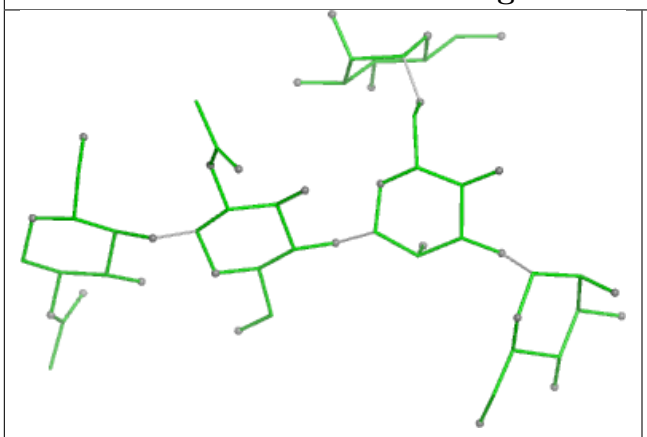
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

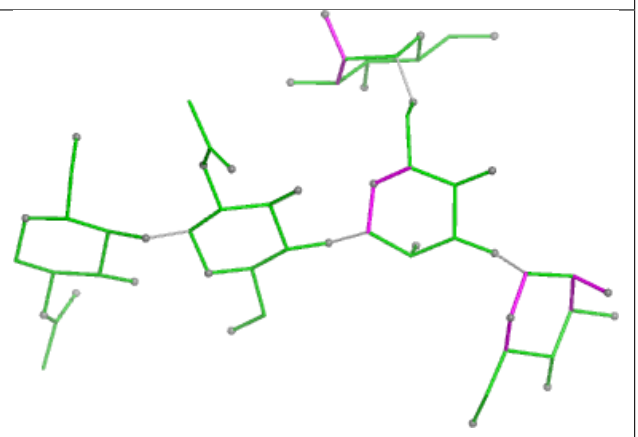
Oligosaccharide Chain D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain E	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

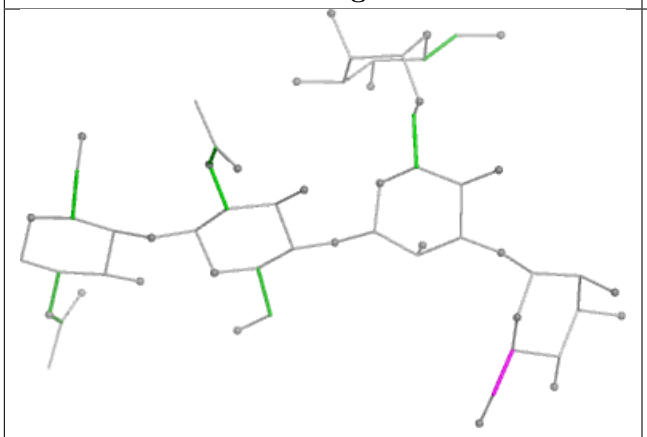
Oligosaccharide Chain F



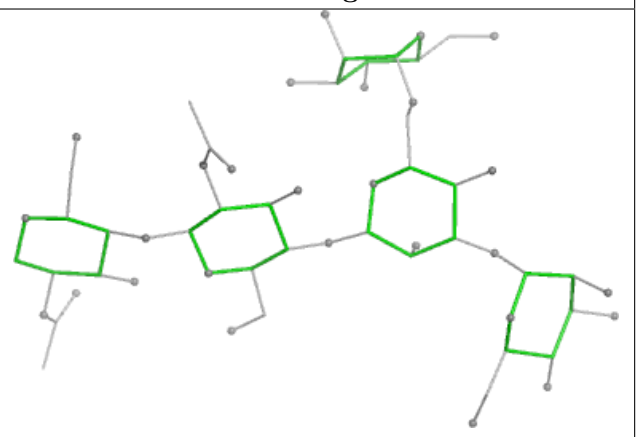
Bond lengths



Bond angles

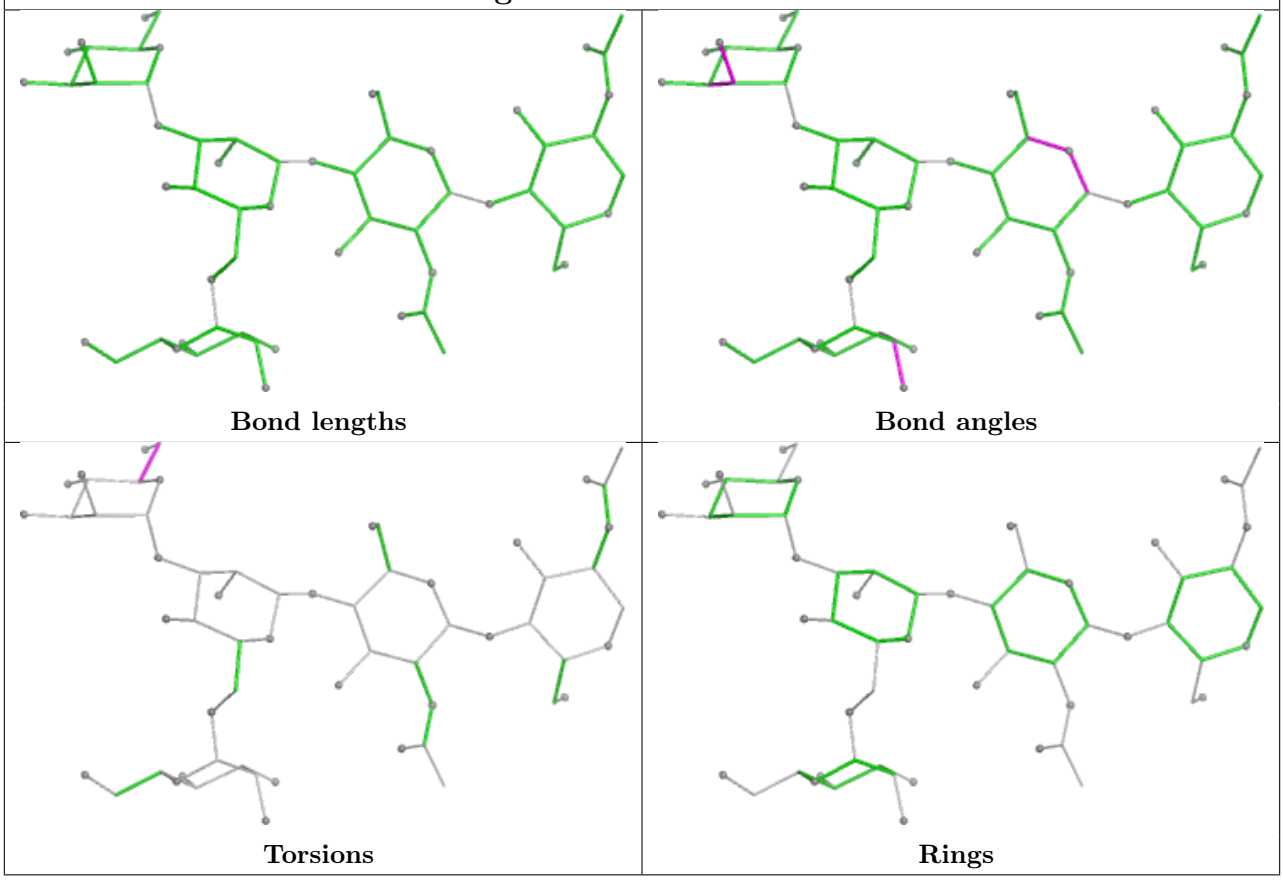


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are modelled with single atom - 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	$\#\|Z\| > 2$
8	A2G	B	1508	2	14,14,15	1.78	5 (35%)	17,19,21	1.12	2 (11%)

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
8	A2G	B	1508	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1508	A2G	C7-N2	3.29	1.45	1.34
8	B	1508	A2G	O5-C1	2.33	1.47	1.43
8	B	1508	A2G	C3-C2	-2.24	1.47	1.52
8	B	1508	A2G	O3-C3	2.12	1.48	1.43
8	B	1508	A2G	C2-N2	2.07	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1508	A2G	C8-C7-N2	2.21	119.85	116.10
8	B	1508	A2G	C2-N2-C7	-2.18	119.80	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1508	A2G	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	651/656 (99%)	-0.37	0	100	100	77, 131, 198, 234	0
2	B	697/767 (90%)	-0.35	0	100	100	76, 118, 190, 231	0
3	C	290/290 (100%)	-0.32	0	100	100	79, 118, 162, 191	0
All	All	1638/1713 (95%)	-0.35	0	100	100	76, 123, 191, 234	0

There are no RSRZ outliers to report.

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
6	MAN	G	5	11/12	0.23	0.08	206,211,223,225	0
6	MAN	F	4	11/12	0.28	0.11	176,188,194,195	0
6	BMA	F	3	11/12	0.37	0.09	190,197,204,208	0
5	NAG	E	2	14/15	0.45	0.10	218,233,237,240	0
4	BMA	D	3	11/12	0.53	0.08	171,178,184,185	0
6	MAN	F	5	11/12	0.55	0.08	174,183,191,194	0
6	MAN	G	4	11/12	0.60	0.09	192,205,209,211	0
5	NAG	E	1	14/15	0.60	0.11	210,214,220,228	0
4	NAG	D	2	14/15	0.62	0.09	181,187,192,199	0
6	BMA	G	3	11/12	0.67	0.07	189,196,206,206	0

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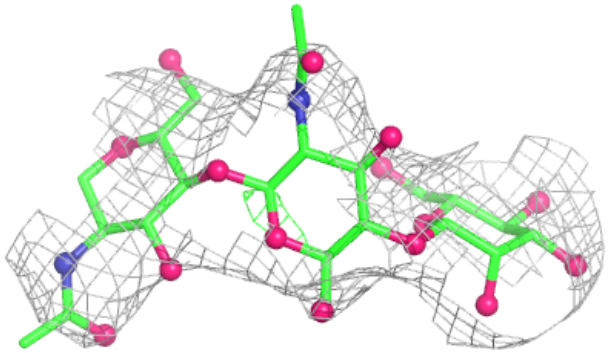
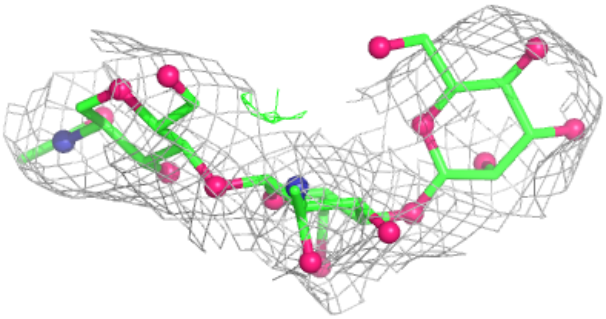
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	2	14/15	0.71	0.09	178,183,185,188	0
6	NAG	F	2	14/15	0.75	0.08	162,194,205,210	0
6	NAG	G	1	14/15	0.80	0.10	171,182,193,197	0
4	NAG	D	1	14/15	0.81	0.09	138,151,167,172	0
6	NAG	F	1	14/15	0.90	0.09	153,155,163,175	0

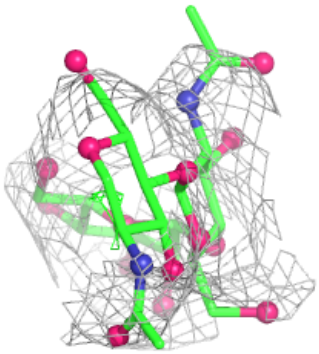
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

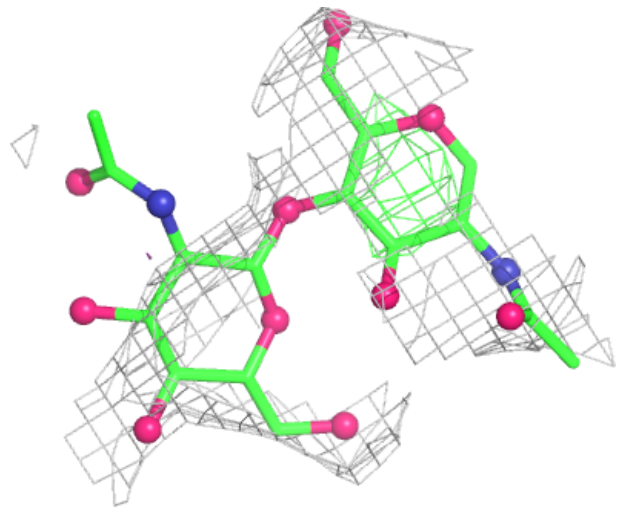


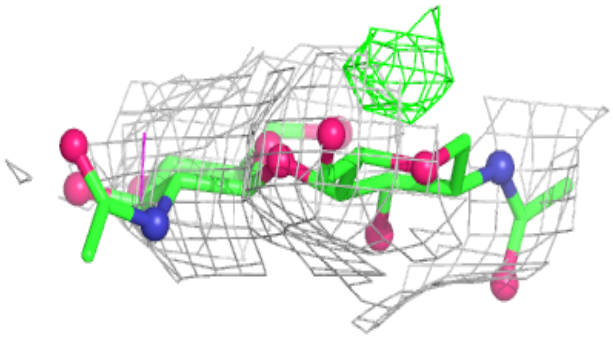


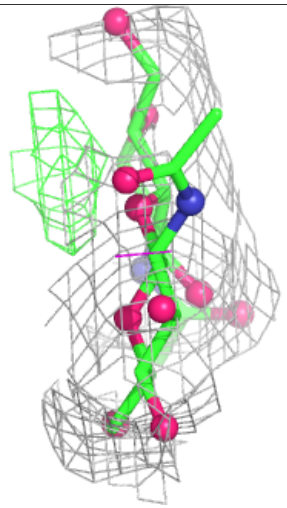


Electron density around Chain E:

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

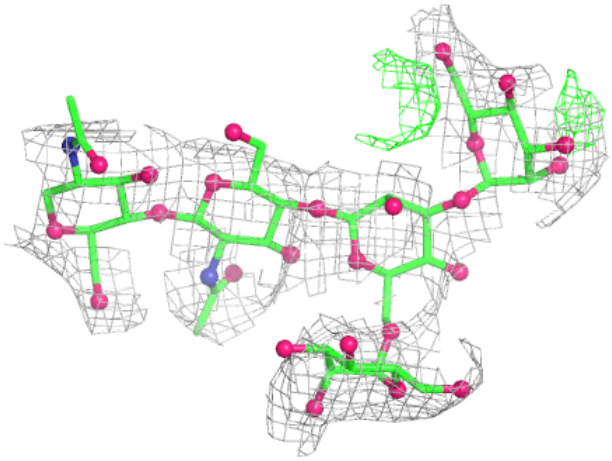


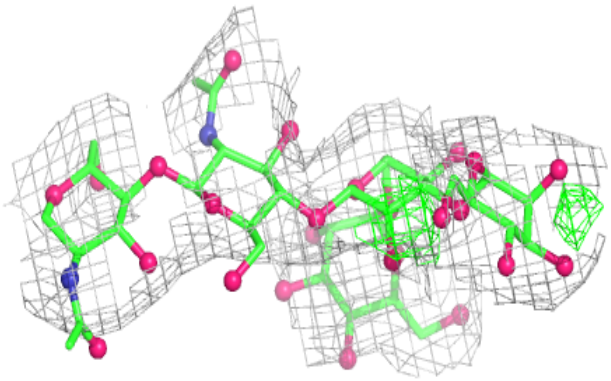


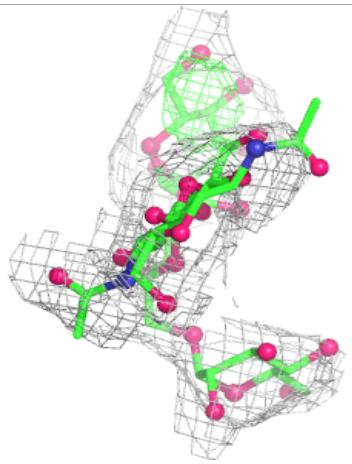


Electron density around Chain F:

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

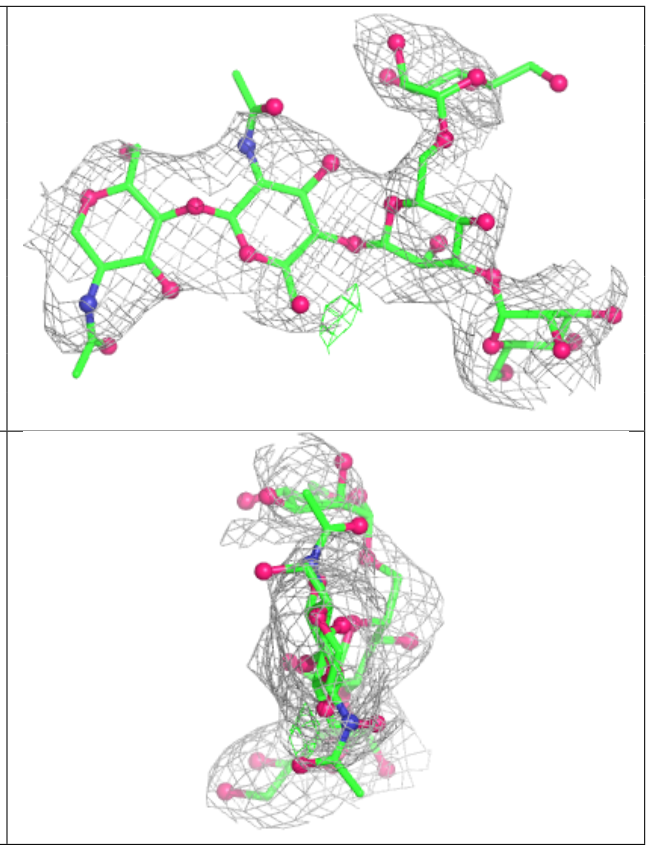






Electron density around Chain G:

$2mF_o$-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
7	PBM	B	1514	1/4	0.66	0.12	142,142,142,142	1
8	A2G	B	1508	14/15	0.86	0.16	157,178,183,184	14
7	PBM	B	1515	1/4	0.91	0.09	137,137,137,137	1
7	PBM	A	704	1/4	0.91	0.09	134,134,134,134	1
7	PBM	C	1801	1/4	0.96	0.09	123,123,123,123	1

6.5 Other polymers (i)

There are no such residues in this entry.