Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:29 PM BST

PDB ID	:	6SEJ
Title	:	Structure of a functional monomeric properdin lacking TSR3
Authors	:	Pedersen, D.V.; Andersen, G.R.
Deposited on	:	2019-07-30
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

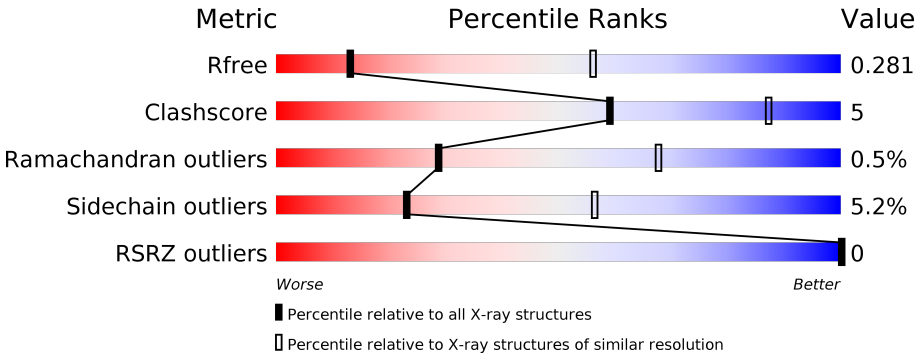
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	170	79% 17%
2	B	221	86% 13%
3	C	2	50% 50%
3	D	2	100%
3	E	2	100%
4	F	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	F	3	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3191 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1244	756	229	238	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLU	-	expression tag	UNP P27918
A	193	ASN	-	expression tag	UNP P27918
A	194	LEU	-	expression tag	UNP P27918
A	195	TYR	-	expression tag	UNP P27918
A	196	PHE	-	expression tag	UNP P27918
A	197	GLN	-	expression tag	UNP P27918

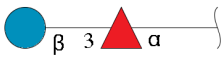
- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1714	1063	319	310	22			

There are 7 discrepancies between the modelled and reference sequences:

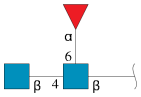
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	expression tag	UNP P27918
B	470	GLU	-	expression tag	UNP P27918
B	471	ASN	-	expression tag	UNP P27918
B	472	LEU	-	expression tag	UNP P27918
B	473	TYR	-	expression tag	UNP P27918
B	474	PHE	-	expression tag	UNP P27918
B	475	GLN	-	expression tag	UNP P27918

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



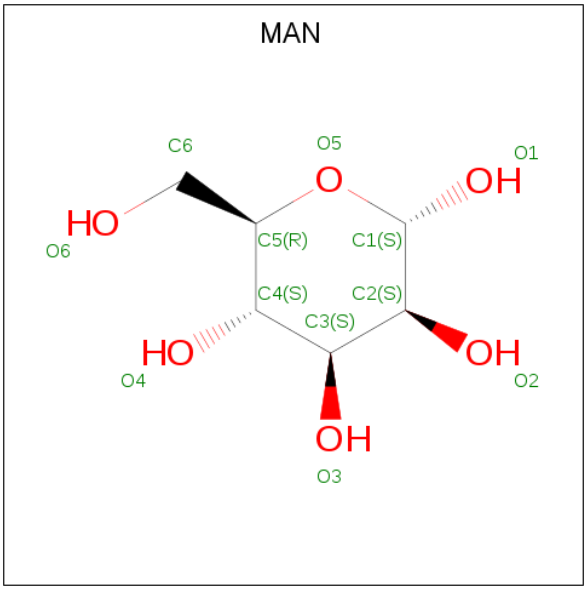
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	2	Total C O 21 12 9	0	0	0
3	D	2	Total C O 21 12 9	0	0	0
3	E	2	Total C O 21 12 9	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	3	Total C N O 38 22 2 14	0	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



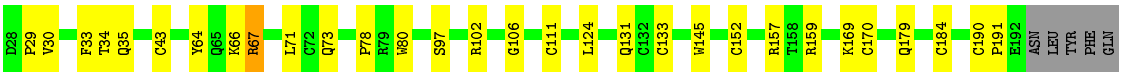
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 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.

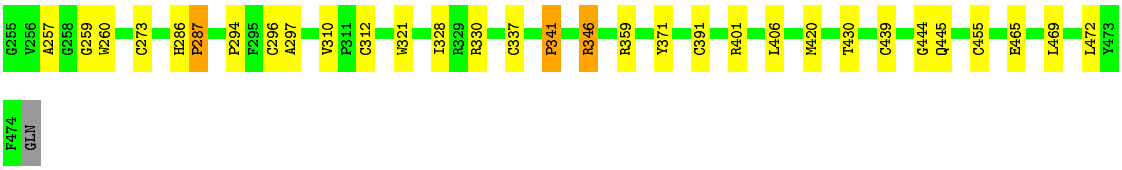
• Molecule 1: Properdin

Chain A:



• Molecule 2: Properdin

Chain B:

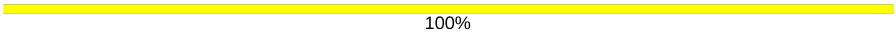


• Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain C:

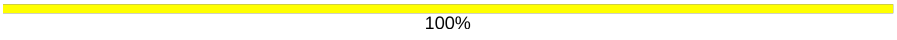
• Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain D:



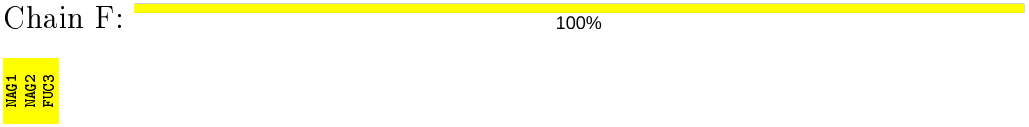
• Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	222.40Å 222.40Å 47.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.50 49.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.73-3.50) 99.8 (49.73-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.242 , 0.266 0.233 , 0.281	Depositor DCC
R_{free} test set	741 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	168.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 120.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.047 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3191	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: FUC, BGC, NAG, 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	0.30	0/1278	0.51	0/1734
2	B	0.36	1/1770 (0.1%)	0.52	0/2410
All	All	0.33	1/3048 (0.0%)	0.51	0/4144

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	2
2	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	PRO	N-CD	5.00	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	67	ARG	Sidechain
2	B	346	ARG	Sidechain

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	1244	0	1135	17	0
2	B	1714	0	1613	13	0
3	C	21	0	19	1	0
3	D	21	0	19	0	0
3	E	21	0	19	0	0
4	F	38	0	34	0	0
5	A	55	0	50	0	0
5	B	77	0	70	0	0
All	All	3191	0	2959	29	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 5.

All (29) 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:66:LYS:O	1:A:67:ARG:HG2	1.74	0.88
1:A:97:SER:HB3	1:A:124:LEU:HD11	1.79	0.64
2:B:330:ARG:HH12	2:B:420:MET:HE3	1.66	0.60
2:B:286:HIS:HB3	2:B:287:PRO:HD3	1.85	0.57
1:A:34:THR:HG23	1:A:35:GLN:HG3	1.87	0.57
1:A:66:LYS:O	1:A:67:ARG:CG	2.49	0.57
2:B:257:ALA:HA	2:B:294:PRO:HG2	1.87	0.57
1:A:29:PRO:O	1:A:30:VAL:HG23	2.07	0.53
2:B:401:ARG:HG3	2:B:455:CYS:SG	2.50	0.52
1:A:29:PRO:O	1:A:30:VAL:CG2	2.59	0.51
2:B:321:TRP:HB3	2:B:346:ARG:HD2	1.93	0.51
2:B:341:PRO:HG3	2:B:371:TYR:HE1	1.76	0.50
1:A:152:CYS:HB3	3:C:1:FUC:H5	1.94	0.50
1:A:33:PHE:CG	1:A:43:CYS:HB3	2.48	0.48
1:A:66:LYS:C	1:A:67:ARG:HG2	2.33	0.47
1:A:29:PRO:C	1:A:30:VAL:HG23	2.35	0.47
2:B:260:TRP:NE1	2:B:297:ALA:O	2.42	0.47
2:B:330:ARG:HH12	2:B:420:MET:CE	2.29	0.45
2:B:259:GLY:O	2:B:287:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:GLU:O	2:B:469:LEU:HG	2.19	0.42
1:A:67:ARG:HH22	1:A:71:LEU:HD12	1.82	0.42
2:B:444:GLY:O	2:B:445:GLN:NE2	2.50	0.41
1:A:80:TRP:NE1	1:A:111:CYS:HB3	2.35	0.41
1:A:78:PRO:HA	1:A:106:GLY:HA3	2.03	0.41
1:A:30:VAL:HG11	1:A:64:TYR:CD1	2.55	0.41
2:B:273:CYS:HA	2:B:310:VAL:HG13	2.03	0.41
1:A:124:LEU:HB3	2:B:391:CYS:HB2	2.02	0.41
1:A:73:GLN:OE1	1:A:106:GLY:N	2.51	0.40
1:A:145:TRP:HB3	1:A:157:ARG:HE	1.85	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	163/170 (96%)	151 (93%)	11 (7%)	1 (1%)	25	64
2	B	218/221 (99%)	202 (93%)	15 (7%)	1 (0%)	29	68
All	All	381/391 (97%)	353 (93%)	26 (7%)	2 (0%)	29	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	PRO
2	B	287	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	136/141 (96%)	128 (94%)	8 (6%)	19 53
2	B	189/190 (100%)	180 (95%)	9 (5%)	25 60
All	All	325/331 (98%)	308 (95%)	17 (5%)	23 56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	133	CYS
1	A	159	ARG
1	A	169	LYS
1	A	170	CYS
1	A	179	GLN
1	A	184	CYS
1	A	190	CYS
2	B	296	CYS
2	B	312	CYS
2	B	328	ILE
2	B	337	CYS
2	B	359	ARG
2	B	406	LEU
2	B	430	THR
2	B	439	CYS
2	B	472	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUC	C	1	1,3	10,10,11	1.63	2 (20%)	14,14,16	1.48	2 (14%)
3	BGC	C	2	3	11,11,12	1.81	2 (18%)	15,15,17	1.62	3 (20%)
3	FUC	D	1	1,3	10,10,11	1.37	1 (10%)	14,14,16	1.37	2 (14%)
3	BGC	D	2	3	11,11,12	1.85	2 (18%)	15,15,17	1.53	3 (20%)
3	FUC	E	1	3,2	10,10,11	1.33	1 (10%)	14,14,16	1.17	2 (14%)
3	BGC	E	2	3	11,11,12	1.91	2 (18%)	15,15,17	1.59	3 (20%)
4	NAG	F	1	2,4	14,14,15	0.67	0	17,19,21	1.09	1 (5%)
4	NAG	F	2	4	14,14,15	1.35	2 (14%)	17,19,21	1.63	3 (17%)
4	FUC	F	3	4	10,10,11	2.00	4 (40%)	14,14,16	1.01	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
3	FUC	C	1	1,3	-	-	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	FUC	D	1	1,3	-	-	0/1/1/1
3	BGC	D	2	3	-	2/2/19/22	0/1/1/1
3	FUC	E	1	3,2	-	-	0/1/1/1
3	BGC	E	2	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	FUC	F	3	4	1/1/4/5	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	BGC	O5-C1	5.23	1.52	1.43
3	D	2	BGC	O5-C1	5.18	1.52	1.43
3	C	2	BGC	O5-C1	4.92	1.51	1.43
4	F	3	FUC	C2-C3	3.86	1.58	1.52
4	F	2	NAG	O5-C1	3.48	1.49	1.43
3	C	1	FUC	C2-C3	3.35	1.57	1.52
4	F	2	NAG	C1-C2	3.29	1.57	1.52
4	F	3	FUC	C4-C3	2.79	1.59	1.52
3	E	1	FUC	C2-C3	2.65	1.56	1.52
3	E	2	BGC	O5-C5	2.61	1.48	1.43
3	C	1	FUC	C1-C2	2.56	1.58	1.52
4	F	3	FUC	C4-C5	2.52	1.58	1.52
4	F	3	FUC	O5-C5	2.45	1.48	1.43
3	D	2	BGC	O5-C5	2.30	1.48	1.43
3	C	2	BGC	O5-C5	2.30	1.48	1.43
3	D	1	FUC	O5-C5	2.26	1.48	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	NAG	C2-N2-C7	4.42	129.20	122.90
4	F	2	NAG	C1-O5-C5	4.01	117.62	112.19
3	D	2	BGC	C2-C3-C4	3.82	117.51	110.89
3	E	2	BGC	C2-C3-C4	3.81	117.48	110.89
3	C	2	BGC	C2-C3-C4	3.58	117.09	110.89
3	C	2	BGC	C1-O5-C5	3.12	116.42	112.19
3	D	1	FUC	C1-O5-C5	3.04	119.67	112.78
3	E	1	FUC	C1-O5-C5	2.98	119.53	112.78
3	D	2	BGC	C1-O5-C5	2.66	115.80	112.19
4	F	1	NAG	C1-O5-C5	2.57	115.68	112.19
3	C	1	FUC	C1-O5-C5	2.54	118.54	112.78
3	C	2	BGC	C1-C2-C3	2.47	112.70	109.67
3	C	1	FUC	C1-C2-C3	2.47	112.70	109.67
3	D	2	BGC	C1-C2-C3	2.42	112.64	109.67
3	E	2	BGC	C1-C2-C3	2.24	112.42	109.67
3	E	2	BGC	C1-O5-C5	2.24	115.22	112.19
3	D	1	FUC	O5-C5-C4	2.19	113.44	109.52
4	F	2	NAG	C1-C2-N2	2.08	114.04	110.49
3	E	1	FUC	O5-C1-C2	2.07	113.96	110.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	FUC	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	BGC	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6
3	D	2	BGC	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	D	2	BGC	O5-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7

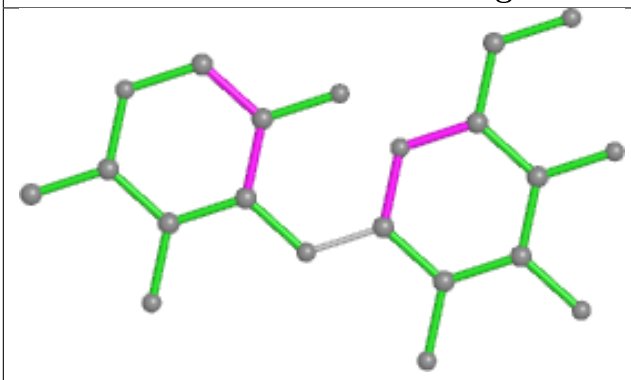
There are no ring outliers.

1 monomer is involved in 1 short contact:

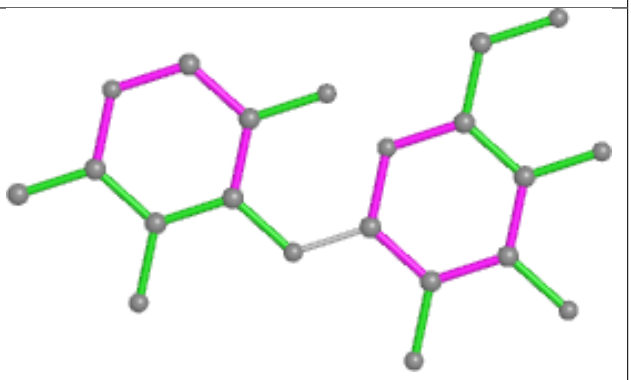
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FUC	1	0

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

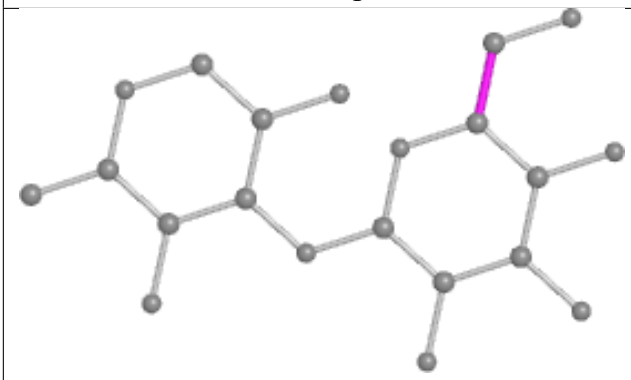
Oligosaccharide Chain C



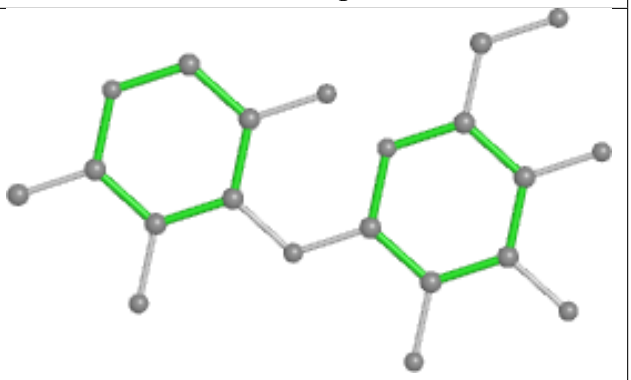
Bond lengths



Bond angles

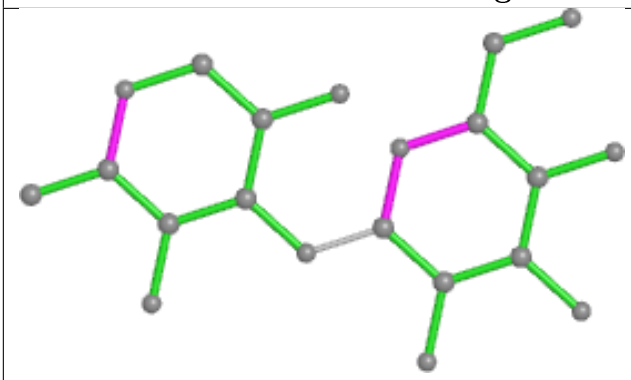


Torsions

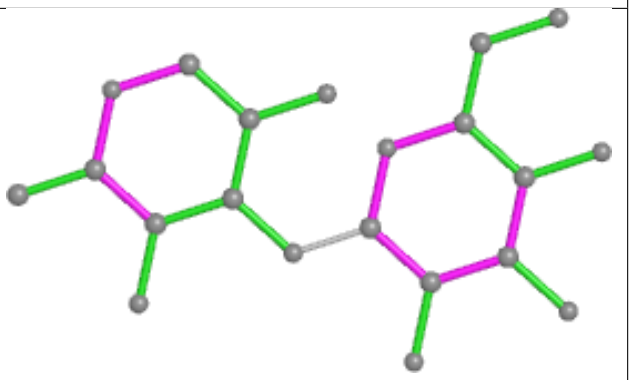


Rings

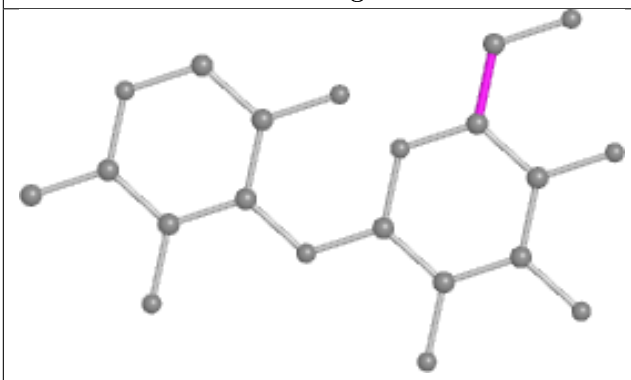
Oligosaccharide Chain D



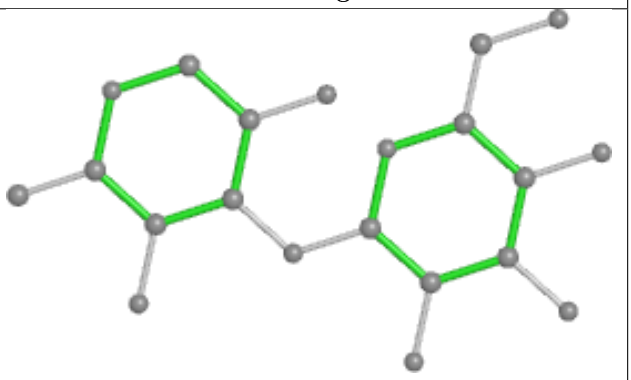
Bond lengths



Bond angles

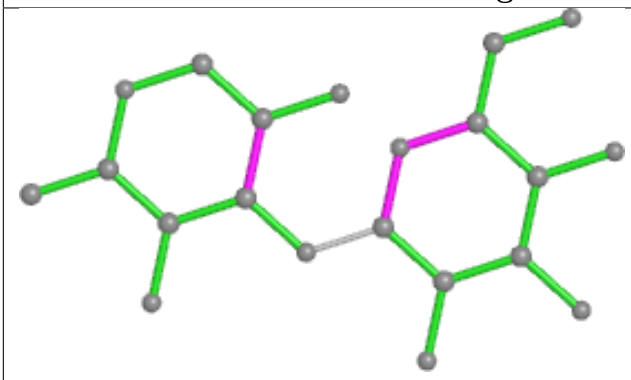


Torsions

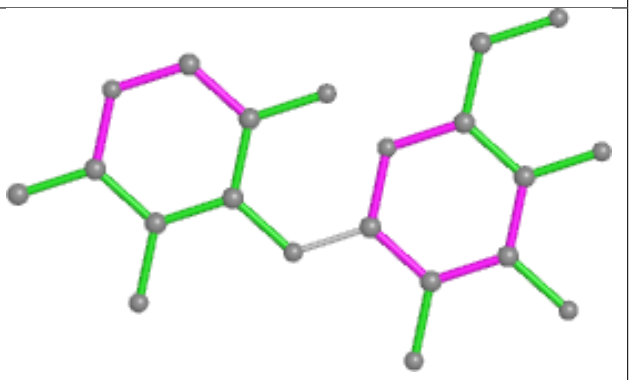


Rings

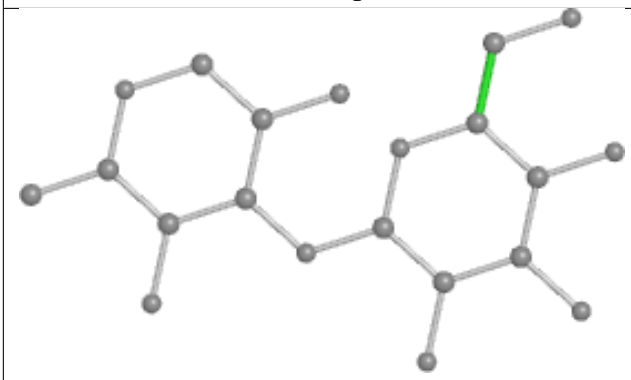
Oligosaccharide Chain E



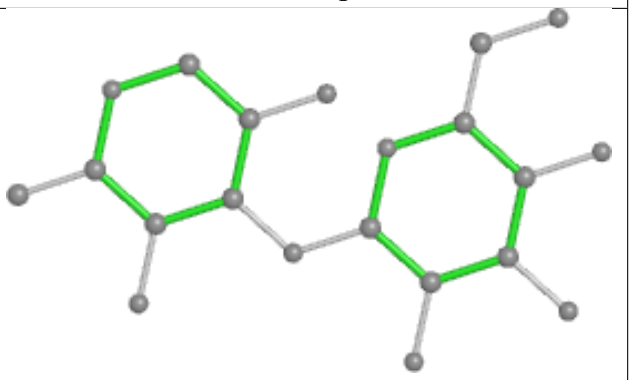
Bond lengths



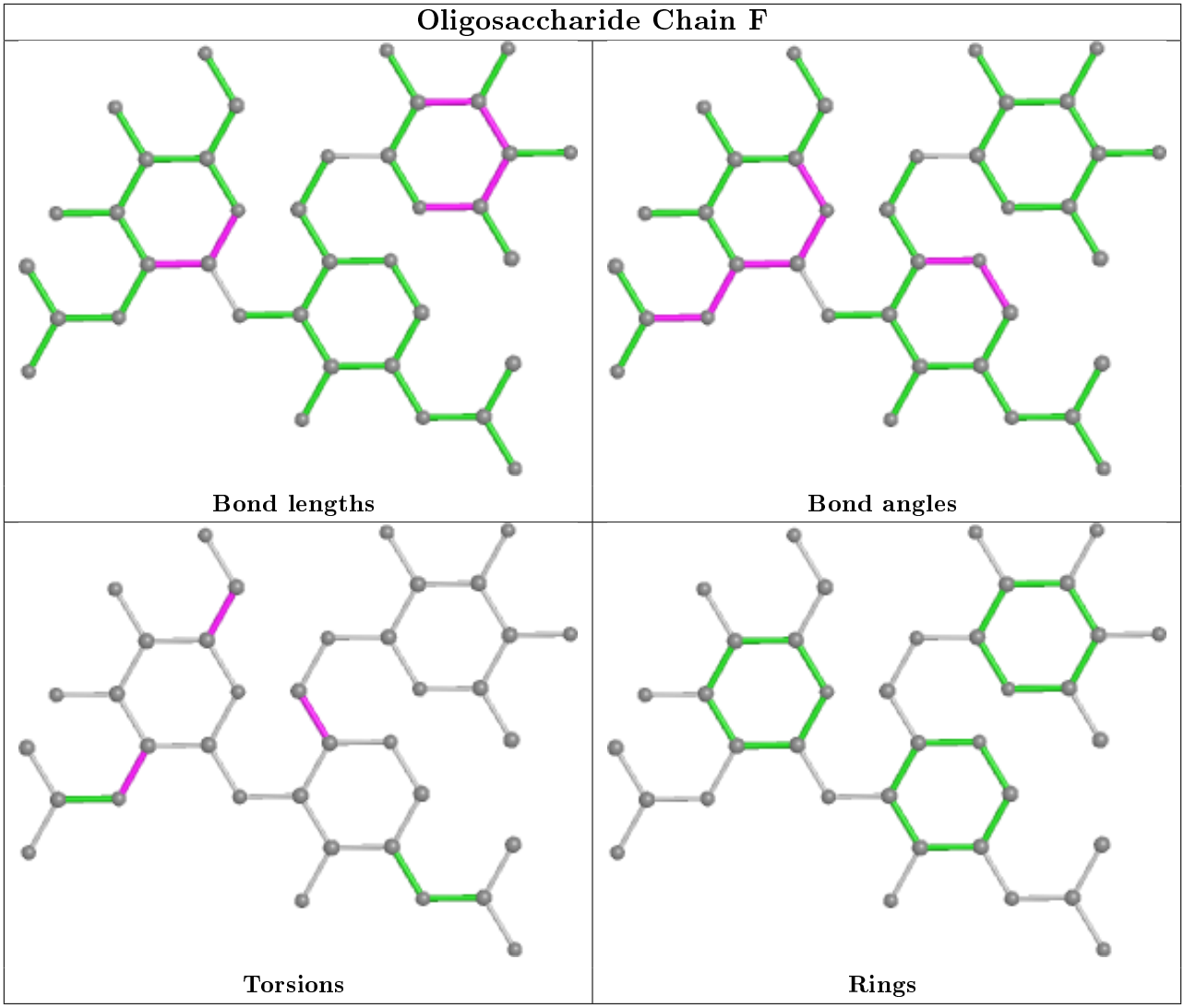
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	A	208	1	11,11,12	1.30	2 (18%)	15,15,17	1.74	2 (13%)
5	MAN	A	207	1	11,11,12	1.32	1 (9%)	15,15,17	1.87	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	A	209	1	11,11,12	1.44	3 (27%)	15,15,17	1.93	2 (13%)
5	MAN	B	504	2	11,11,12	1.24	1 (9%)	15,15,17	1.94	3 (20%)
5	MAN	B	509	2	11,11,12	1.39	2 (18%)	15,15,17	1.88	3 (20%)
5	MAN	A	204	1	11,11,12	1.33	2 (18%)	15,15,17	2.23	4 (26%)
5	MAN	B	505	2	11,11,12	1.31	3 (27%)	15,15,17	2.03	4 (26%)
5	MAN	B	511	2	11,11,12	1.29	1 (9%)	15,15,17	2.09	3 (20%)
5	MAN	B	503	2	11,11,12	1.28	1 (9%)	15,15,17	1.68	2 (13%)
5	MAN	B	512	2	11,11,12	1.27	2 (18%)	15,15,17	2.28	3 (20%)
5	MAN	A	203	1	11,11,12	1.30	2 (18%)	15,15,17	1.94	2 (13%)
5	MAN	B	510	2	11,11,12	1.13	1 (9%)	15,15,17	1.88	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	208	1	-	0/2/19/22	0/1/1/1
5	MAN	A	207	1	-	0/2/19/22	0/1/1/1
5	MAN	A	209	1	-	0/2/19/22	0/1/1/1
5	MAN	B	504	2	-	0/2/19/22	0/1/1/1
5	MAN	B	509	2	-	0/2/19/22	0/1/1/1
5	MAN	A	204	1	-	1/2/19/22	0/1/1/1
5	MAN	B	505	2	-	0/2/19/22	0/1/1/1
5	MAN	B	511	2	-	0/2/19/22	0/1/1/1
5	MAN	B	503	2	-	0/2/19/22	0/1/1/1
5	MAN	B	512	2	-	0/2/19/22	0/1/1/1
5	MAN	A	203	1	-	0/2/19/22	0/1/1/1
5	MAN	B	510	2	-	1/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	209	MAN	O2-C2	-3.05	1.36	1.43
5	A	207	MAN	O5-C5	2.65	1.48	1.43
5	B	509	MAN	O5-C5	2.61	1.48	1.43
5	A	203	MAN	O2-C2	-2.54	1.38	1.43
5	B	503	MAN	O5-C5	2.49	1.48	1.43
5	A	203	MAN	O5-C5	2.48	1.48	1.43
5	B	504	MAN	O5-C5	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	511	MAN	O5-C5	2.42	1.48	1.43
5	B	505	MAN	O5-C5	2.39	1.48	1.43
5	B	512	MAN	O5-C5	2.38	1.48	1.43
5	A	204	MAN	O5-C5	2.35	1.48	1.43
5	B	512	MAN	C2-C3	2.33	1.55	1.52
5	A	209	MAN	C4-C5	2.32	1.57	1.53
5	A	209	MAN	O5-C5	2.30	1.48	1.43
5	A	208	MAN	O5-C5	2.25	1.48	1.43
5	B	505	MAN	C1-C2	2.19	1.57	1.52
5	B	510	MAN	O5-C5	2.18	1.47	1.43
5	A	204	MAN	C2-C3	2.14	1.55	1.52
5	B	505	MAN	C4-C5	2.06	1.57	1.53
5	A	208	MAN	C2-C3	2.05	1.55	1.52
5	B	509	MAN	C2-C3	2.03	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	512	MAN	C1-O5-C5	7.20	121.95	112.19
5	B	511	MAN	C1-O5-C5	6.54	121.06	112.19
5	A	204	MAN	C1-O5-C5	6.04	120.38	112.19
5	A	209	MAN	C1-O5-C5	5.86	120.12	112.19
5	A	203	MAN	C1-O5-C5	5.75	119.98	112.19
5	B	510	MAN	C1-O5-C5	5.72	119.94	112.19
5	B	504	MAN	C1-O5-C5	5.52	119.67	112.19
5	B	505	MAN	C1-O5-C5	5.28	119.35	112.19
5	B	509	MAN	C1-O5-C5	5.26	119.31	112.19
5	A	207	MAN	C1-O5-C5	5.09	119.08	112.19
5	A	208	MAN	C1-O5-C5	5.06	119.04	112.19
5	B	503	MAN	C1-O5-C5	4.41	118.17	112.19
5	A	204	MAN	C1-C2-C3	3.75	114.28	109.67
5	A	203	MAN	O2-C2-C3	-3.06	104.01	110.14
5	B	512	MAN	O5-C1-C2	3.02	115.44	110.77
5	A	209	MAN	O2-C2-C3	-3.01	104.12	110.14
5	B	510	MAN	O2-C2-C3	-2.95	104.22	110.14
5	B	505	MAN	O2-C2-C3	-2.85	104.44	110.14
5	B	505	MAN	O5-C1-C2	2.77	115.04	110.77
5	B	511	MAN	O5-C1-C2	2.70	114.94	110.77
5	B	505	MAN	C1-C2-C3	2.63	112.90	109.67
5	B	504	MAN	O2-C2-C3	-2.49	105.15	110.14
5	A	207	MAN	O2-C2-C3	-2.48	105.17	110.14
5	B	503	MAN	O2-C2-C3	-2.42	105.29	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	204	MAN	O2-C2-C3	-2.41	105.31	110.14
5	B	509	MAN	O2-C2-C3	-2.39	105.36	110.14
5	B	512	MAN	O2-C2-C3	-2.38	105.37	110.14
5	B	509	MAN	C1-C2-C3	2.37	112.58	109.67
5	A	204	MAN	O5-C1-C2	2.27	114.27	110.77
5	A	207	MAN	O5-C1-C2	2.22	114.20	110.77
5	B	511	MAN	O2-C2-C3	-2.19	105.76	110.14
5	B	504	MAN	C1-C2-C3	2.15	112.31	109.67
5	A	208	MAN	C1-C2-C3	2.12	112.28	109.67
5	A	207	MAN	C1-C2-C3	2.02	112.15	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	204	MAN	O5-C5-C6-O6
5	B	510	MAN	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

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	165/170 (97%)	-0.52	0	100	100	142, 195, 252, 284	0
2	B	220/221 (99%)	-0.44	0	100	100	143, 189, 250, 282	0
All	All	385/391 (98%)	-0.48	0	100	100	142, 191, 251, 284	0

There are no RSRZ outliers to report.

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

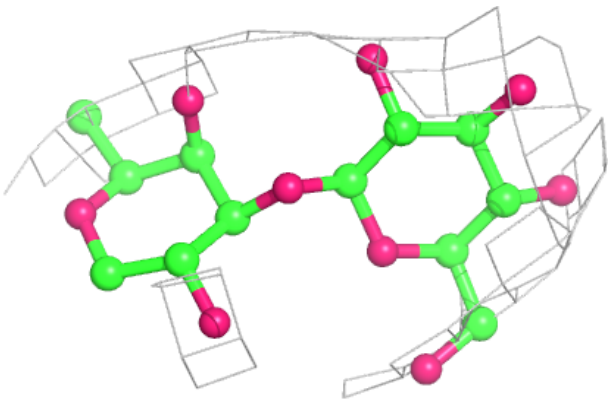
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

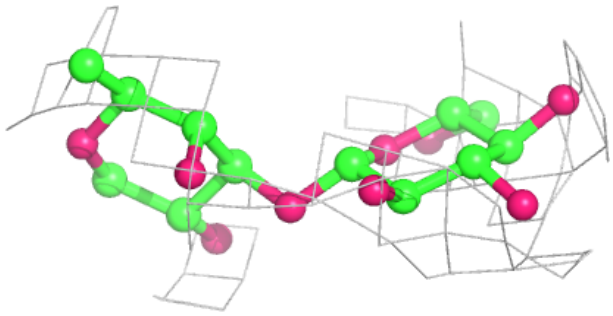
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	E	2	11/12	0.87	0.52	222,245,299,308	0
4	NAG	F	2	14/15	0.87	0.15	228,298,340,355	0
3	FUC	D	1	10/11	0.90	0.16	190,211,229,239	0
3	FUC	C	1	10/11	0.91	0.25	161,184,210,214	0
4	NAG	F	1	14/15	0.91	0.15	248,282,308,329	0
4	FUC	F	3	10/11	0.92	0.22	221,254,297,308	0
3	BGC	D	2	11/12	0.92	0.28	207,242,252,287	0
3	BGC	C	2	11/12	0.93	0.21	196,222,247,247	0
3	FUC	E	1	10/11	0.97	0.21	172,208,240,284	0

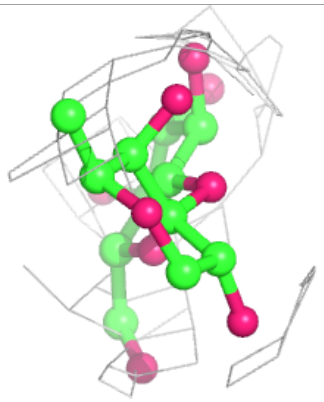
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

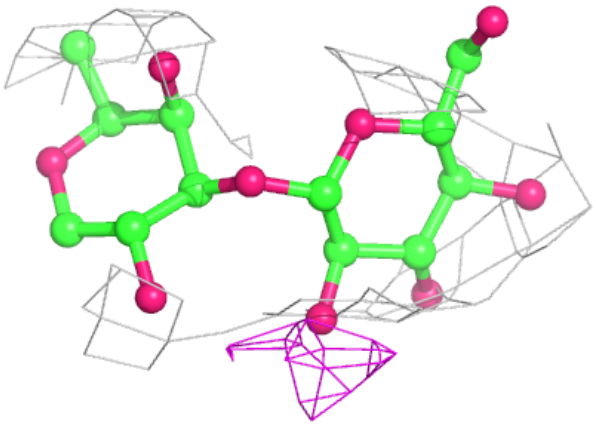


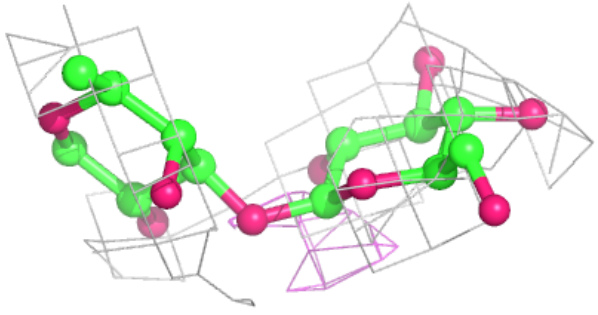


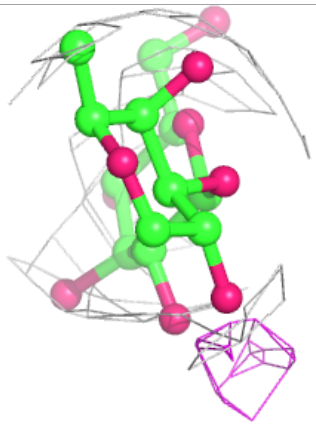


Electron density around Chain D:

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

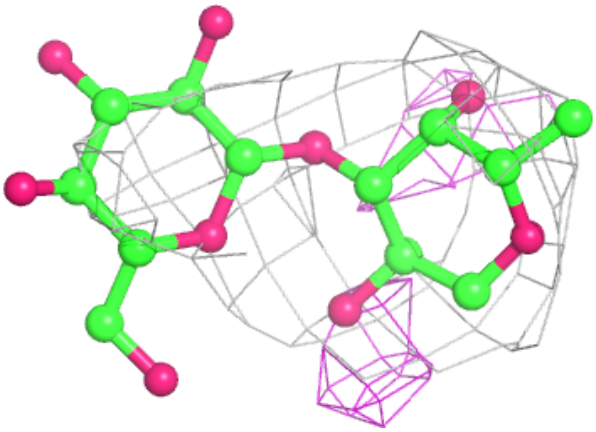


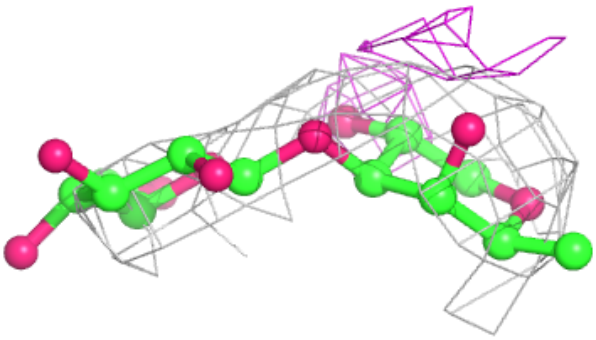


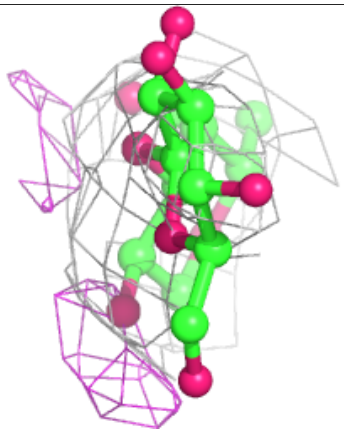


Electron density around Chain E:

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

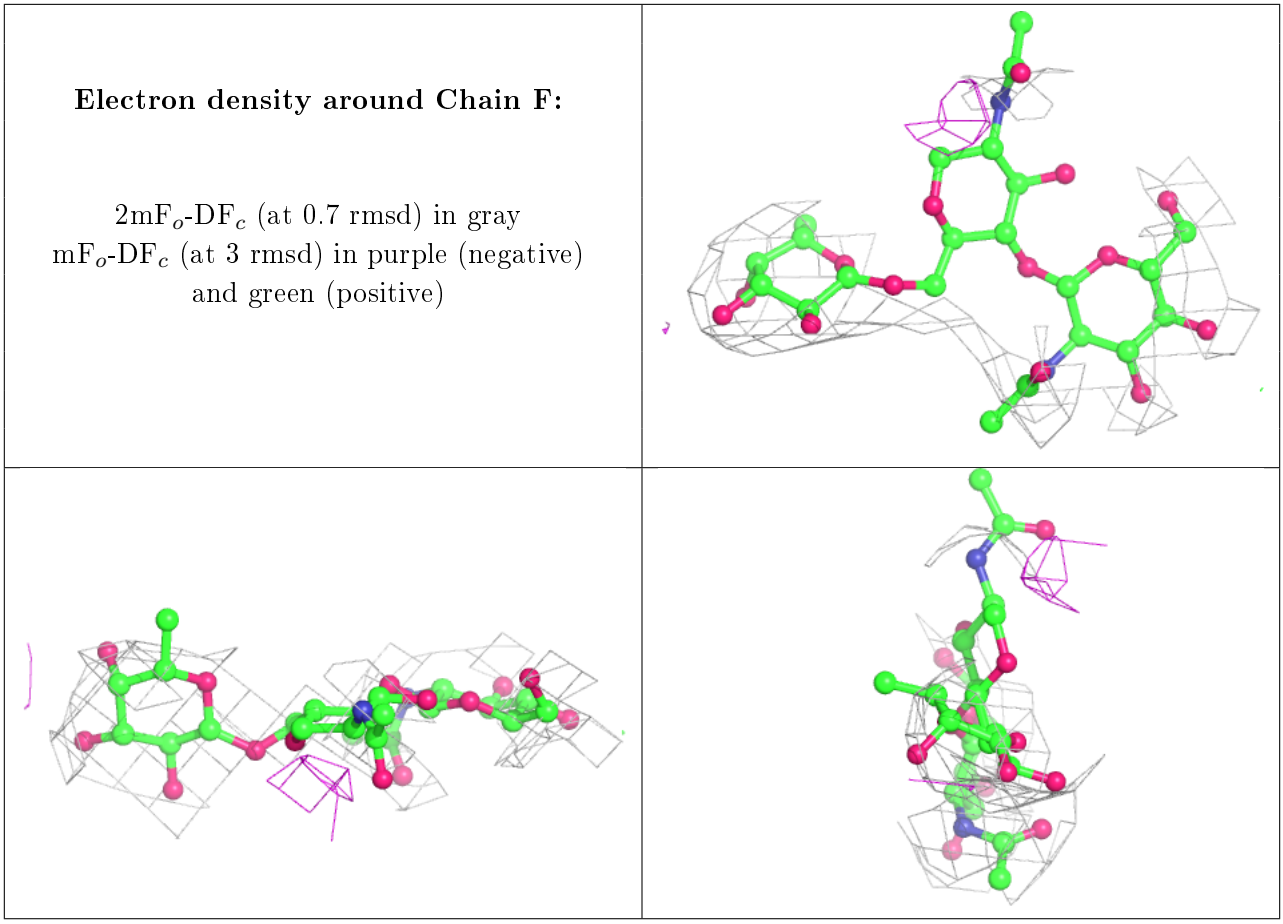






Electron density around Chain F:

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



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
5	MAN	B	512	11/12	0.91	0.21	197,232,263,270	0
5	MAN	B	503	11/12	0.92	0.21	177,203,248,248	0
5	MAN	A	204	11/12	0.92	0.16	215,244,256,274	0
5	MAN	A	208	11/12	0.92	0.12	220,251,285,294	0
5	MAN	A	209	11/12	0.93	0.11	244,281,299,304	0
5	MAN	A	207	11/12	0.93	0.14	213,256,278,294	0
5	MAN	B	505	11/12	0.93	0.12	169,193,224,238	0
5	MAN	B	504	11/12	0.93	0.17	150,191,217,224	0
5	MAN	A	203	11/12	0.93	0.24	155,191,246,247	0
5	MAN	B	509	11/12	0.94	0.13	171,200,240,248	0
5	MAN	B	511	11/12	0.94	0.11	213,256,274,295	0
5	MAN	B	510	11/12	0.95	0.12	170,219,268,272	0

6.5 Other polymers (i)

There are no such residues in this entry.