



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:47 PM UTC

PDB ID : 7NOZ / pdb_00007noz
Title : Structure of the nanobody stablized properdin bound alternative pathway pro-convertase C3b:FB:FP
Authors : Lorenzen, J.; Pedersen, D.V.; Andersen, G.R.
Deposited on : 2021-02-26
Resolution : 3.90 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

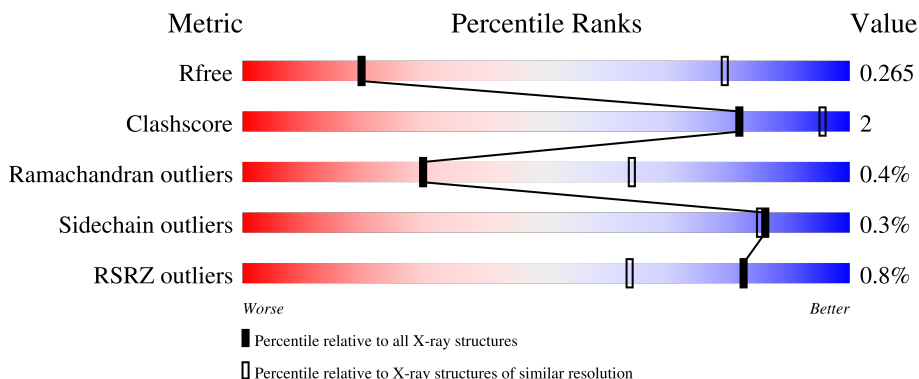
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



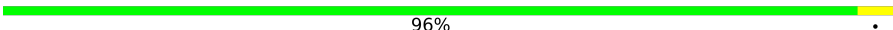
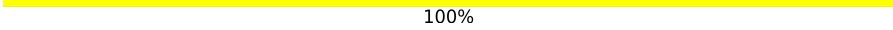
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	2% 93% 7%
2	B	912	90% 9% .
3	C	163	92% 8%
4	D	207	89% 10% .
5	F	731	% 91% 7% .

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Mol	Chain	Length	Quality of chain
6	R	124	 96%
7	E	3	 33% 67%
7	G	3	 33% 67%
7	L	3	 33% 67%
8	H	2	 50% 50%
8	I	2	 100%
8	J	2	 50% 50%
9	K	4	 50% 50%
9	M	4	 25% 75%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21994 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 C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	906	Total	C	N	O	S	0	0	0
			7236	4584	1215	1399	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	conflict	UNP P01024

- Molecule 3 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	163	Total	C	N	O	S	0	0	0
			1228	746	227	234	21			

- Molecule 4 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	207	Total	C	N	O	S	0	0	0
			1594	987	303	282	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	255	GLY	PRO	conflict	UNP P27918

- Molecule 5 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	712	Total	C	N	O	S	0	0	0
			5615	3529	978	1075	33			

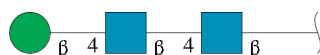
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	279	GLY	ASP	engineered mutation	UNP P00751
F	765	ALA	-	expression tag	UNP P00751

- Molecule 6 is a protein called hFPNb1 nanobody.

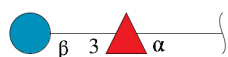
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	124	Total	C	N	O	S	0	0	0
			951	588	172	187	4			

- Molecule 7 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
7	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



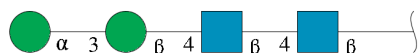
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	H	2	Total	C	O	0	0	0
			21	12	9			
8	I	2	Total	C	O	0	0	0
			21	12	9			

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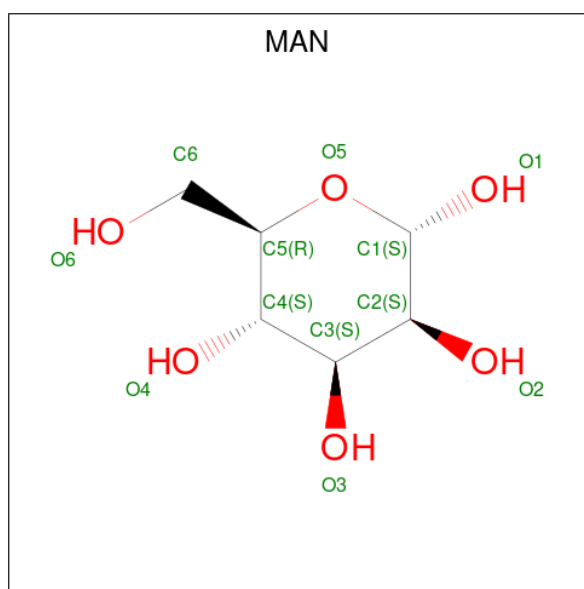
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	J	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
9	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
9	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



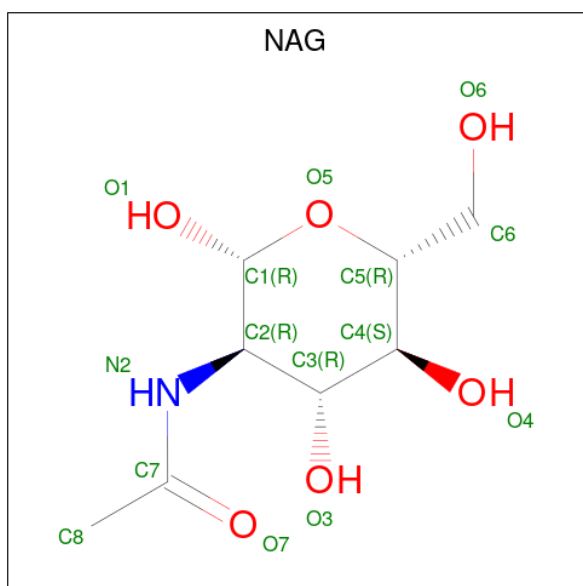
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		

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



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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	F	1	Total	Mg	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	O	0	0
			1	1		

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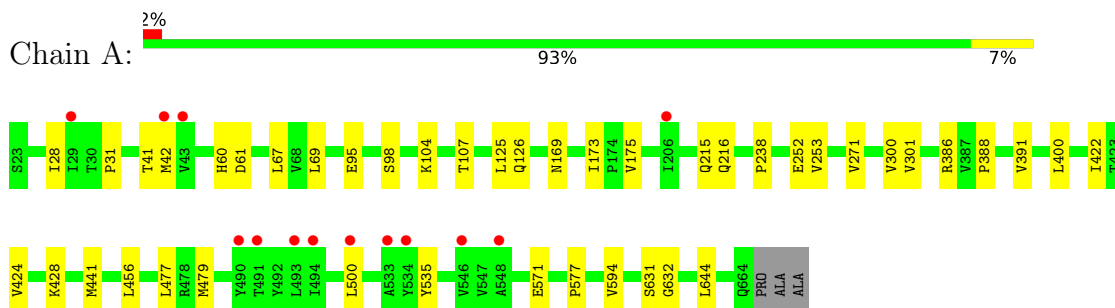
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	F	1	Total	O	0	0
			1	1		

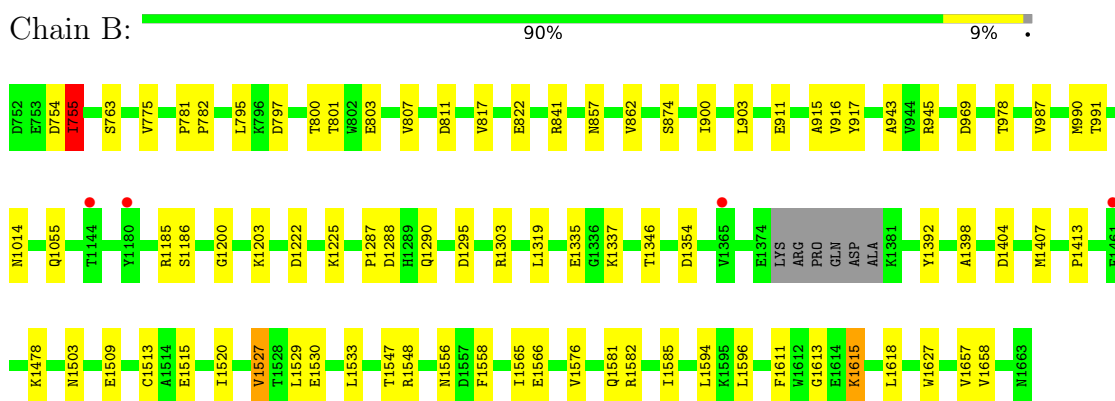
3 Residue-property plots

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

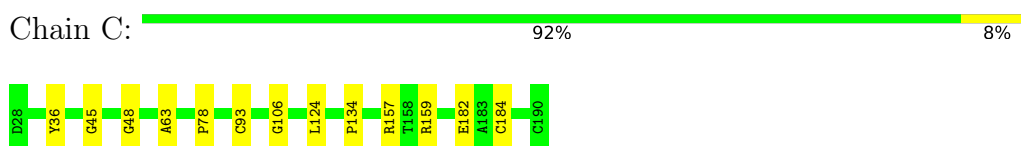
- Molecule 1: Complement C3 beta chain



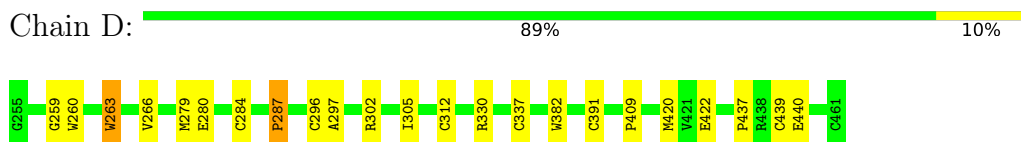
- Molecule 2: Complement C3 alpha chain



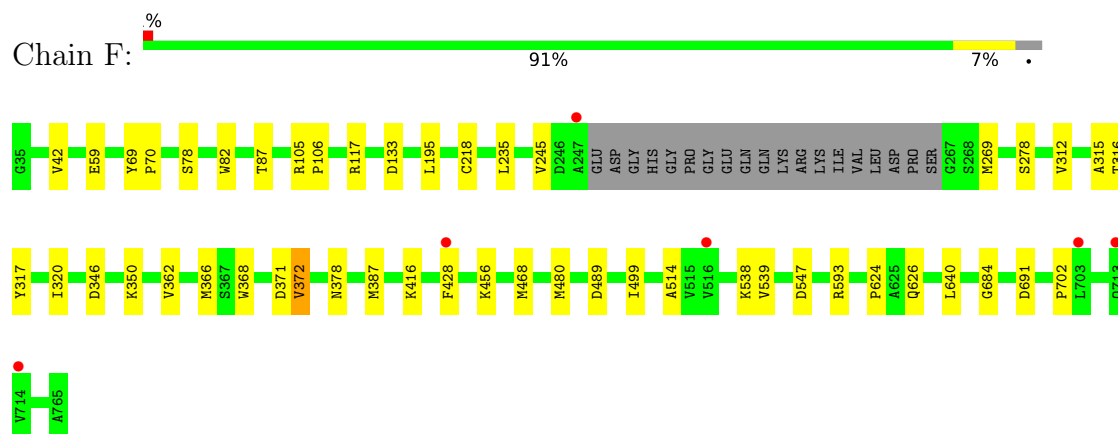
- Molecule 3: Properdin



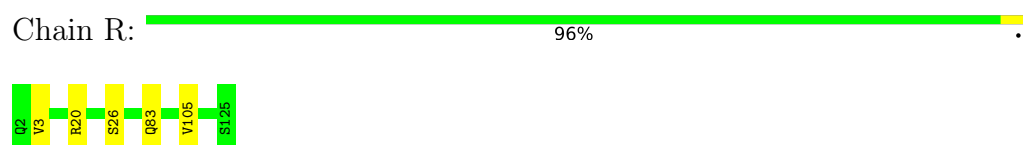
- Molecule 4: Properdin



- Molecule 5: Complement factor B



- Molecule 6: hFPNb1 nanobody



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain I:  100%

FUC1
BGC2

- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain J:  50% 50%

FUC1
BGC2

- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2
BNA3
MAN4

- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  25% 75%

MAG1
MAG2
BNA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	148.69Å 179.46Å 192.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 3.90 48.59 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.59-3.90) 99.9 (48.59-3.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.249 , 0.265 0.252 , 0.265	Depositor DCC
R_{free} test set	45798 reflections (96.04%)	wwPDB-VP
Wilson B-factor (Å ²)	196.3	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 222.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21994	wwPDB-VP
Average B, all atoms (Å ²)	288.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, BGC, NAG, FUC, 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	0.16	0/5108	0.37	0/6940
2	B	0.17	0/7380	0.42	4/9992 (0.0%)
3	C	0.19	0/1261	0.45	0/1710
4	D	0.19	0/1647	0.46	0/2244
5	F	0.16	0/5742	0.39	0/7773
6	R	0.12	0/967	0.31	0/1305
All	All	0.17	0/22105	0.40	4/29964 (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
3	C	0	1
4	D	0	1
5	F	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	ASP	CA-C-N	6.33	133.35	121.97
2	B	754	ASP	C-N-CA	6.33	133.35	121.97
2	B	755	ILE	N-CA-CB	5.63	120.53	111.23
2	B	1615	LYS	CB-CA-C	5.17	120.35	110.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	159	ARG	Sidechain
4	D	263	TRP	Peptide
5	F	372	VAL	Peptide
5	F	69	TYR	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	5007	0	5064	24	0
2	B	7236	0	7153	49	0
3	C	1228	0	1122	5	0
4	D	1594	0	1508	12	0
5	F	5615	0	5468	27	0
6	R	951	0	923	3	0
7	E	39	0	34	0	0
7	G	39	0	34	0	0
7	L	39	0	34	0	0
8	H	21	0	19	0	0
8	I	21	0	19	0	0
8	J	21	0	19	0	0
9	K	50	0	43	0	0
9	M	50	0	43	0	0
10	C	33	0	30	0	0
10	D	33	0	30	0	0
11	F	14	0	13	0	0
12	F	1	0	0	0	0
13	B	1	0	0	0	0
13	F	1	0	0	1	0
All	All	21994	0	21556	108	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 2.

The worst 5 of 108 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)
2:B:1503:ASN:N	2:B:1515:GLU:OE2	2.17	0.72
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.81	0.63
1:A:386:ARG:HG3	1:A:400:LEU:HD21	1.83	0.61
1:A:125:LEU:HB2	1:A:215:GLN:HE22	1.69	0.58
2:B:1404:ASP:HB3	2:B:1478:LYS:HB3	1.86	0.58

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	640/645 (99%)	614 (96%)	25 (4%)	1 (0%)	43	74
2	B	902/912 (99%)	849 (94%)	47 (5%)	6 (1%)	18	53
3	C	161/163 (99%)	147 (91%)	12 (8%)	2 (1%)	10	41
4	D	205/207 (99%)	195 (95%)	9 (4%)	1 (0%)	24	59
5	F	708/731 (97%)	674 (95%)	32 (4%)	2 (0%)	36	69
6	R	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
All	All	2738/2782 (98%)	2597 (95%)	129 (5%)	12 (0%)	30	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	755	ILE
2	B	1527	VAL
3	C	134	PRO
2	B	1615	LYS
4	D	287	PRO

5.3.2 Protein sidechains ⓘ

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	566/567 (100%)	566 (100%)	0	100	100
2	B	802/807 (99%)	802 (100%)	0	100	100
3	C	134/134 (100%)	132 (98%)	2 (2%)	57	70
4	D	175/176 (99%)	170 (97%)	5 (3%)	37	58
5	F	619/635 (98%)	618 (100%)	1 (0%)	87	87
6	R	100/100 (100%)	100 (100%)	0	100	100
All	All	2396/2419 (99%)	2388 (100%)	8 (0%)	86	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	378	ASN
4	D	439	CYS
4	D	312	CYS
4	D	296	CYS
4	D	337	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1473	GLN
4	D	331	ASN
6	R	114	HIS
2	B	1663	ASN
4	D	343	GLN

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 ⓘ

23 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	E	1	1,7	14,14,15	0.48	0	17,19,21	0.49	0
7	NAG	E	2	7	14,14,15	0.47	0	17,19,21	1.42	3 (17%)
7	BMA	E	3	7	11,11,12	0.93	1 (9%)	15,15,17	1.35	1 (6%)
7	NAG	G	1	7,2	14,14,15	0.76	1 (7%)	17,19,21	0.83	1 (5%)
7	NAG	G	2	7	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
7	BMA	G	3	7	11,11,12	0.83	0	15,15,17	0.79	0
8	FUC	H	1	3,8	10,10,11	0.80	0	14,14,16	0.83	0
8	BGC	H	2	8	11,11,12	1.71	3 (27%)	15,15,17	0.92	0
8	FUC	I	1	3,8	10,10,11	1.14	1 (10%)	14,14,16	0.91	0
8	BGC	I	2	8	11,11,12	1.63	1 (9%)	15,15,17	1.88	3 (20%)
8	FUC	J	1	4,8	10,10,11	0.93	0	14,14,16	0.86	0
8	BGC	J	2	8	11,11,12	1.72	3 (27%)	15,15,17	1.08	1 (6%)
9	NAG	K	1	4,9	14,14,15	0.39	0	17,19,21	0.72	0
9	NAG	K	2	9	14,14,15	1.16	1 (7%)	17,19,21	2.35	3 (17%)
9	BMA	K	3	9	11,11,12	0.91	0	15,15,17	0.69	0
9	MAN	K	4	9	11,11,12	0.88	1 (9%)	15,15,17	1.49	2 (13%)
7	NAG	L	1	5,7	14,14,15	0.43	0	17,19,21	0.52	0
7	NAG	L	2	7	14,14,15	0.78	1 (7%)	17,19,21	0.75	1 (5%)
7	BMA	L	3	7	11,11,12	0.83	0	15,15,17	0.91	1 (6%)
9	NAG	M	1	9,5	14,14,15	0.63	1 (7%)	17,19,21	0.97	1 (5%)
9	NAG	M	2	9	14,14,15	0.37	0	17,19,21	0.53	0
9	BMA	M	3	9	11,11,12	0.83	0	15,15,17	0.97	1 (6%)
9	MAN	M	4	9	11,11,12	0.96	1 (9%)	15,15,17	1.49	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
7	NAG	E	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	BMA	E	3	7	-	1/2/19/22	0/1/1/1
7	NAG	G	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	1/2/19/22	0/1/1/1
8	FUC	H	1	3,8	-	-	0/1/1/1
8	BGC	H	2	8	-	2/2/19/22	0/1/1/1
8	FUC	I	1	3,8	-	-	0/1/1/1
8	BGC	I	2	8	-	2/2/19/22	0/1/1/1
8	FUC	J	1	4,8	-	-	0/1/1/1
8	BGC	J	2	8	-	2/2/19/22	0/1/1/1
9	NAG	K	1	4,9	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	4/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	2/2/19/22	0/1/1/1
7	NAG	L	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	1/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	2	BGC	O5-C1	4.51	1.51	1.43
8	J	2	BGC	O5-C1	4.49	1.51	1.43
8	H	2	BGC	O5-C1	4.40	1.51	1.43
9	K	2	NAG	C1-C2	3.72	1.57	1.52
9	K	4	MAN	O5-C5	2.49	1.48	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	2	NAG	C2-N2-C7	8.21	133.90	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	4	MAN	C1-O5-C5	4.99	118.87	112.19
9	K	4	MAN	C1-O5-C5	4.94	118.80	112.19
8	I	2	BGC	C1-C2-C3	4.60	116.35	109.64
7	E	3	BMA	C1-O5-C5	4.28	117.93	112.19

There are no chirality outliers.

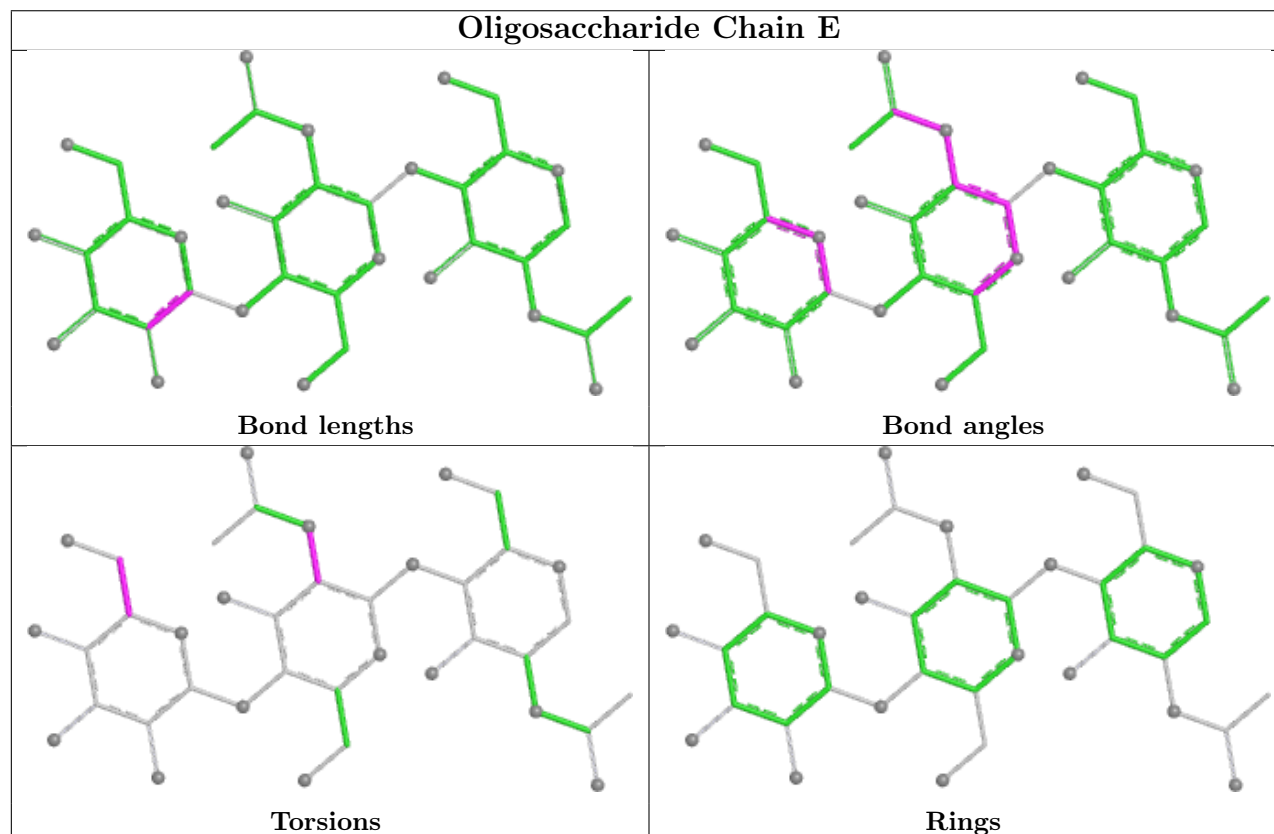
5 of 24 torsion outliers are listed below:

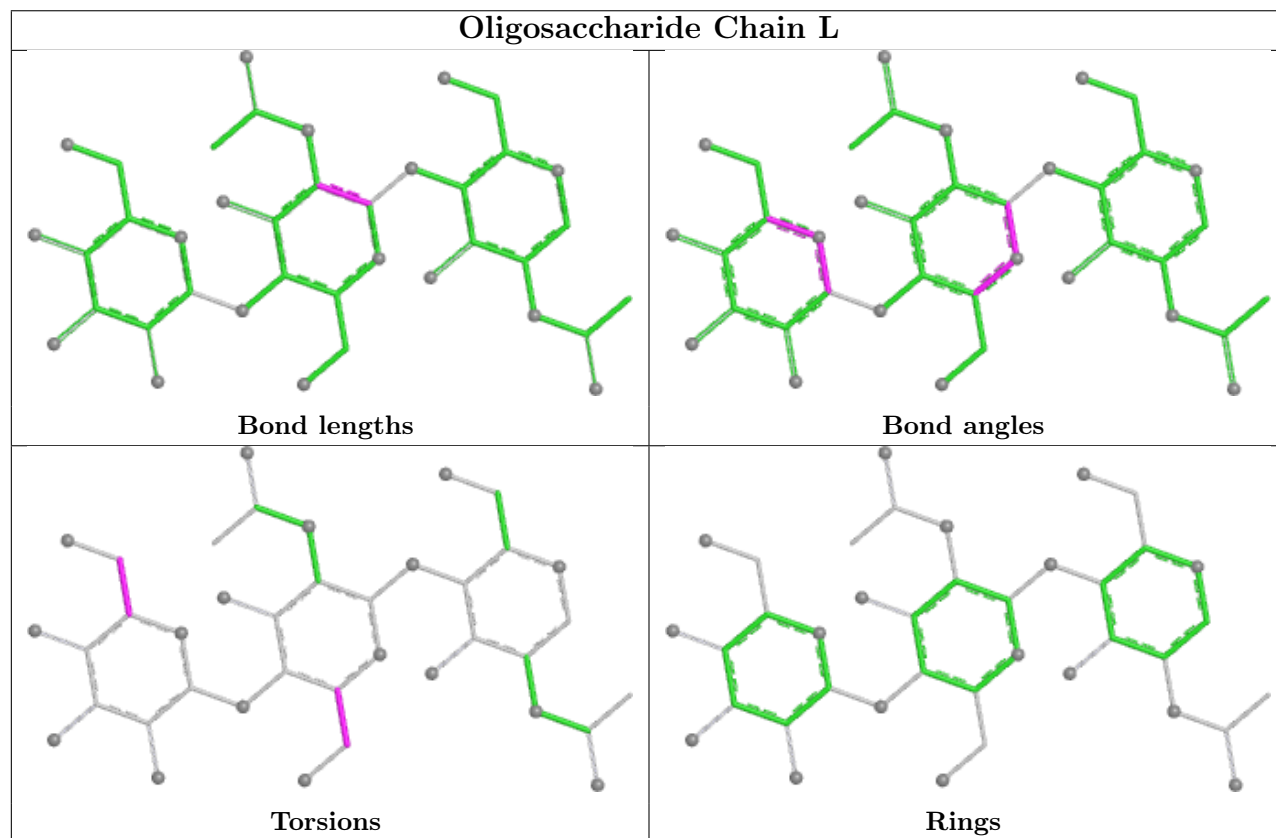
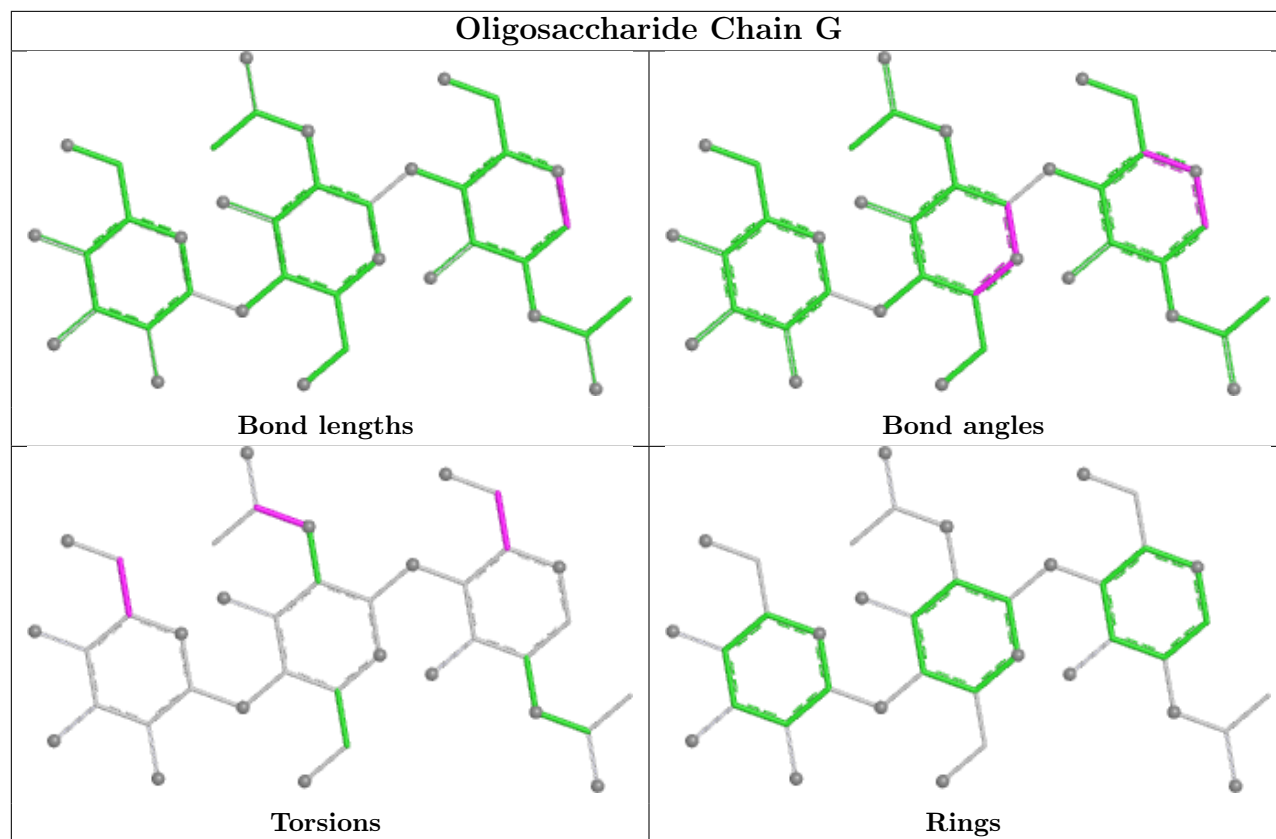
Mol	Chain	Res	Type	Atoms
7	G	1	NAG	O5-C5-C6-O6
8	H	2	BGC	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6

There are no ring outliers.

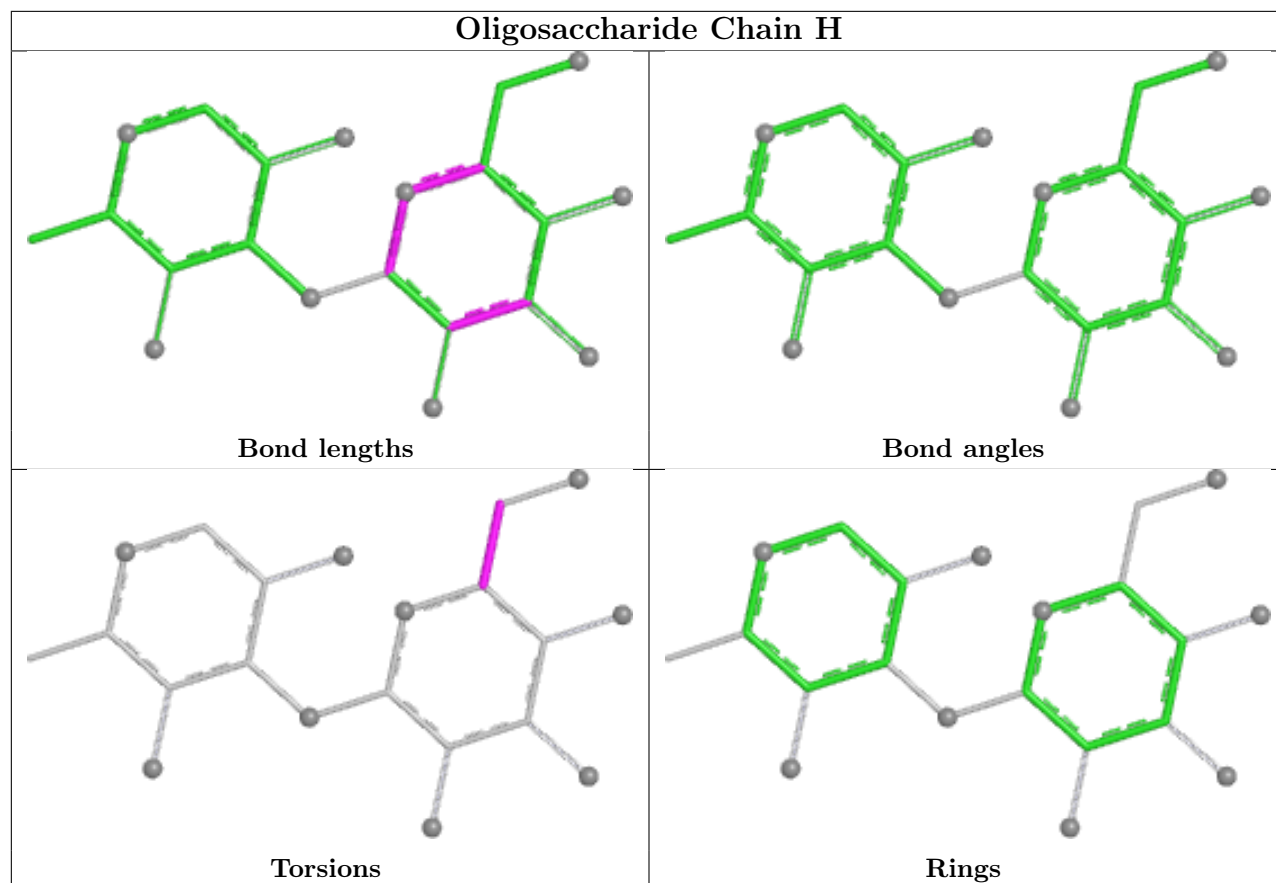
No monomer is involved in short contacts.

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

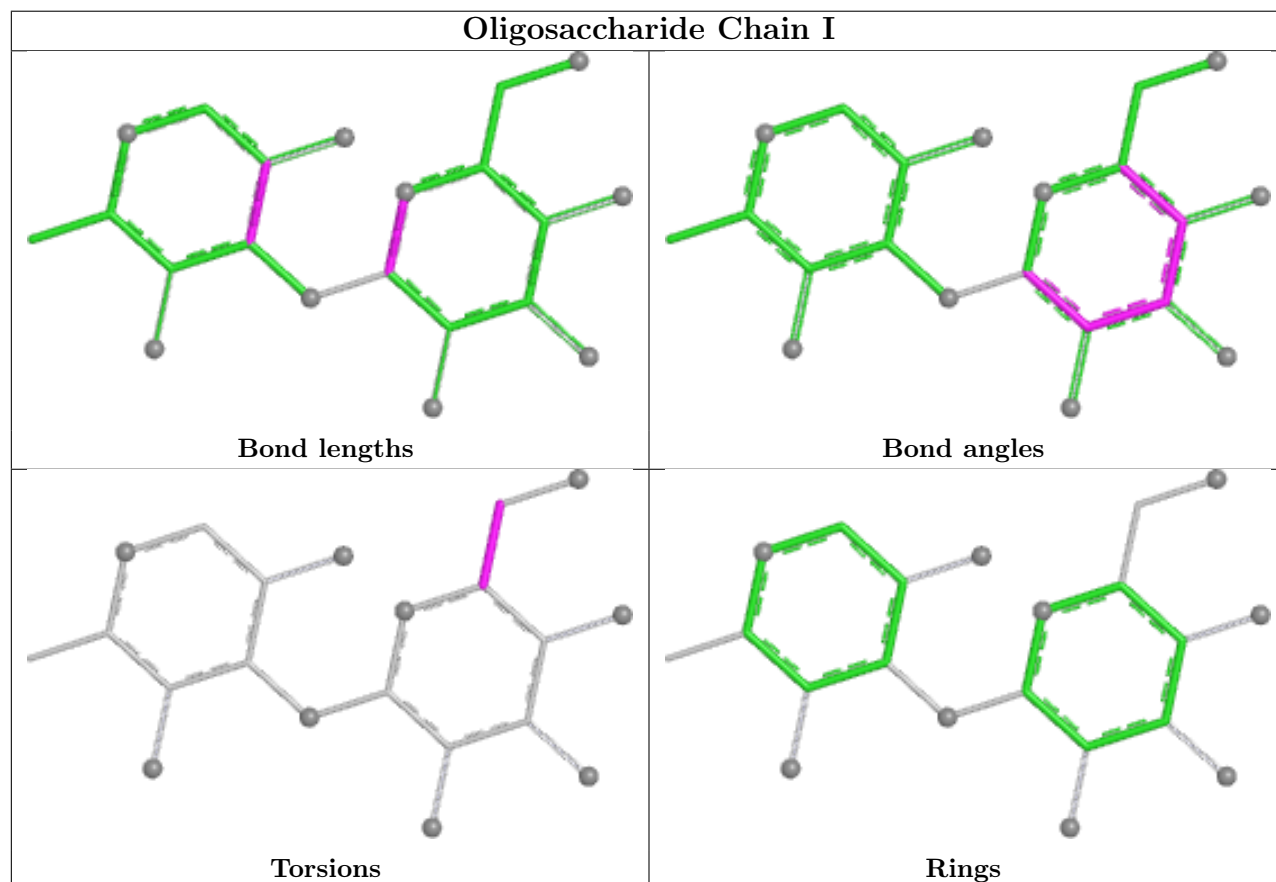




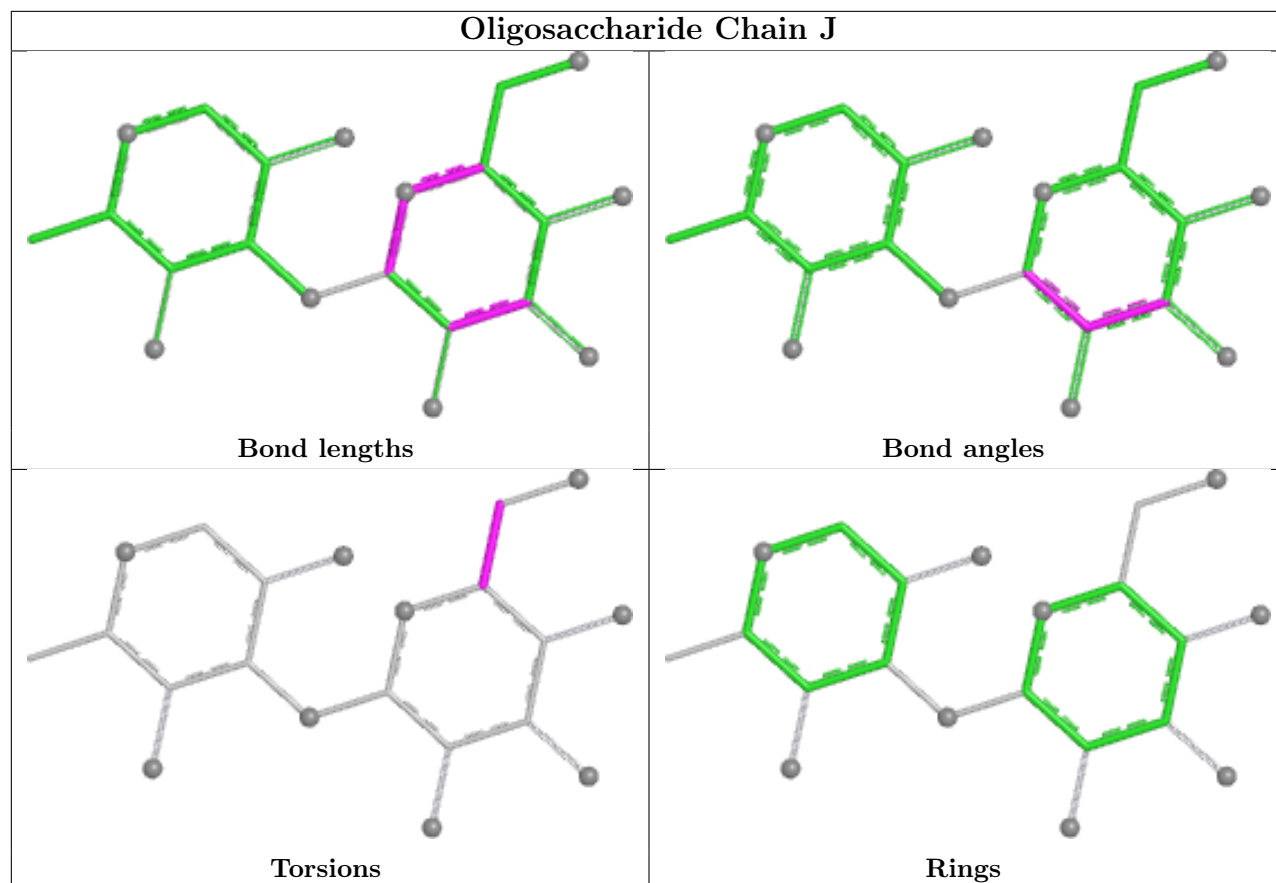
Oligosaccharide Chain H



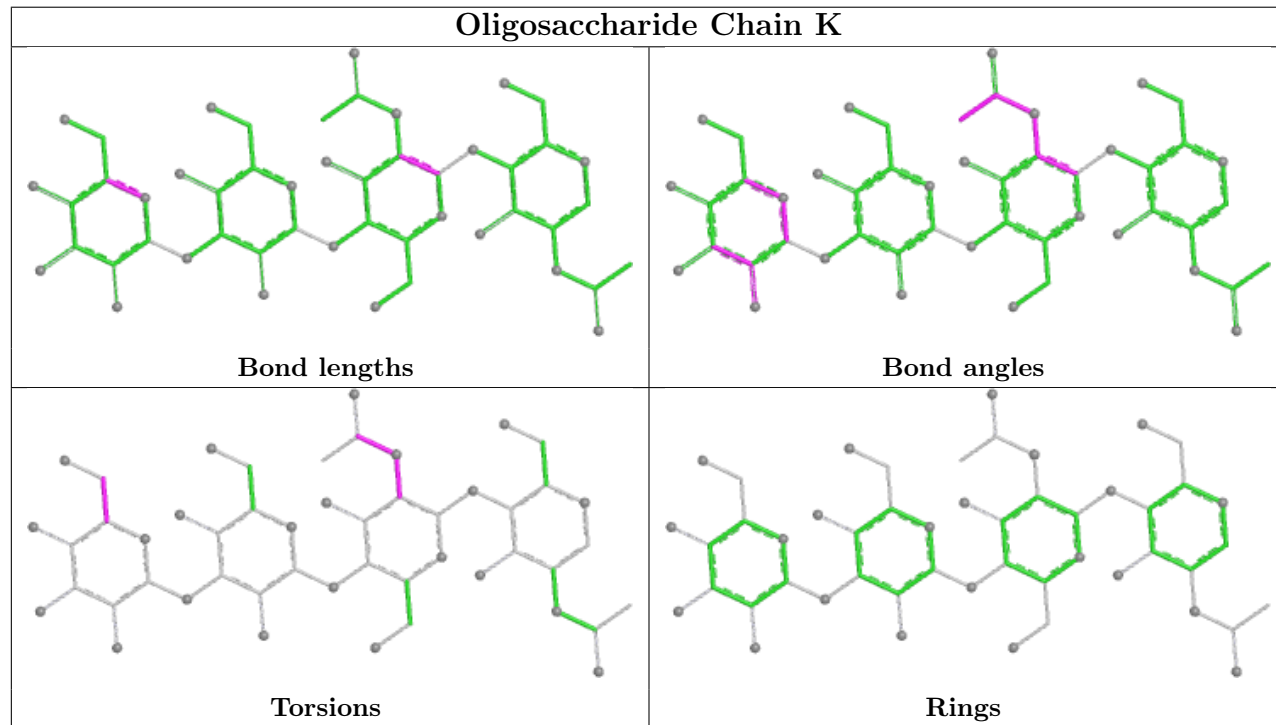
Oligosaccharide Chain I

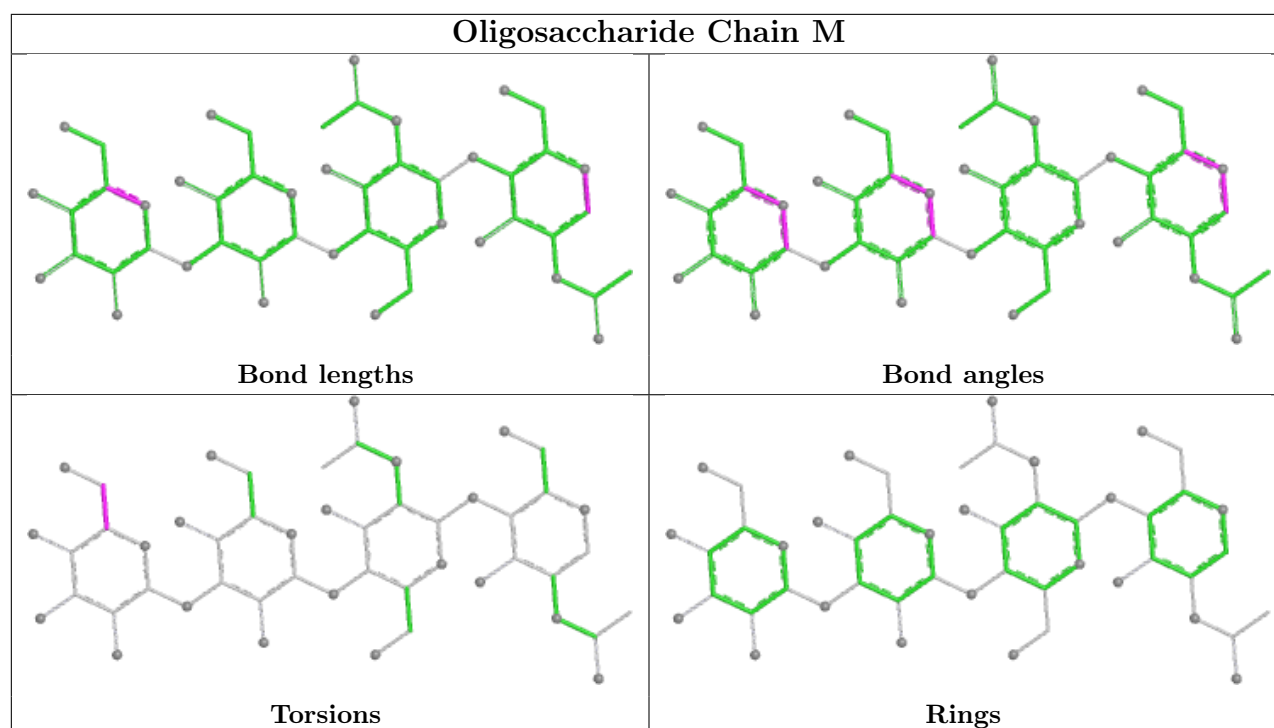


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z > 2$
10	MAN	D	501	4	11,11,12	1.05	0	15,15,17	1.47	2 (13%)
10	MAN	C	201	3	11,11,12	1.13	0	15,15,17	1.24	2 (13%)
10	MAN	C	203	3	11,11,12	1.03	0	15,15,17	1.48	2 (13%)
10	MAN	C	202	3	11,11,12	1.13	0	15,15,17	1.26	2 (13%)
11	NAG	F	801	5	14,14,15	0.53	0	17,19,21	1.05	1 (5%)
10	MAN	D	502	4	11,11,12	1.02	0	15,15,17	1.45	2 (13%)
10	MAN	D	503	4	11,11,12	1.28	2 (18%)	15,15,17	1.70	3 (20%)

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
10	MAN	D	501	4	-	0/2/19/22	0/1/1/1
10	MAN	C	201	3	-	2/2/19/22	0/1/1/1
10	MAN	C	203	3	-	0/2/19/22	0/1/1/1
10	MAN	C	202	3	-	0/2/19/22	0/1/1/1
11	NAG	F	801	5	-	4/6/23/26	0/1/1/1
10	MAN	D	502	4	-	1/2/19/22	0/1/1/1
10	MAN	D	503	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	MAN	C4-C5	2.55	1.58	1.53
10	D	503	MAN	O5-C5	2.43	1.48	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	MAN	C1-O5-C5	4.81	118.63	112.19
10	D	502	MAN	C1-O5-C5	4.12	117.71	112.19
10	D	501	MAN	C1-O5-C5	4.01	117.56	112.19
10	C	203	MAN	C1-O5-C5	3.84	117.34	112.19
11	F	801	NAG	C2-N2-C7	3.21	127.20	122.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	801	NAG	C4-C5-C6-O6
11	F	801	NAG	O5-C5-C6-O6
10	C	201	MAN	C4-C5-C6-O6
10	D	503	MAN	C4-C5-C6-O6
10	C	201	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 [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	642/645 (99%)	-0.39	13 (2%) 65 45	164, 224, 308, 343	0
2	B	906/912 (99%)	-0.55	4 (0%) 88 74	161, 255, 453, 489	0
3	C	163/163 (100%)	-0.74	0 100 100	347, 395, 626, 674	0
4	D	207/207 (100%)	-0.72	0 100 100	279, 352, 493, 532	0
5	F	712/731 (97%)	-0.41	6 (0%) 82 64	190, 233, 342, 367	0
6	R	124/124 (100%)	-0.71	0 100 100	383, 465, 510, 524	0
All	All	2754/2782 (98%)	-0.51	23 (0%) 82 64	161, 256, 475, 674	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	ALA	4.5
1	A	534	TYR	4.3
1	A	493	LEU	4.1
1	A	533	ALA	3.9
1	A	42	MET	3.5

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

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

6.3 Carbohydrates [i](#)

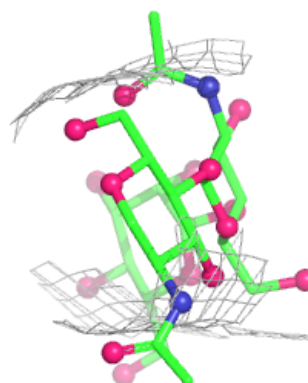
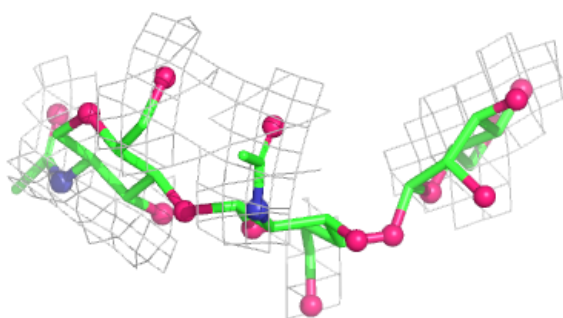
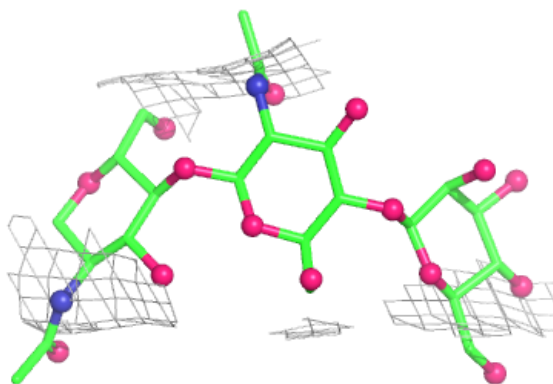
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	E	1	14/15	-	-	265,266,268,268	0
7	NAG	E	2	14/15	-	-	267,269,271,271	0
7	BMA	E	3	11/12	-	-	270,271,272,273	0
7	BMA	L	3	11/12	0.22	0.09	344,349,373,383	0
8	BGC	I	2	11/12	0.26	0.08	445,466,477,478	0
8	BGC	J	2	11/12	0.35	0.06	302,319,344,348	0
8	FUC	I	1	10/11	0.50	0.07	466,472,482,491	0
9	NAG	M	2	14/15	0.53	0.09	296,296,296,296	0
7	BMA	G	3	11/12	0.55	0.10	334,351,381,382	0
8	FUC	H	1	10/11	-	-	635,694,745,767	0
8	BGC	H	2	11/12	-	-	726,765,818,828	0
7	NAG	G	2	14/15	0.55	0.08	293,317,341,341	0
8	FUC	J	1	10/11	0.60	0.05	310,320,332,340	0
9	BMA	M	3	11/12	0.64	0.06	296,296,296,296	0
7	NAG	L	2	14/15	0.65	0.07	313,322,336,345	0
9	NAG	K	1	14/15	-	-	292,296,303,305	0
9	NAG	K	2	14/15	-	-	301,312,321,322	0
9	BMA	K	3	11/12	-	-	326,332,339,340	0
9	MAN	K	4	11/12	-	-	326,339,345,350	0
9	NAG	M	1	14/15	0.80	0.07	296,296,296,296	0
7	NAG	L	1	14/15	0.83	0.06	277,287,300,302	0
7	NAG	G	1	14/15	0.85	0.06	247,265,283,287	0
9	MAN	M	4	11/12	-	-	296,296,296,296	0

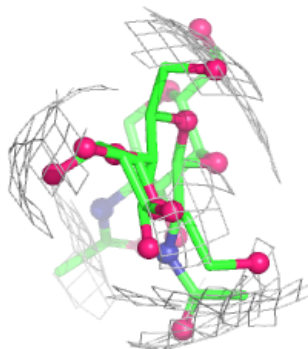
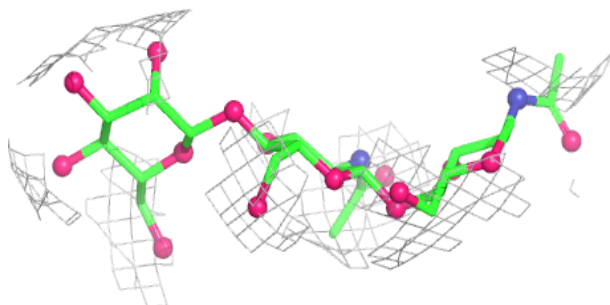
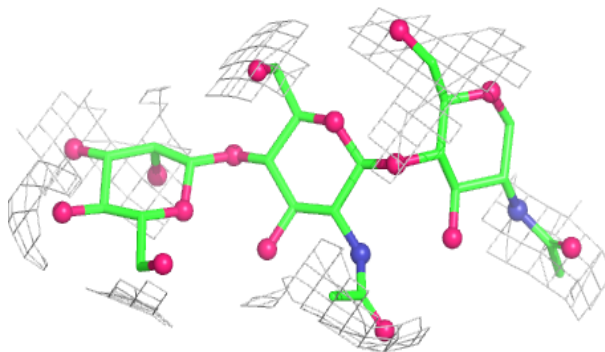
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

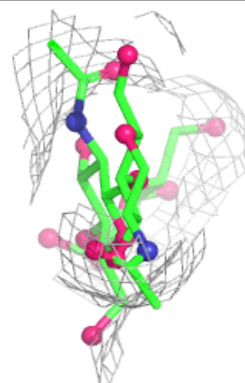
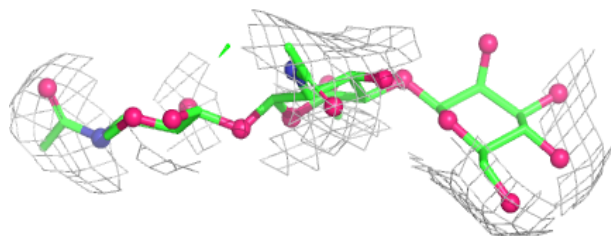
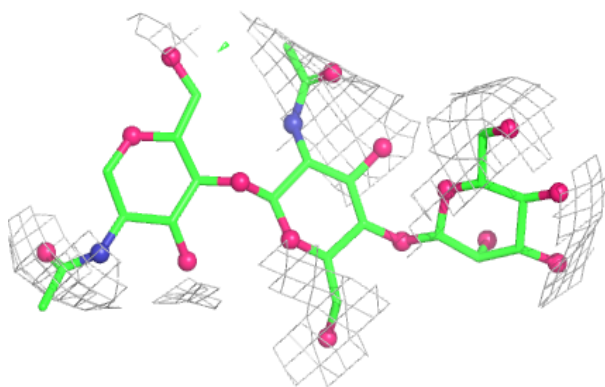
**Electron density around Chain G:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



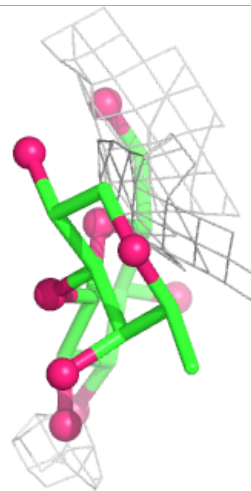
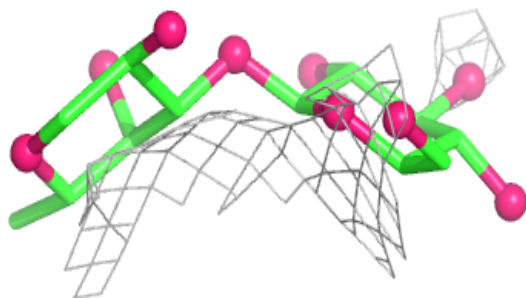
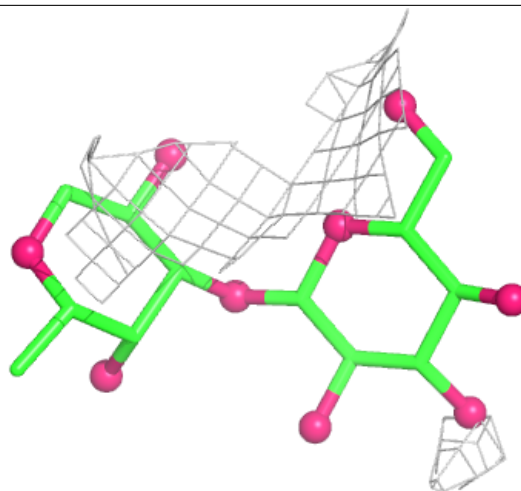
Electron density around Chain L:

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



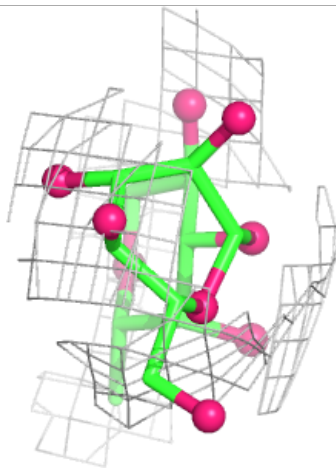
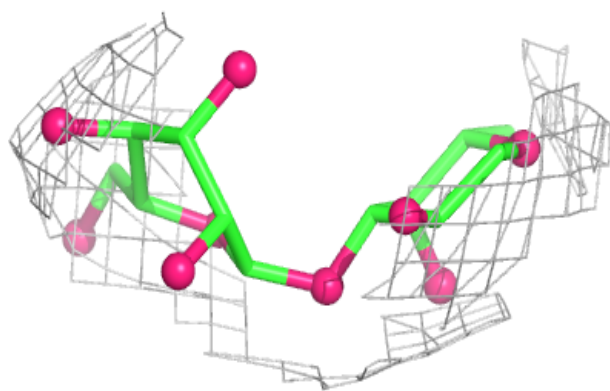
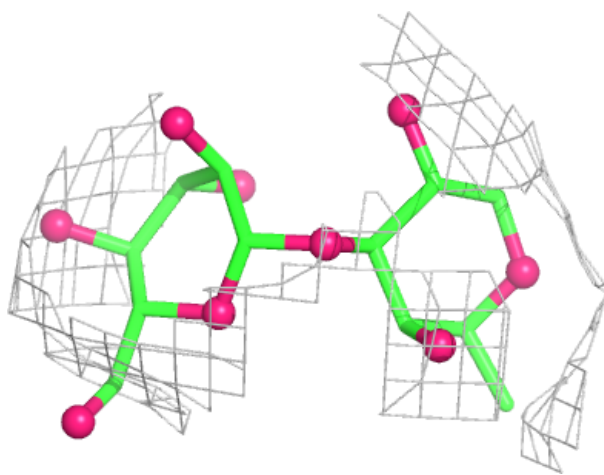
Electron density around Chain H:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



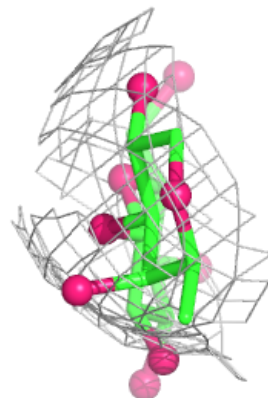
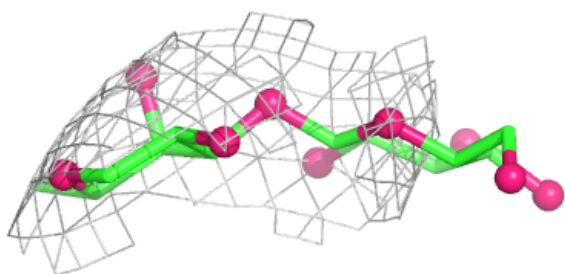
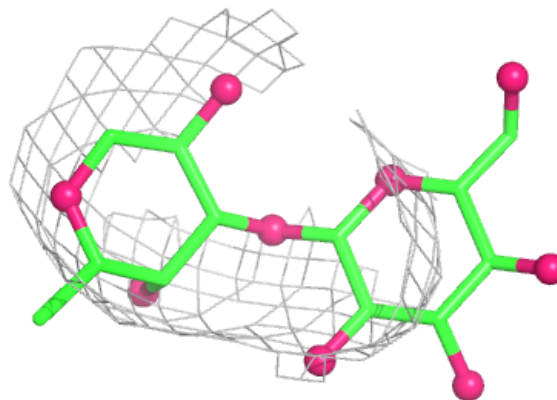
Electron density around Chain I:

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



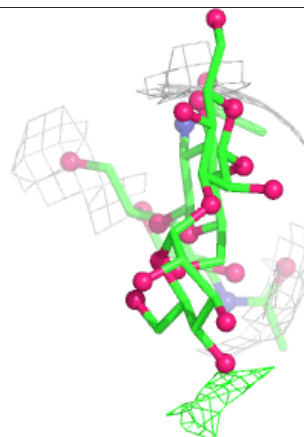
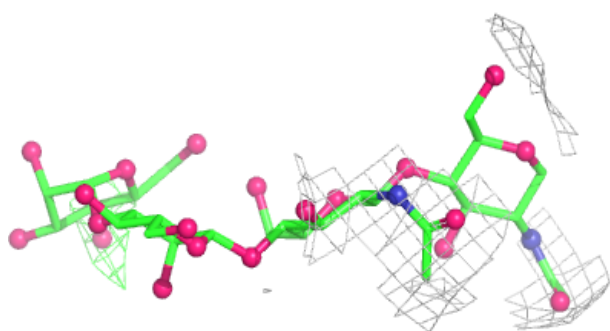
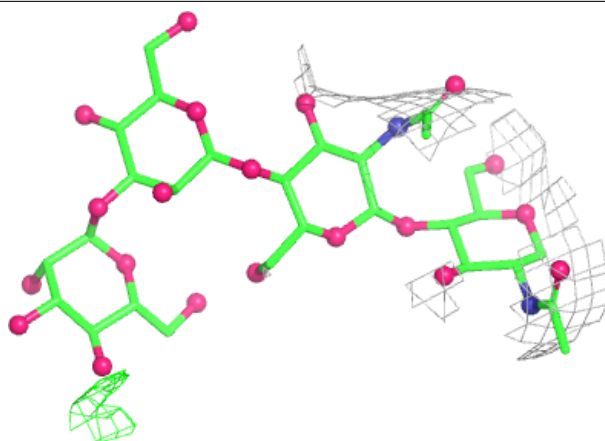
Electron density around Chain J:

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

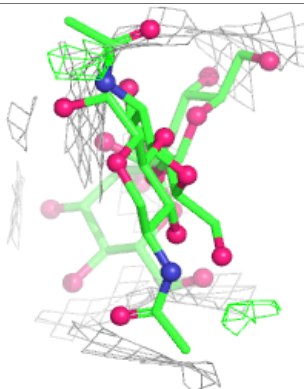
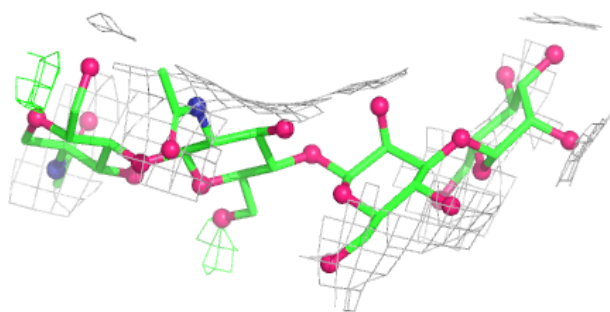
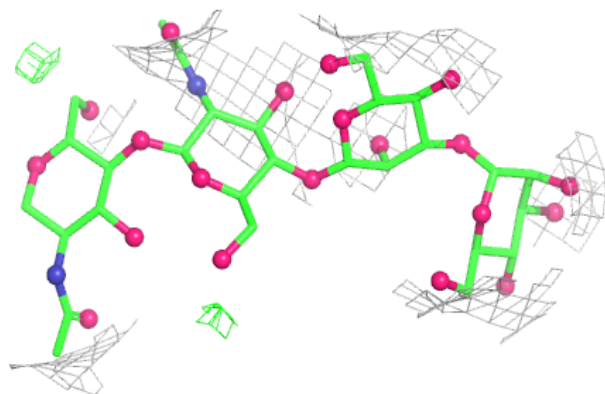


Electron density around Chain K:

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

**Electron density around Chain M:**

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



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
10	MAN	D	503	11/12	0.29	0.07	309,315,322,324	0
10	MAN	C	203	11/12	0.56	0.06	435,439,457,459	0
10	MAN	C	201	11/12	0.76	0.08	296,304,319,322	0
10	MAN	C	202	11/12	0.78	0.04	367,378,392,392	0
10	MAN	D	501	11/12	0.86	0.04	243,253,260,262	0
11	NAG	F	801	14/15	0.90	0.06	266,286,294,301	0
10	MAN	D	502	11/12	0.92	0.04	242,250,255,257	0
12	MG	F	802	1/1	0.98	0.03	226,226,226,226	0

6.5 Other polymers [i](#)

There are no such residues in this entry.