Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 07:29 pm BST

PDB ID	:	8A0Y
Title	:	Crystal structure of mouse contactin 2 immunoglobulin domains
Authors	:	Chataigner, L.M.P.; Janssen, B.J.C.
Deposited on	:	2022-05-30
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

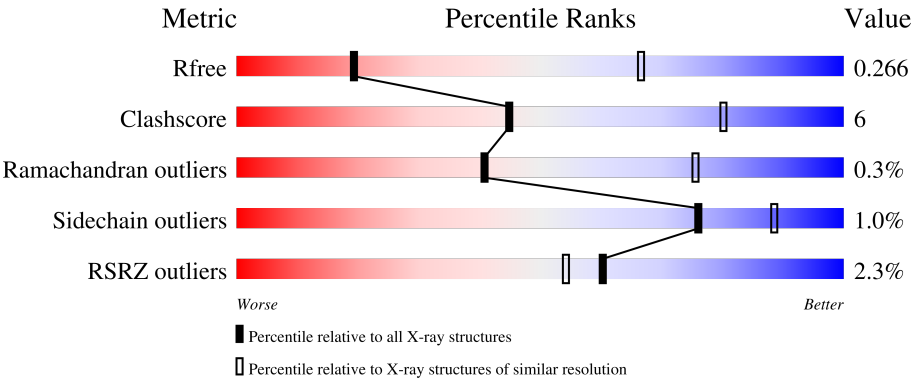
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	588	3% 82% 15%
1	B	588	% 85% 13%
1	C	588	3% 84% 13%
2	D	4	25% 75%
2	G	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	E	3	67% 33%
3	I	3	100%
3	K	3	100%
4	F	6	50% 17% 33%
5	H	2	100%
5	L	2	100%
6	J	5	40% 40% 20%
7	M	7	14% 57% 29%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26854 atoms, of which 12967 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 Contactin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	574	Total	C	H	N	O	S	0	0	0
			8747	2781	4323	778	843	22			
1	B	574	Total	C	H	N	O	S	0	0	0
			8746	2781	4322	778	843	22			
1	C	574	Total	C	H	N	O	S	0	0	0
			8746	2781	4322	778	843	22			

There are 21 discrepancies between the modelled and reference sequences:

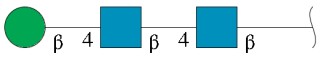
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q61330
A	609	HIS	-	expression tag	UNP Q61330
A	610	HIS	-	expression tag	UNP Q61330
A	611	HIS	-	expression tag	UNP Q61330
A	612	HIS	-	expression tag	UNP Q61330
A	613	HIS	-	expression tag	UNP Q61330
A	614	HIS	-	expression tag	UNP Q61330
B	27	GLY	-	expression tag	UNP Q61330
B	609	HIS	-	expression tag	UNP Q61330
B	610	HIS	-	expression tag	UNP Q61330
B	611	HIS	-	expression tag	UNP Q61330
B	612	HIS	-	expression tag	UNP Q61330
B	613	HIS	-	expression tag	UNP Q61330
B	614	HIS	-	expression tag	UNP Q61330
C	27	GLY	-	expression tag	UNP Q61330
C	609	HIS	-	expression tag	UNP Q61330
C	610	HIS	-	expression tag	UNP Q61330
C	611	HIS	-	expression tag	UNP Q61330
C	612	HIS	-	expression tag	UNP Q61330
C	613	HIS	-	expression tag	UNP Q61330
C	614	HIS	-	expression tag	UNP Q61330

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

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

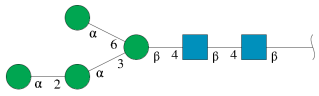
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.

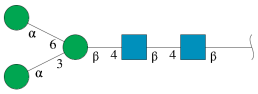


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

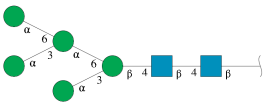
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



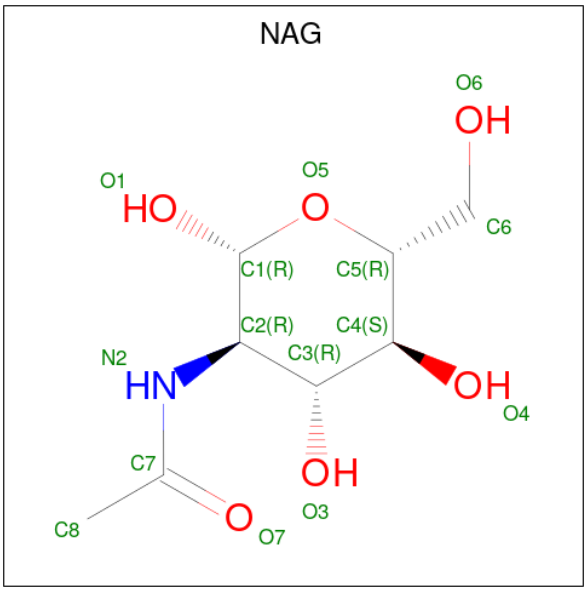
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
7	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



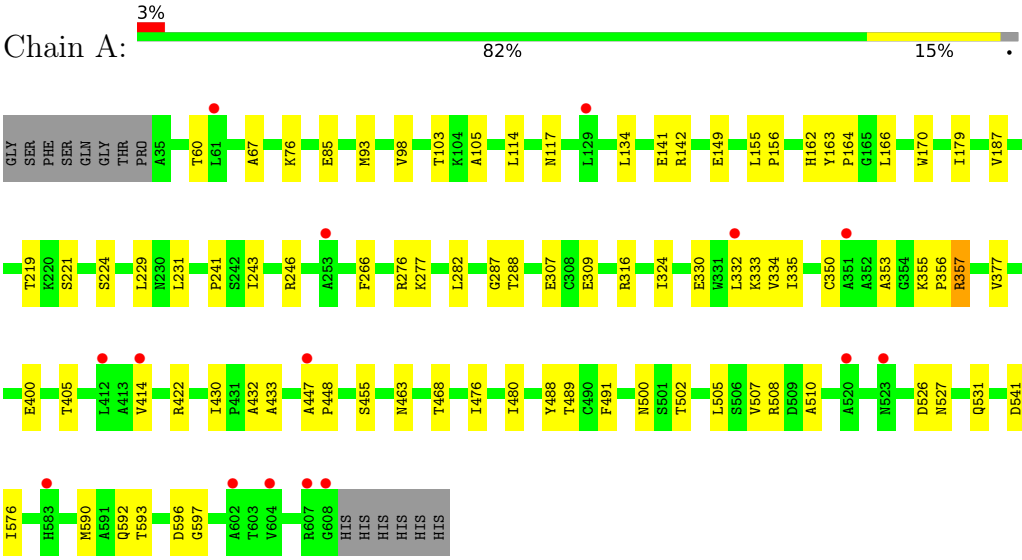
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total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

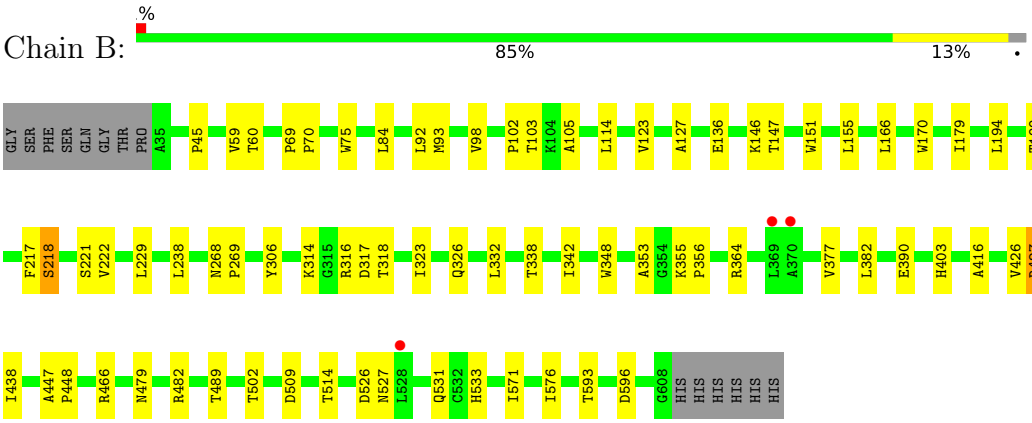
• Molecule 1: Contactin-2

Chain A:



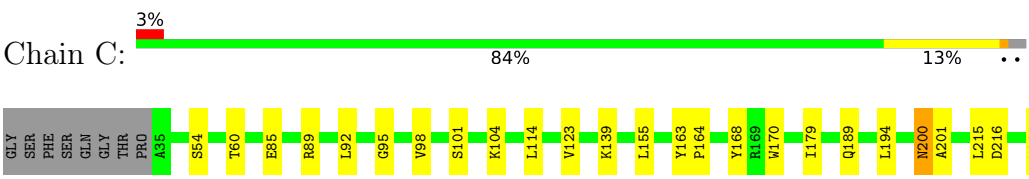
• Molecule 1: Contactin-2

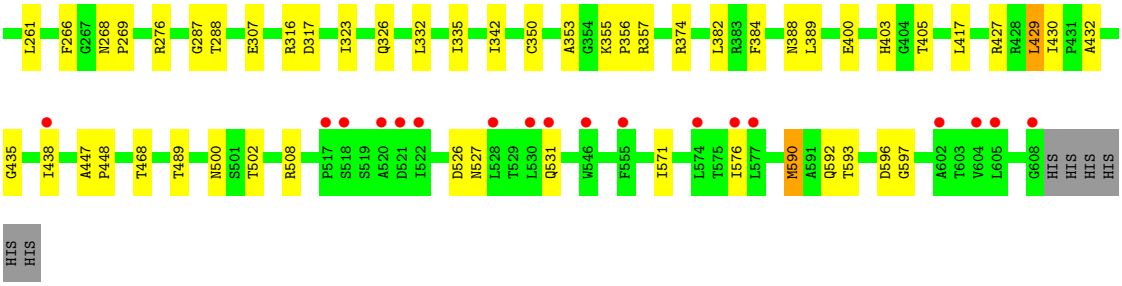
Chain B:



• Molecule 1: Contactin-2

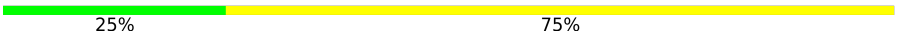
Chain C:





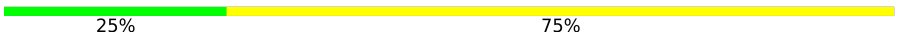
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 2: 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 G:



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

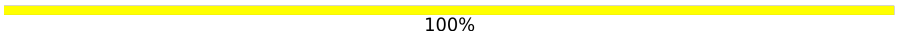
Chain E:

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

Chain I:

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

Chain K:



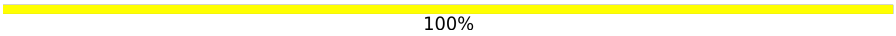
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam

ido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain H:

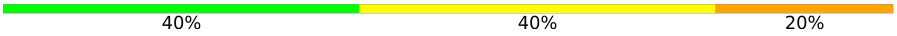


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• 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 J:



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.93Å 159.78Å 227.89Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	59.82 – 3.50 59.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (59.82-3.50) 99.2 (59.82-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.225 , 0.264 0.225 , 0.266	Depositor DCC
R_{free} test set	2977 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	172.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 166.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26854	wwPDB-VP
Average B, all atoms (Å^2)	251.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: BMA, 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	0.25	0/4528	0.47	0/6160
1	B	0.25	0/4528	0.47	0/6160
1	C	0.25	0/4528	0.47	0/6160
All	All	0.25	0/13584	0.47	0/18480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4424	4323	4323	66	0
1	B	4424	4322	4322	50	0
1	C	4424	4322	4323	48	0
2	D	50	0	43	1	0
2	G	50	0	43	1	0
3	E	39	0	34	4	0
3	I	39	0	34	0	0
3	K	39	0	32	3	0
4	F	72	0	61	1	0
5	H	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	28	0	25	0	0
6	J	61	0	52	3	0
7	M	83	0	70	7	0
8	A	42	0	39	1	0
8	B	42	0	39	1	0
8	C	42	0	39	3	0
All	All	13887	12967	13504	178	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 6.

All (178) 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)
3:K:1:NAG:H83	3:K:1:NAG:H3	1.50	0.92
1:C:60:THR:HG22	1:C:98:VAL:HG22	1.49	0.91
1:A:60:THR:HG22	1:A:98:VAL:HG22	1.54	0.89
3:E:1:NAG:H83	3:E:1:NAG:H3	1.55	0.89
1:B:60:THR:HG22	1:B:98:VAL:HG22	1.59	0.84
7:M:1:NAG:H83	7:M:1:NAG:H3	1.62	0.80
1:A:219:THR:OG1	1:B:222:VAL:HG13	1.80	0.80
1:B:482:ARG:NH2	1:B:509:ASP:OD1	2.15	0.80
1:A:432:ALA:HB3	1:A:507:VAL:HG22	1.67	0.76
1:B:136:GLU:HA	1:B:222:VAL:HG11	1.69	0.74
6:J:2:NAG:O7	6:J:2:NAG:O3	2.07	0.73
1:A:221:SER:HG	1:B:221:SER:HG	1.29	0.72
1:A:377:VAL:HG22	1:A:382:LEU:HD13	1.72	0.71
1:A:432:ALA:HB3	1:A:507:VAL:CG2	2.22	0.70
1:C:114:LEU:HD23	1:C:123:VAL:HG22	1.74	0.69
6:J:2:NAG:O7	6:J:5:MAN:O4	2.10	0.69
1:C:447:ALA:HB3	1:C:448:PRO:CD	2.27	0.65
1:C:114:LEU:CD2	1:C:123:VAL:HG22	2.27	0.65
1:A:447:ALA:HB3	1:A:448:PRO:CD	2.27	0.64
1:A:400:GLU:CB	1:A:405:THR:HG22	2.28	0.63
1:C:590:MET:SD	1:C:592:GLN:NE2	2.72	0.63
1:B:377:VAL:HG22	1:B:382:LEU:CD1	2.29	0.63
1:C:374:ARG:NH1	1:C:388:ASN:OD1	2.31	0.63
1:B:377:VAL:HG22	1:B:382:LEU:HD13	1.81	0.62
1:A:277:LYS:HB2	1:A:282:LEU:HD13	1.82	0.62
1:B:466:ARG:NH1	1:B:479:ASN:O	2.33	0.62
3:K:1:NAG:H3	3:K:1:NAG:C8	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ASP:OD1	1:A:597:GLY:N	2.32	0.61
1:B:447:ALA:HB3	1:B:448:PRO:CD	2.28	0.61
1:A:334:VAL:HG22	1:C:429:LEU:HD21	1.82	0.61
1:A:141:GLU:OE1	1:A:141:GLU:N	2.34	0.61
1:C:596:ASP:OD1	1:C:597:GLY:N	2.32	0.60
1:B:59:VAL:HG13	1:B:102:PRO:HG2	1.84	0.60
1:A:377:VAL:HG22	1:A:382:LEU:CD1	2.32	0.59
1:A:400:GLU:HB3	1:A:405:THR:HG22	1.83	0.59
1:C:326:GLN:OE1	1:C:403:HIS:NE2	2.34	0.59
1:B:526:ASP:OD1	8:B:703:NAG:H82	2.02	0.59
1:A:489:THR:OG1	1:A:502:THR:HG22	2.03	0.59
1:B:526:ASP:OD1	1:B:527:ASN:N	2.34	0.58
7:M:1:NAG:C1	7:M:1:NAG:H82	2.33	0.58
1:C:139:LYS:O	1:C:225:LYS:NZ	2.32	0.58
1:A:526:ASP:OD1	1:A:527:ASN:N	2.36	0.58
1:B:317:ASP:OD1	1:B:318:THR:N	2.37	0.57
1:A:134:LEU:HD22	1:A:213:SER:HB2	1.85	0.57
1:C:435:GLY:O	8:C:703:NAG:H82	2.05	0.57
1:C:526:ASP:OD1	1:C:527:ASN:N	2.37	0.57
3:K:2:NAG:O3	3:K:3:BMA:O5	2.19	0.57
1:A:276:ARG:NH2	1:A:307:GLU:OE1	2.38	0.57
3:E:1:NAG:H3	3:E:1:NAG:C8	2.31	0.56
1:B:489:THR:OG1	1:B:502:THR:HG22	2.06	0.56
1:B:531:GLN:OE1	1:B:571:ILE:HD11	2.05	0.56
1:C:200:ASN:OD1	1:C:201:ALA:N	2.39	0.55
1:C:489:THR:OG1	1:C:502:THR:HG22	2.08	0.54
1:A:355:LYS:HB3	1:A:356:PRO:HD3	1.89	0.54
1:C:261:LEU:HD21	1:C:323:ILE:HD11	1.90	0.54
3:E:1:NAG:C1	3:E:1:NAG:H82	2.38	0.54
1:A:324:ILE:HG23	1:A:324:ILE:O	2.08	0.54
1:B:342:ILE:HD11	1:B:416:ALA:HB2	1.89	0.53
1:C:155:LEU:HD12	1:C:194:LEU:HD23	1.89	0.53
1:A:333:LYS:HA	1:C:429:LEU:HD23	1.89	0.53
1:B:426:VAL:O	1:B:427:ARG:HB2	2.09	0.53
1:C:92:LEU:HD21	1:C:95:GLY:H	1.74	0.53
1:A:531:GLN:OE1	1:A:571:ILE:HD11	2.08	0.53
1:A:500:ASN:N	1:A:500:ASN:OD1	2.42	0.52
1:A:330:GLU:OE2	1:C:508:ARG:NH1	2.42	0.52
4:F:4:MAN:O3	4:F:5:MAN:H2	2.09	0.52
1:A:400:GLU:HB2	1:A:405:THR:HG22	1.92	0.51
1:A:392:SER:HB2	1:A:414:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ALA:HB3	1:B:448:PRO:HD3	1.92	0.51
1:C:170:TRP:HB2	1:C:179:ILE:HD12	1.93	0.51
1:C:468:THR:HG21	8:C:702:NAG:H62	1.93	0.51
1:A:541:ASP:OD2	1:C:357:ARG:NH1	2.45	0.50
1:A:204:LEU:HD13	1:A:231:LEU:HB2	1.94	0.50
7:M:2:NAG:O7	7:M:4:MAN:H5	2.12	0.50
1:B:364:ARG:NH1	1:B:390:GLU:O	2.44	0.50
1:B:204:LEU:HD12	1:B:229:LEU:O	2.12	0.49
1:C:400:GLU:HG2	1:C:405:THR:HG23	1.93	0.49
1:C:447:ALA:HB3	1:C:448:PRO:HD2	1.95	0.49
1:C:89:ARG:NH1	1:C:101:SER:O	2.45	0.49
1:B:170:TRP:HB2	1:B:179:ILE:HD12	1.93	0.49
1:B:217:PHE:O	1:B:218:SER:CB	2.59	0.49
1:A:204:LEU:HD12	1:A:229:LEU:O	2.12	0.49
1:B:332:LEU:HD11	1:B:353:ALA:HB2	1.94	0.49
5:H:1:NAG:O7	5:H:1:NAG:O3	2.28	0.49
1:A:309:GLU:OE2	1:A:316:ARG:HD2	2.12	0.48
7:M:4:MAN:H62	7:M:6:MAN:H2	1.53	0.48
1:B:432:ALA:CB	1:B:438:ILE:HD11	2.43	0.48
1:C:531:GLN:OE1	1:C:571:ILE:HD11	2.12	0.48
7:M:1:NAG:C1	7:M:1:NAG:C8	2.92	0.48
1:A:76:LYS:HE3	1:A:114:LEU:HD11	1.95	0.48
5:H:1:NAG:H62	5:H:2:NAG:C7	2.43	0.48
1:A:170:TRP:HB2	1:A:179:ILE:HD12	1.94	0.48
6:J:2:NAG:HO3	6:J:2:NAG:C7	2.22	0.48
1:A:170:TRP:CB	1:A:179:ILE:HD12	2.44	0.48
1:B:326:GLN:OE1	1:B:403:HIS:NE2	2.42	0.47
1:A:488:TYR:CE1	1:A:505:LEU:HD13	2.49	0.47
1:B:593:THR:HG23	1:B:596:ASP:H	1.79	0.47
8:A:701:NAG:O3	8:A:701:NAG:H82	2.15	0.47
7:M:1:NAG:H3	7:M:1:NAG:C8	2.38	0.47
1:A:243:ILE:HG22	1:A:246:ARG:HG2	1.97	0.47
1:C:417:LEU:N	1:C:447:ALA:HB2	2.29	0.47
1:C:168:TYR:O	1:C:189:GLN:NE2	2.48	0.47
1:C:447:ALA:CB	1:C:448:PRO:CD	2.93	0.47
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.97	0.46
1:A:67:ALA:HB1	1:A:117:ASN:ND2	2.30	0.46
1:B:355:LYS:HB3	1:B:356:PRO:HD3	1.98	0.46
1:B:155:LEU:HD12	1:B:194:LEU:HD23	1.96	0.46
1:A:187:VAL:HG23	1:A:187:VAL:O	2.15	0.46
1:C:200:ASN:OD1	8:C:701:NAG:N2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:MET:HG3	1:A:592:GLN:HG3	1.98	0.46
1:A:241:PRO:HA	1:A:266:PHE:O	2.16	0.46
1:A:455:SER:HG	1:A:491:PHE:HE1	1.63	0.46
1:C:335:ILE:HG23	1:C:350:CYS:SG	2.56	0.45
1:C:276:ARG:NE	1:C:307:GLU:OE1	2.46	0.45
1:C:355:LYS:HB3	1:C:356:PRO:HD3	1.98	0.45
1:A:162:HIS:CG	1:A:166:LEU:HD11	2.52	0.45
1:A:447:ALA:HB3	1:A:448:PRO:HD2	1.99	0.45
1:A:93:MET:CE	1:A:98:VAL:HG21	2.46	0.45
1:A:447:ALA:CB	1:A:448:PRO:CD	2.94	0.45
1:B:426:VAL:O	1:B:427:ARG:CB	2.66	0.44
1:C:200:ASN:OD1	1:C:200:ASN:C	2.55	0.44
2:D:1:NAG:H61	2:D:2:NAG:N2	2.31	0.44
1:A:142:ARG:NH1	1:A:156:PRO:O	2.50	0.44
1:A:430:ILE:O	1:A:430:ILE:HG22	2.18	0.44
1:C:432:ALA:CB	1:C:438:ILE:HD11	2.47	0.44
3:E:1:NAG:C8	3:E:1:NAG:C1	2.96	0.44
1:A:287:GLY:O	1:A:288:THR:OG1	2.28	0.44
1:C:500:ASN:OD1	7:M:1:NAG:O5	2.36	0.44
1:A:480:ILE:HG21	1:A:507:VAL:HG11	2.00	0.44
1:A:335:ILE:HG23	1:A:350:CYS:SG	2.58	0.44
1:A:149:GLU:HB2	1:A:231:LEU:HG	1.98	0.44
1:B:268:ASN:HB3	1:B:269:PRO:HD3	1.99	0.43
1:B:114:LEU:N	1:B:114:LEU:HD12	2.33	0.43
1:B:151:TRP:O	1:B:199:THR:OG1	2.37	0.43
1:C:593:THR:HG23	1:C:596:ASP:H	1.82	0.43
1:B:84:LEU:HB3	1:B:92:LEU:HG	2.01	0.43
1:B:75:TRP:CD1	1:B:92:LEU:HD21	2.54	0.43
1:A:103:THR:HG22	1:A:105:ALA:H	1.84	0.42
1:C:268:ASN:HB3	1:C:269:PRO:HD3	2.02	0.42
2:G:1:NAG:H61	2:G:2:NAG:C7	2.49	0.42
1:A:155:LEU:HD12	1:A:194:LEU:HD23	2.01	0.42
1:B:114:LEU:HG	1:B:123:VAL:HG12	2.01	0.42
1:B:146:LYS:O	1:B:147:THR:HG23	2.20	0.42
1:C:287:GLY:O	1:C:288:THR:OG1	2.32	0.42
1:C:163:TYR:HB3	1:C:164:PRO:HD3	2.02	0.42
1:A:468:THR:OG1	1:A:476:ILE:HB	2.20	0.42
1:A:356:PRO:O	1:A:357:ARG:C	2.59	0.42
1:B:84:LEU:HD22	1:B:92:LEU:HG	2.02	0.42
1:B:338:THR:HG1	1:B:348:TRP:HZ2	1.68	0.42
1:A:142:ARG:NH2	1:A:224:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ILE:HD11	1:C:389:LEU:HG	2.01	0.41
1:A:433:ALA:HB1	1:A:510:ALA:CB	2.50	0.41
1:A:334:VAL:HG22	1:C:429:LEU:CD2	2.50	0.41
1:B:151:TRP:O	1:B:199:THR:HG23	2.20	0.41
1:C:215:LEU:HD12	1:C:216:ASP:N	2.35	0.41
1:C:429:LEU:C	1:C:430:ILE:HD12	2.41	0.41
1:A:433:ALA:HB1	1:A:510:ALA:HB2	2.02	0.41
1:A:593:THR:HG23	1:A:596:ASP:H	1.85	0.41
1:B:103:THR:HG22	1:B:105:ALA:H	1.86	0.41
1:B:238:LEU:HB3	1:B:314:LYS:HG3	2.02	0.41
1:B:306:TYR:CE1	1:B:323:ILE:HD12	2.55	0.41
1:B:447:ALA:CB	1:B:448:PRO:CD	2.96	0.41
1:B:45:PRO:HB2	1:B:127:ALA:HB2	2.03	0.41
1:C:332:LEU:HD11	1:C:353:ALA:HB2	2.03	0.41
1:A:432:ALA:CB	1:A:507:VAL:HG22	2.46	0.41
1:C:382:LEU:HD21	1:C:384:PHE:CZ	2.56	0.41
1:C:576:ILE:N	1:C:576:ILE:HD12	2.36	0.41
1:A:576:ILE:N	1:A:576:ILE:HD12	2.36	0.41
1:B:69:PRO:O	1:B:70:PRO:C	2.60	0.41
1:C:241:PRO:HA	1:C:266:PHE:O	2.21	0.41
1:A:93:MET:HE1	1:A:98:VAL:HG21	2.02	0.40
1:A:163:TYR:HB3	1:A:164:PRO:HD3	2.03	0.40
1:A:332:LEU:HD11	1:A:353:ALA:HB2	2.04	0.40
1:B:84:LEU:HD22	1:B:92:LEU:HD21	2.03	0.40
1:B:514:THR:N	1:B:533:HIS:O	2.55	0.40
1:B:576:ILE:HD12	1:B:576:ILE:N	2.36	0.40
1:A:221:SER:OG	1:B:221:SER:OG	2.09	0.40
1:B:166:LEU:HD13	1:B:211:ALA:HB1	2.03	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	572/588 (97%)	534 (93%)	38 (7%)	0	100	100
1	B	572/588 (97%)	535 (94%)	35 (6%)	2 (0%)	41	75
1	C	572/588 (97%)	534 (93%)	35 (6%)	3 (0%)	29	68
All	All	1716/1764 (97%)	1603 (93%)	108 (6%)	5 (0%)	41	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	SER
1	C	54	SER
1	B	427	ARG
1	C	427	ARG
1	C	85	GLU

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	477/489 (98%)	472 (99%)	5 (1%)	76	88
1	B	477/489 (98%)	475 (100%)	2 (0%)	91	96
1	C	477/489 (98%)	470 (98%)	7 (2%)	65	84
All	All	1431/1467 (98%)	1417 (99%)	14 (1%)	76	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	357	ARG
1	A	422	ARG
1	A	463	ASN
1	A	508	ARG
1	B	93	MET
1	B	316	ARG
1	C	104	LYS

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Mol	Chain	Res	Type
1	C	200	ASN
1	C	239	PHE
1	C	316	ARG
1	C	317	ASP
1	C	429	LEU
1	C	590	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	424	ASN
1	C	592	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

39 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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.52	0
2	BMA	D	3	2	11,11,12	0.63	0	15,15,17	0.66	0
2	MAN	D	4	2	11,11,12	0.68	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	1	1,3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	BMA	E	3	3	11,11,12	0.62	0	15,15,17	0.68	0
4	NAG	F	1	1,4	14,14,15	0.56	0	17,19,21	0.62	0
4	NAG	F	2	4	14,14,15	0.21	0	17,19,21	0.43	0
4	BMA	F	3	4	11,11,12	0.56	0	15,15,17	0.82	0
4	MAN	F	4	4	11,11,12	0.60	0	15,15,17	0.97	1 (6%)
4	MAN	F	5	4	11,11,12	0.62	0	15,15,17	1.00	2 (13%)
4	MAN	F	6	4	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
2	NAG	G	1	1,2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	G	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	BMA	G	3	2	11,11,12	0.55	0	15,15,17	0.69	0
2	MAN	G	4	2	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.28	0	17,19,21	0.36	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	I	1	1,3	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.39	0
3	BMA	I	3	3	11,11,12	0.62	0	15,15,17	0.72	0
6	NAG	J	1	6,1	14,14,15	0.21	0	17,19,21	0.36	0
6	NAG	J	2	6	14,14,15	0.31	0	17,19,21	0.46	0
6	BMA	J	3	6	11,11,12	0.51	0	15,15,17	0.70	0
6	MAN	J	4	6	11,11,12	0.66	0	15,15,17	0.91	2 (13%)
6	MAN	J	5	6	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.31	0	17,19,21	0.60	0
3	NAG	K	2	3	14,14,15	0.27	0	17,19,21	0.40	0
3	BMA	K	3	3	11,11,12	0.56	0	15,15,17	0.71	0
5	NAG	L	1	5,1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	L	2	5	14,14,15	0.25	0	17,19,21	0.39	0
7	NAG	M	1	1,7	14,14,15	0.22	0	17,19,21	0.53	0
7	NAG	M	2	7	14,14,15	0.24	0	17,19,21	0.37	0
7	BMA	M	3	7	11,11,12	0.60	0	15,15,17	0.80	0
7	MAN	M	4	7	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
7	MAN	M	5	7	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
7	MAN	M	6	7	11,11,12	0.55	0	15,15,17	1.04	2 (13%)
7	MAN	M	7	7	11,11,12	0.61	0	15,15,17	1.03	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
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
7	NAG	M	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	BMA	M	3	7	-	2/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	1/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
7	MAN	M	6	7	-	0/2/19/22	0/1/1/1
7	MAN	M	7	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	4	MAN	C1-O5-C5	3.40	116.80	112.19
7	M	6	MAN	C1-O5-C5	2.77	115.94	112.19
2	D	4	MAN	C1-O5-C5	2.57	115.67	112.19
6	J	5	MAN	C1-O5-C5	2.49	115.56	112.19
4	F	5	MAN	C1-O5-C5	2.49	115.56	112.19
7	M	7	MAN	C1-O5-C5	2.47	115.54	112.19
4	F	4	MAN	C1-O5-C5	2.37	115.40	112.19
7	M	5	MAN	C1-O5-C5	2.32	115.34	112.19
4	F	6	MAN	C1-O5-C5	2.31	115.32	112.19
7	M	5	MAN	O2-C2-C3	-2.25	105.63	110.14
7	M	7	MAN	O2-C2-C3	-2.24	105.66	110.14
6	J	4	MAN	O2-C2-C3	-2.21	105.71	110.14
2	D	4	MAN	O2-C2-C3	-2.21	105.71	110.14
7	M	6	MAN	O2-C2-C3	-2.21	105.72	110.14
7	M	4	MAN	O2-C2-C3	-2.20	105.72	110.14
2	G	4	MAN	O2-C2-C3	-2.19	105.75	110.14
6	J	5	MAN	O2-C2-C3	-2.18	105.77	110.14
4	F	6	MAN	O2-C2-C3	-2.15	105.83	110.14
4	F	5	MAN	O2-C2-C3	-2.08	105.98	110.14
6	J	4	MAN	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
7	M	3	BMA	O5-C5-C6-O6
5	H	1	NAG	C1-C2-N2-C7
6	J	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
7	M	3	BMA	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
6	J	2	NAG	C3-C2-N2-C7
4	F	4	MAN	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
4	F	4	MAN	O5-C5-C6-O6
5	L	1	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
7	M	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C3-C2-N2-C7
7	M	1	NAG	C3-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	4	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
6	J	2	NAG	3	0
2	D	1	NAG	1	0
3	K	3	BMA	1	0
5	H	1	NAG	2	0
4	F	4	MAN	1	0
6	J	5	MAN	1	0
7	M	6	MAN	1	0
3	E	1	NAG	4	0

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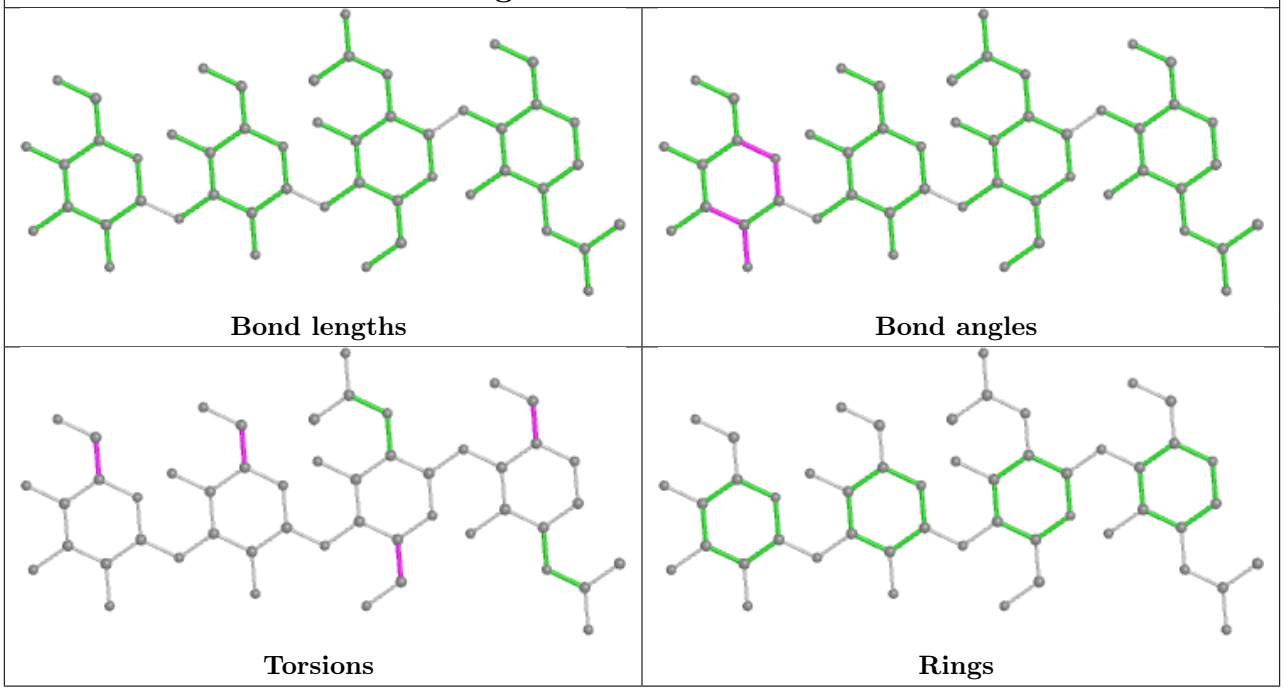
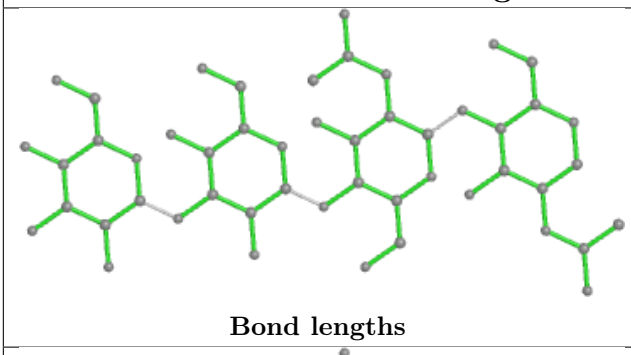
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	4	MAN	2	0
3	K	2	NAG	1	0
3	K	1	NAG	2	0
2	G	1	NAG	1	0
5	H	2	NAG	1	0
7	M	2	NAG	1	0
2	D	2	NAG	1	0
7	M	1	NAG	5	0
4	F	5	MAN	1	0

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

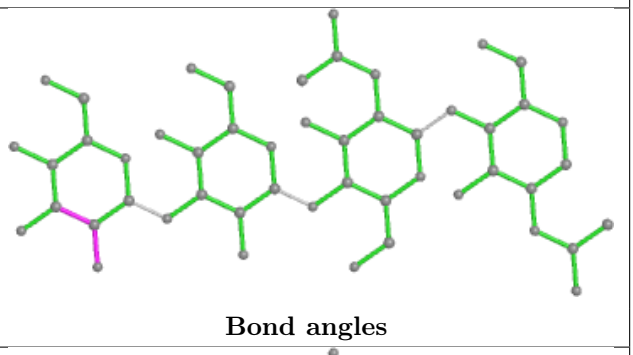
Oligosaccharide Chain D



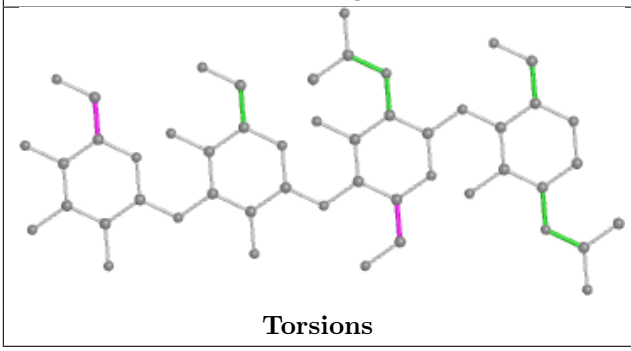
Oligosaccharide Chain G



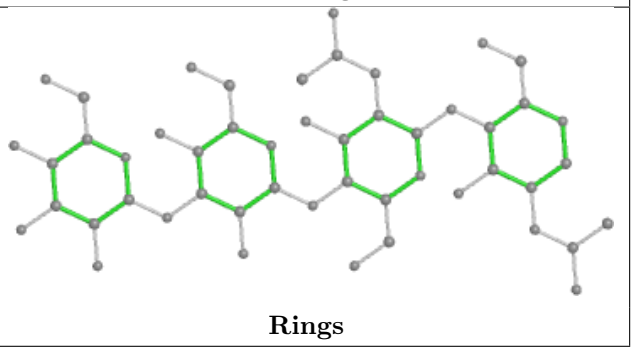
Bond lengths



Bond angles

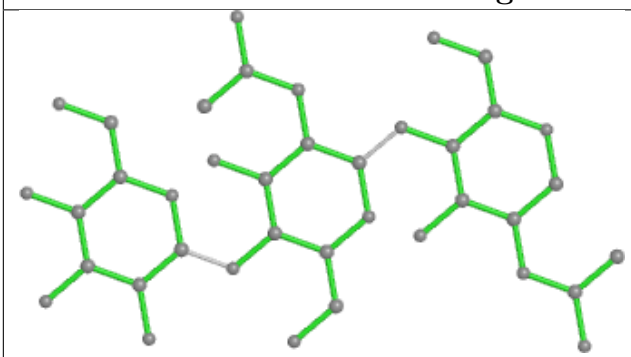


Torsions

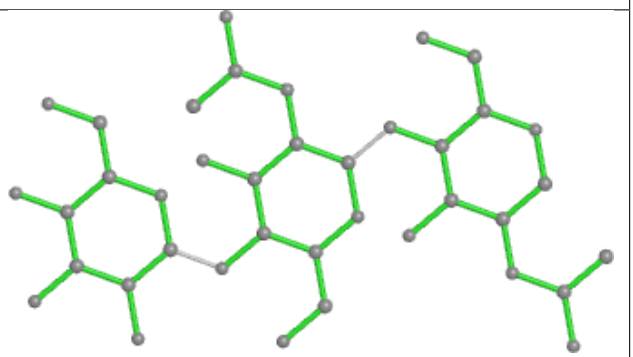


Rings

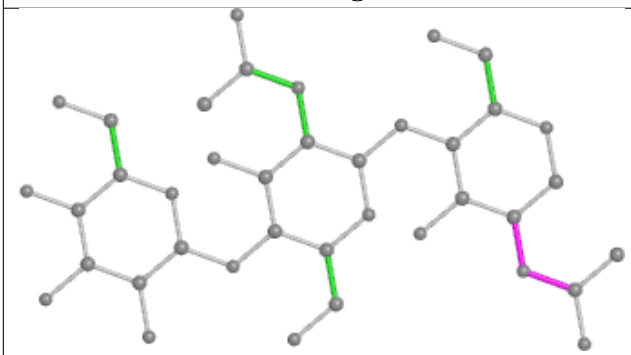
Oligosaccharide Chain E



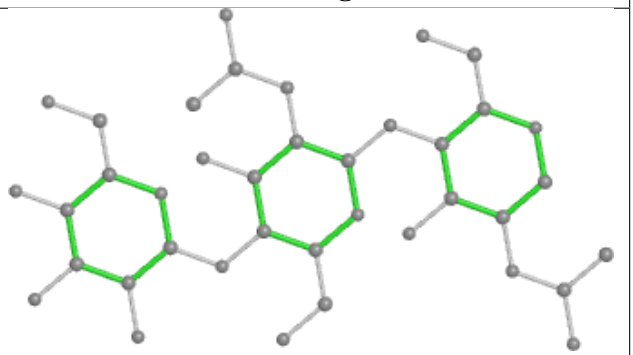
Bond lengths



Bond angles

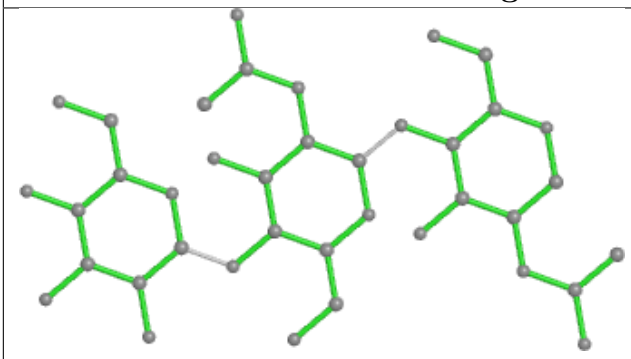


Torsions

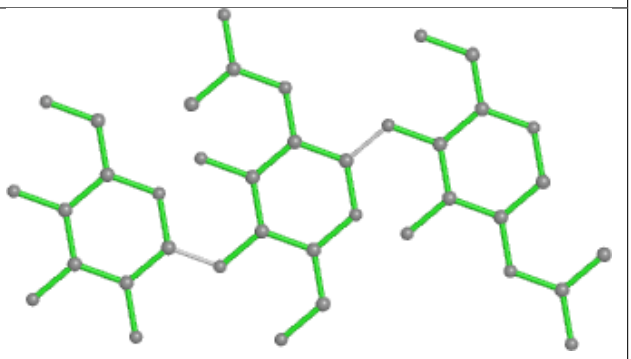


Rings

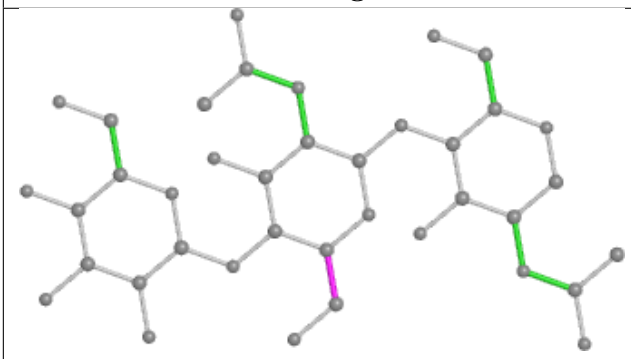
Oligosaccharide Chain I



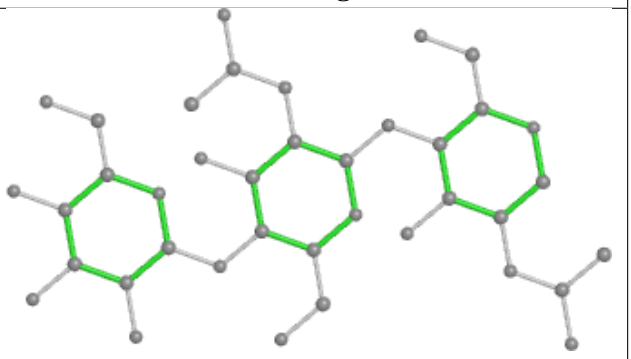
Bond lengths



Bond angles

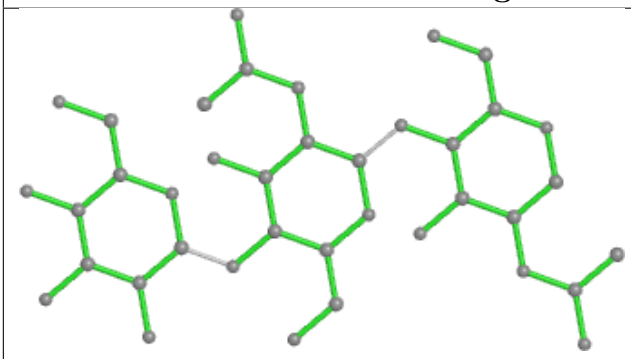


Torsions

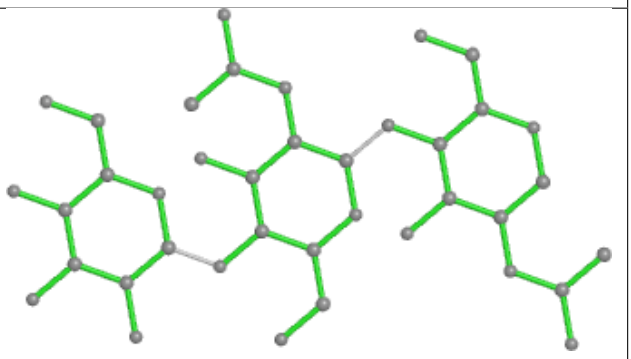


Rings

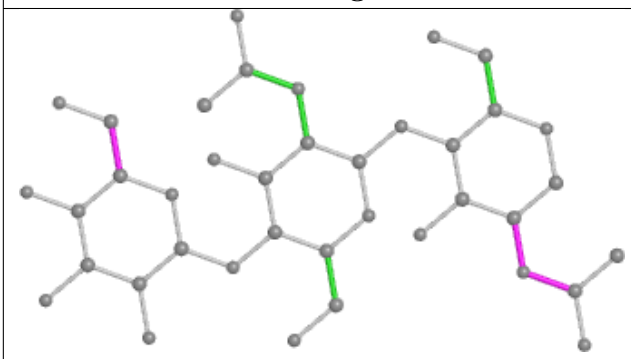
Oligosaccharide Chain K



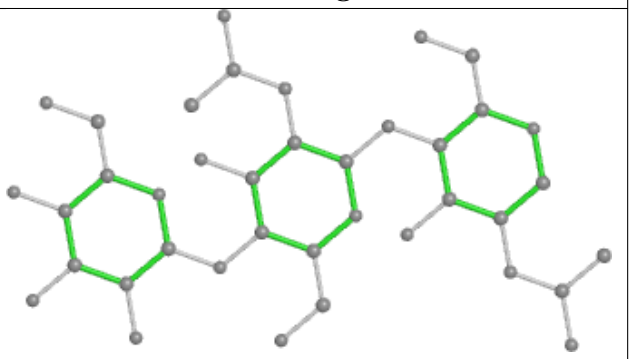
Bond lengths



Bond angles

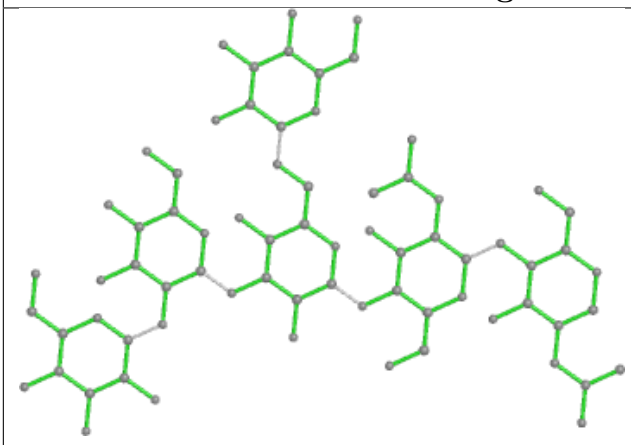


Torsions

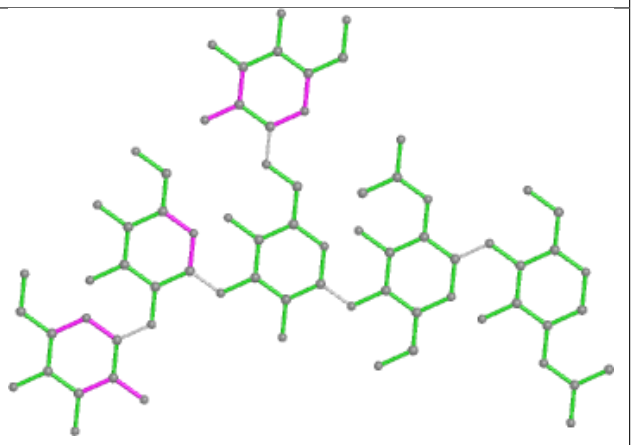


Rings

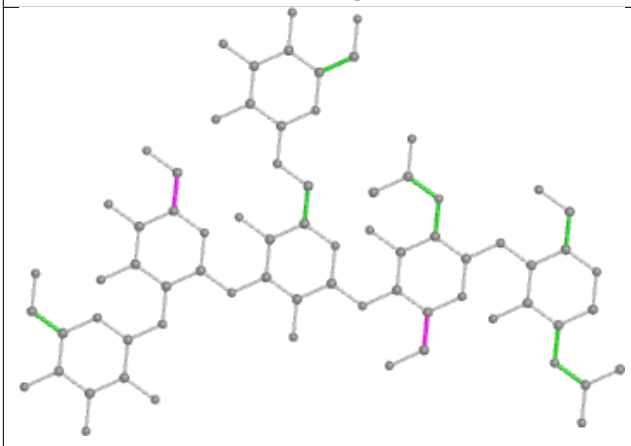
Oligosaccharide Chain F



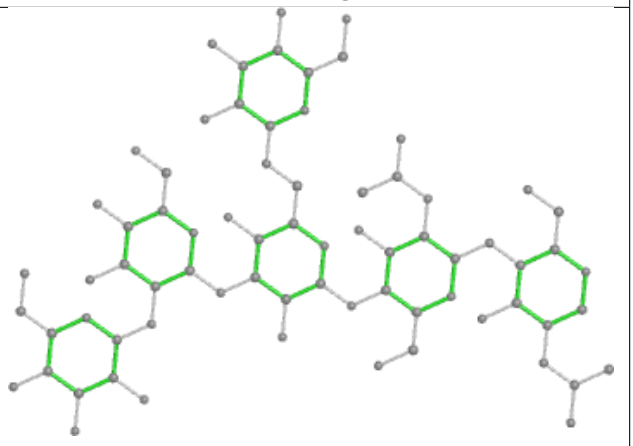
Bond lengths



Bond angles

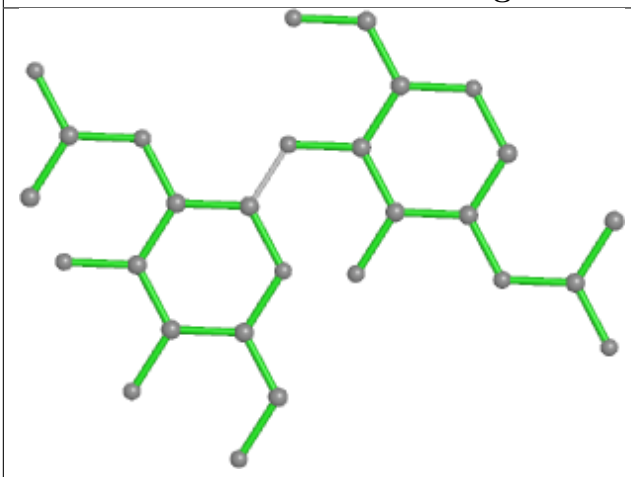


Torsions

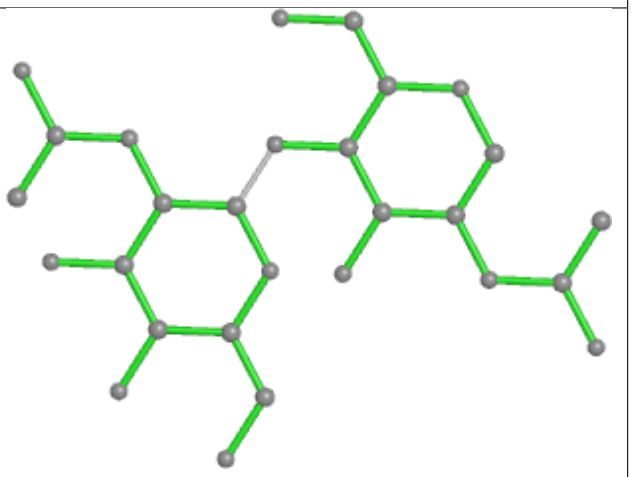


Rings

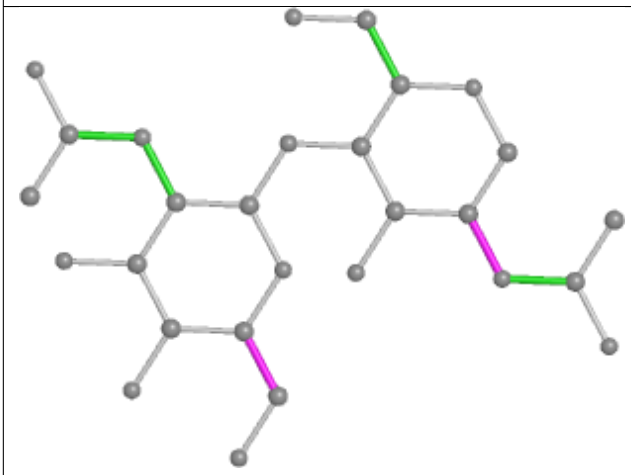
Oligosaccharide Chain H



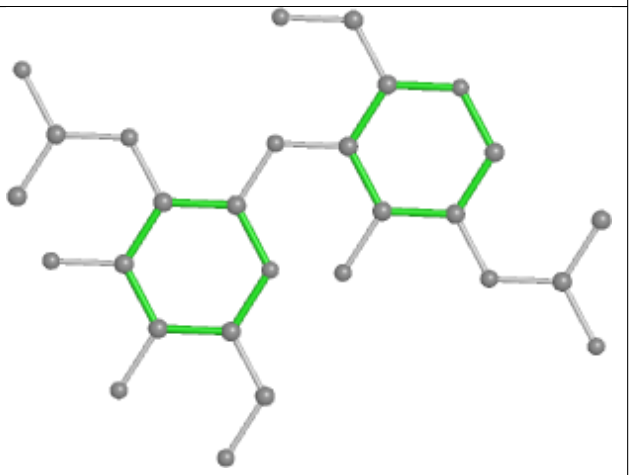
Bond lengths



Bond angles

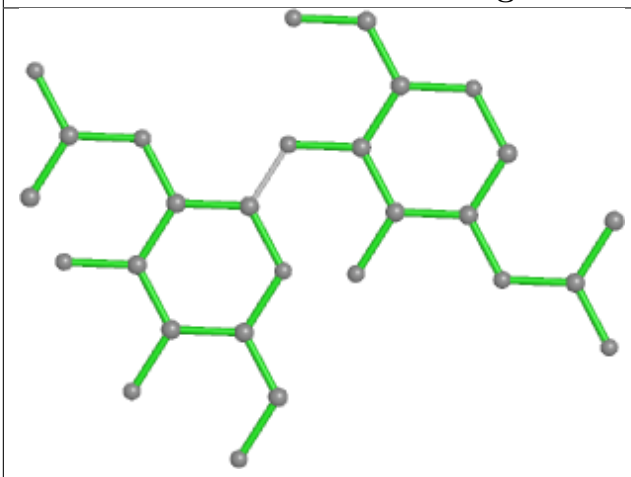


Torsions

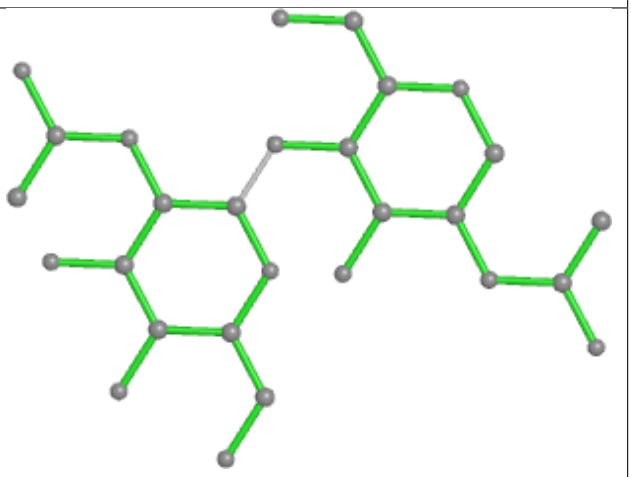


Rings

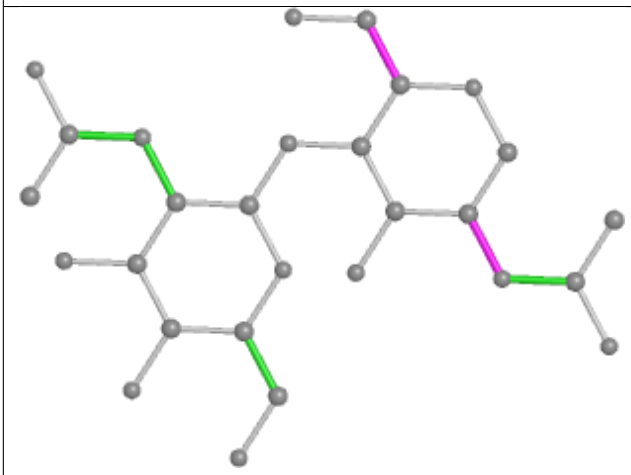
Oligosaccharide Chain L



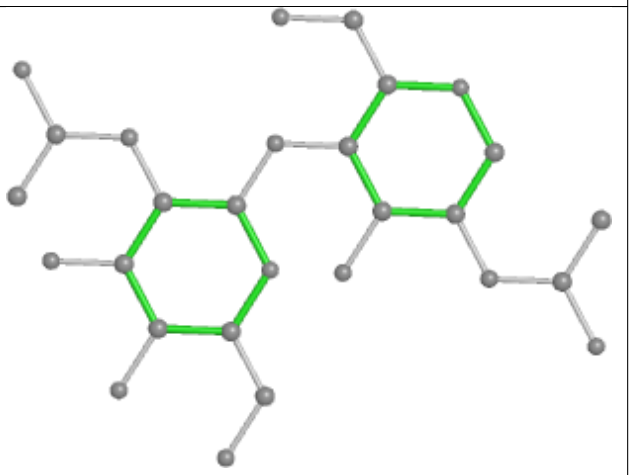
Bond lengths



Bond angles

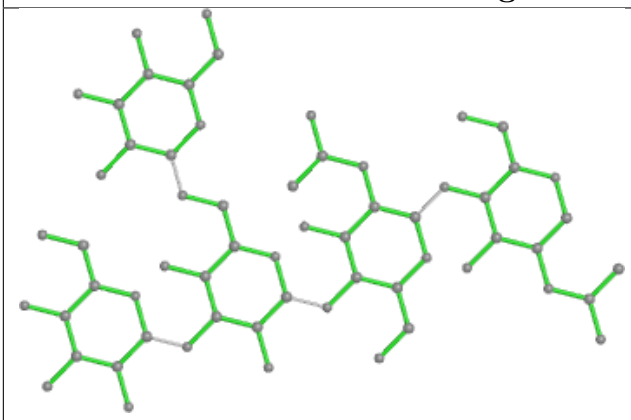


Torsions

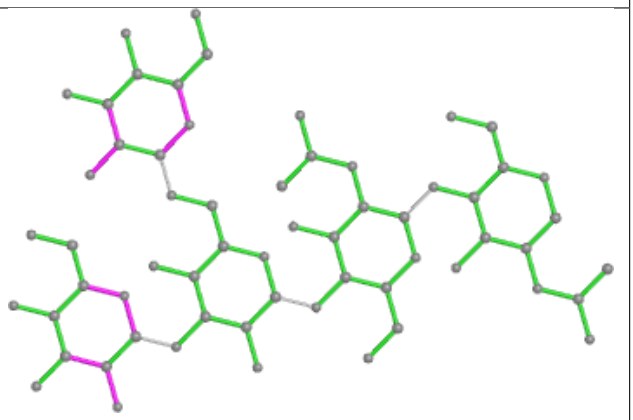


Rings

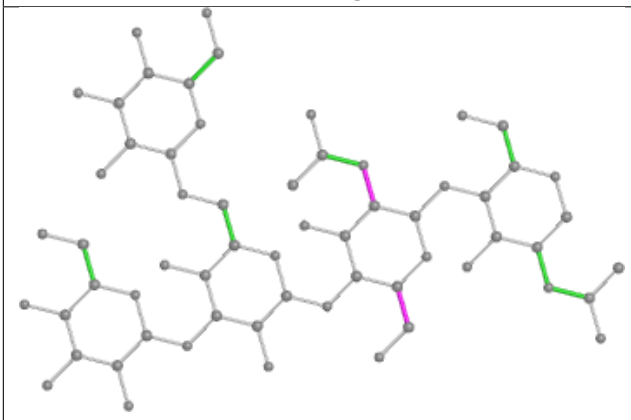
Oligosaccharide Chain J



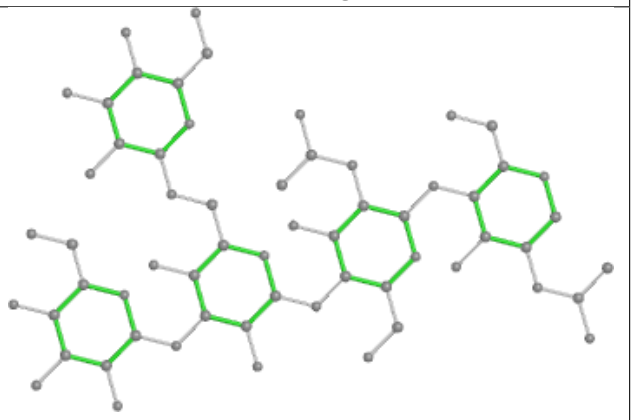
Bond lengths



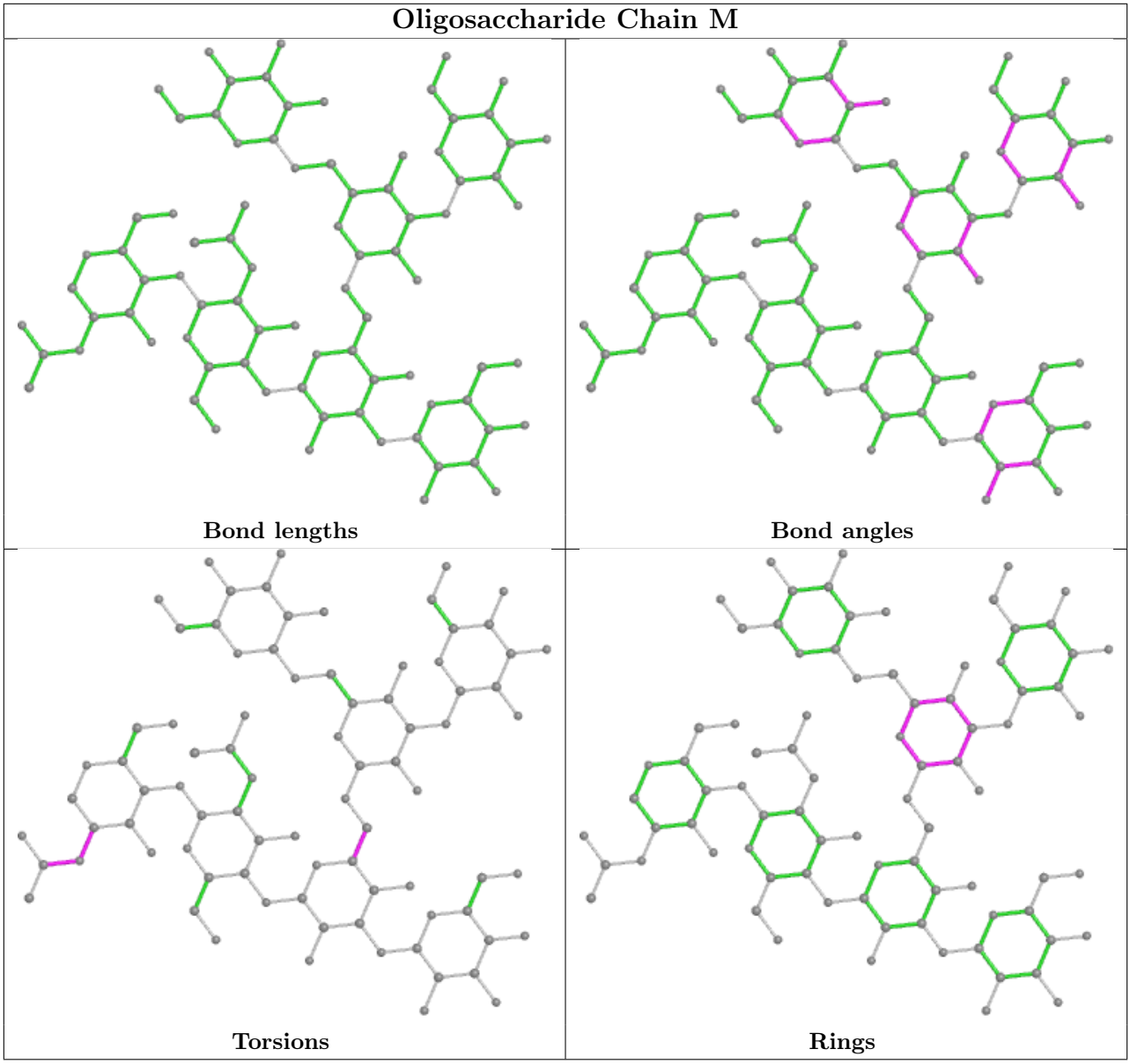
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	703	1	14,14,15	0.28	0	17,19,21	0.43	0
8	NAG	C	702	1	14,14,15	0.29	0	17,19,21	0.45	0
8	NAG	B	703	1	14,14,15	0.19	0	17,19,21	0.37	0
8	NAG	B	702	1	14,14,15	0.22	0	17,19,21	0.52	0
8	NAG	C	701	1	14,14,15	0.26	0	17,19,21	0.43	0
8	NAG	B	701	1	14,14,15	0.20	0	17,19,21	0.43	0
8	NAG	A	701	1	14,14,15	0.21	0	17,19,21	0.34	0
8	NAG	A	702	1	14,14,15	0.21	0	17,19,21	0.38	0
8	NAG	C	703	1	14,14,15	0.23	0	17,19,21	0.46	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
8	NAG	A	703	1	-	0/6/23/26	0/1/1/1
8	NAG	C	702	1	-	2/6/23/26	0/1/1/1
8	NAG	B	703	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	1	-	2/6/23/26	0/1/1/1
8	NAG	C	701	1	-	1/6/23/26	0/1/1/1
8	NAG	B	701	1	-	3/6/23/26	0/1/1/1
8	NAG	A	701	1	-	4/6/23/26	0/1/1/1
8	NAG	A	702	1	-	0/6/23/26	0/1/1/1
8	NAG	C	703	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	703	NAG	C4-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	A	701	NAG	C8-C7-N2-C2
8	A	701	NAG	O7-C7-N2-C2
8	B	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	703	NAG	O5-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	A	701	NAG	C4-C5-C6-O6
8	B	701	NAG	C1-C2-N2-C7
8	B	702	NAG	O5-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6
8	C	702	NAG	C4-C5-C6-O6
8	C	703	NAG	C4-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	C	702	NAG	O5-C5-C6-O6
8	C	701	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	702	NAG	1	0
8	B	703	NAG	1	0
8	C	701	NAG	1	0
8	A	701	NAG	1	0
8	C	703	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	574/588 (97%)	-0.16	17 (2%) 50 44	136, 232, 371, 444	0
1	B	574/588 (97%)	-0.15	4 (0%) 87 83	149, 211, 309, 395	0
1	C	574/588 (97%)	-0.02	18 (3%) 49 43	122, 203, 369, 462	0
All	All	1722/1764 (97%)	-0.11	39 (2%) 60 54	122, 217, 349, 462	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	GLY	6.8
1	C	608	GLY	6.0
1	A	332	LEU	4.9
1	C	577	LEU	4.7
1	C	531	GLN	4.3
1	C	574	LEU	4.2
1	A	607	ARG	3.7
1	C	517	PRO	3.6
1	C	605	LEU	3.5
1	C	576	ILE	3.5
1	C	528	LEU	3.4
1	C	520	ALA	3.4
1	C	530	LEU	3.2
1	B	428	ARG	3.1
1	A	520	ALA	3.1
1	A	447	ALA	3.1
1	A	414	VAL	3.1
1	A	395	TYR	2.9
1	A	602	ALA	2.9
1	A	253	ALA	2.8
1	A	583	HIS	2.7
1	A	61	LEU	2.6
1	A	604	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	518	SER	2.5
1	B	369	LEU	2.5
1	A	412	LEU	2.4
1	C	602	ALA	2.4
1	A	351	ALA	2.4
1	A	523	ASN	2.4
1	C	555	PHE	2.3
1	C	438	ILE	2.3
1	C	604	VAL	2.3
1	B	370	ALA	2.2
1	B	528	LEU	2.1
1	C	546	TRP	2.1
1	C	521	ASP	2.1
1	C	522	ILE	2.1
1	A	129	LEU	2.1
1	A	558	PRO	2.0

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, 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
7	MAN	M	5	11/12	0.38	0.21	259,321,341,343	0
3	BMA	E	3	11/12	0.55	0.16	224,308,344,345	0
3	BMA	I	3	11/12	0.57	0.33	204,272,280,282	0
6	BMA	J	3	11/12	0.59	0.10	230,301,318,325	0
4	MAN	F	4	11/12	0.63	0.14	165,283,313,326	0
7	MAN	M	4	11/12	0.71	0.11	269,302,337,343	0
4	MAN	F	5	11/12	0.72	0.17	181,269,306,310	0
6	MAN	J	5	11/12	0.72	0.14	201,291,310,310	0
2	MAN	D	4	11/12	0.74	0.27	260,300,326,332	0
5	NAG	H	2	14/15	0.76	0.40	178,274,287,319	0
2	BMA	G	3	11/12	0.78	0.21	218,281,316,333	0
2	NAG	D	2	14/15	0.78	0.20	224,267,299,312	0

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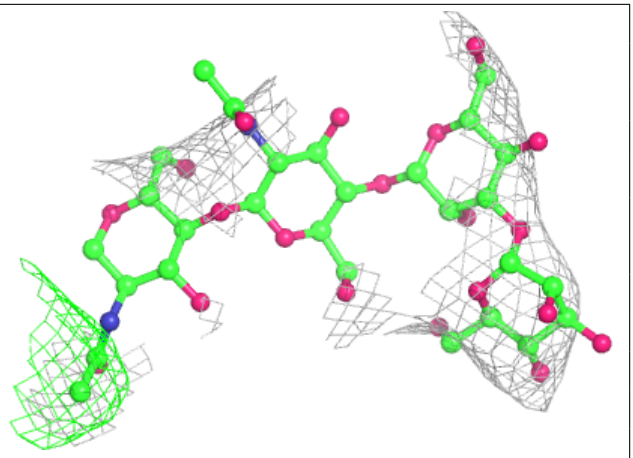
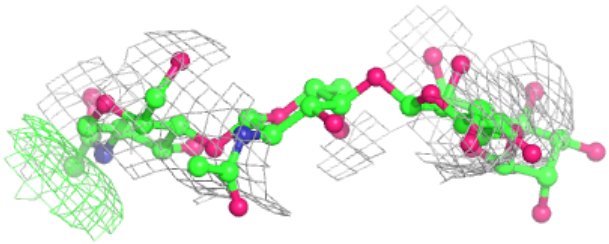
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.81	0.18	235,297,331,353	0
6	MAN	J	4	11/12	0.82	0.24	255,311,332,333	0
3	NAG	E	1	14/15	0.82	0.16	159,256,288,297	0
4	BMA	F	3	11/12	0.83	0.12	236,286,307,311	0
3	NAG	E	2	14/15	0.83	0.12	212,304,336,339	0
4	NAG	F	2	14/15	0.83	0.19	163,235,295,311	0
2	NAG	D	1	14/15	0.87	0.16	154,215,250,254	0
7	BMA	M	3	11/12	0.87	0.17	259,282,290,310	0
7	MAN	M	7	11/12	0.87	0.12	228,312,328,328	0
4	MAN	F	6	11/12	0.89	0.09	204,267,308,316	0
3	NAG	I	2	14/15	0.89	0.21	216,273,293,296	0
2	MAN	G	4	11/12	0.89	0.13	233,283,314,319	0
3	NAG	K	1	14/15	0.90	0.24	173,226,254,261	0
7	NAG	M	1	14/15	0.91	0.32	140,222,242,253	0
5	NAG	L	2	14/15	0.91	0.26	210,264,283,306	0
2	NAG	G	2	14/15	0.91	0.26	206,255,286,296	0
5	NAG	H	1	14/15	0.91	0.14	132,207,273,285	0
4	NAG	F	1	14/15	0.91	0.18	193,251,277,283	0
3	NAG	I	1	14/15	0.92	0.12	157,210,242,243	0
6	NAG	J	2	14/15	0.92	0.10	226,258,312,314	0
5	NAG	L	1	14/15	0.92	0.13	146,188,234,254	0
7	NAG	M	2	14/15	0.92	0.24	194,229,297,301	0
3	BMA	K	3	11/12	0.93	0.30	199,281,299,307	0
6	NAG	J	1	14/15	0.93	0.19	197,232,257,269	0
2	NAG	G	1	14/15	0.93	0.34	177,233,276,287	0
7	MAN	M	6	11/12	0.94	0.11	237,268,285,307	0
3	NAG	K	2	14/15	0.95	0.19	164,243,274,284	0

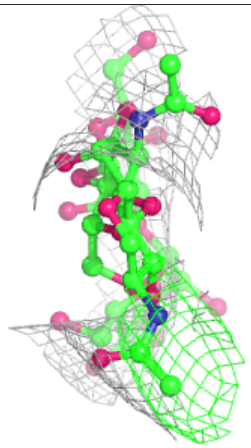
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

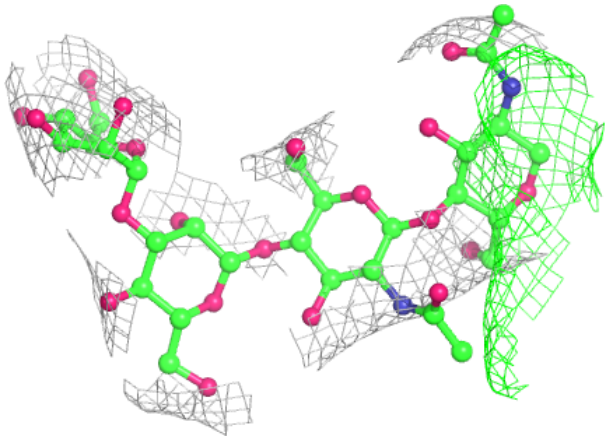


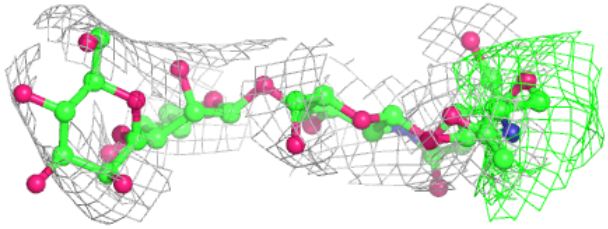


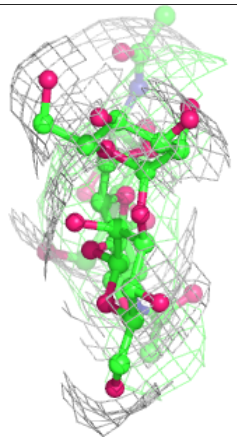


Electron density around Chain G:

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

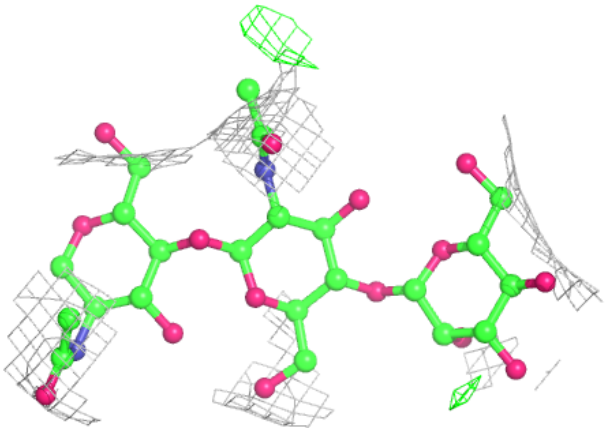


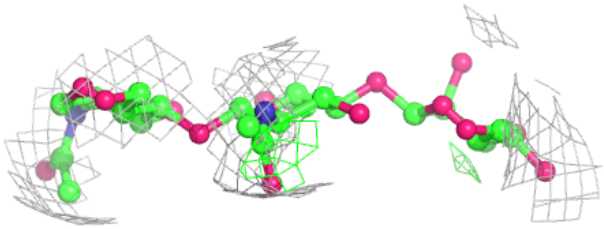


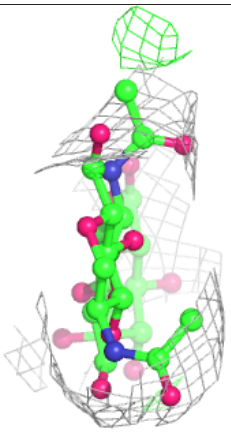


Electron density around Chain E:

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

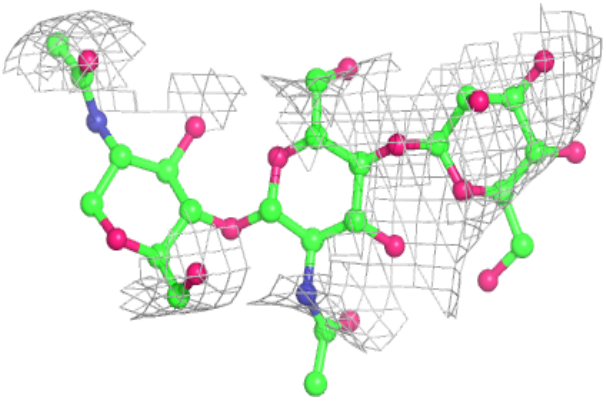


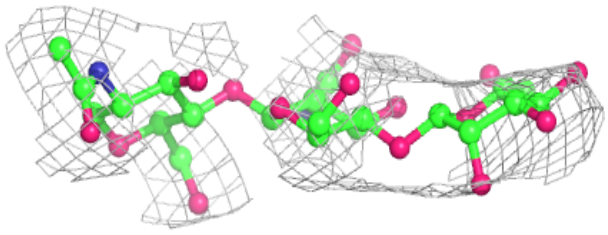


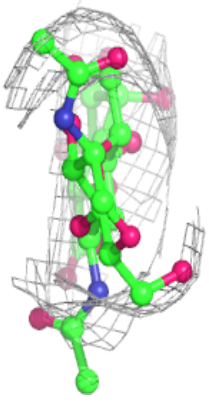


Electron density around Chain I:

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

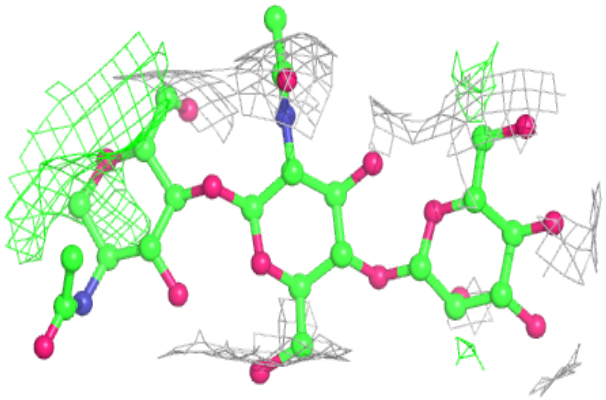


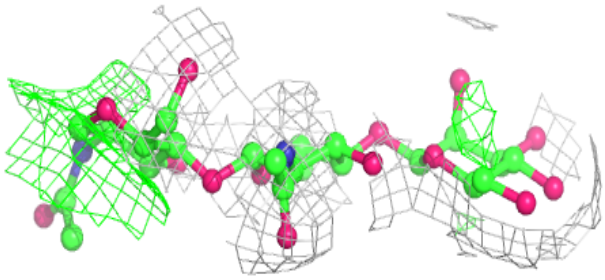


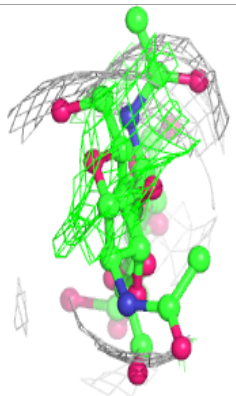


Electron density around Chain K:

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

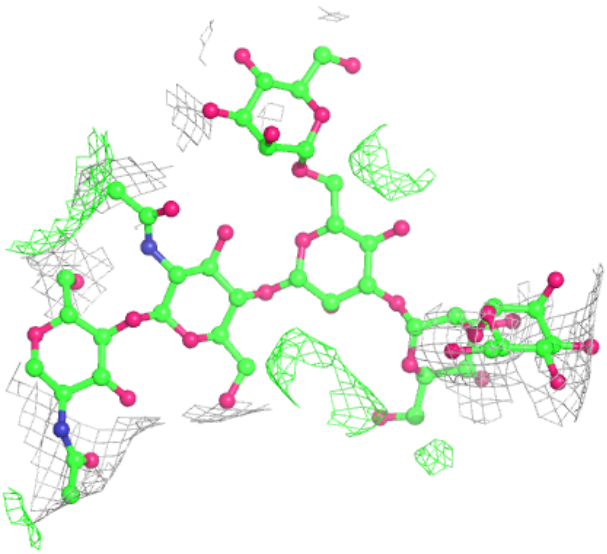


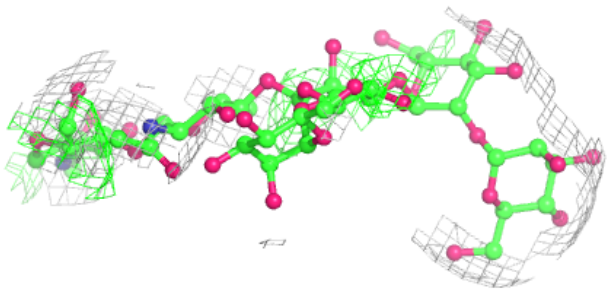


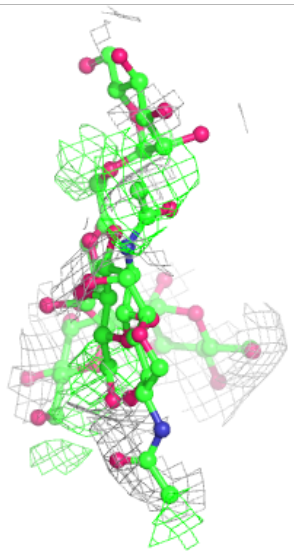


Electron density around Chain F:

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

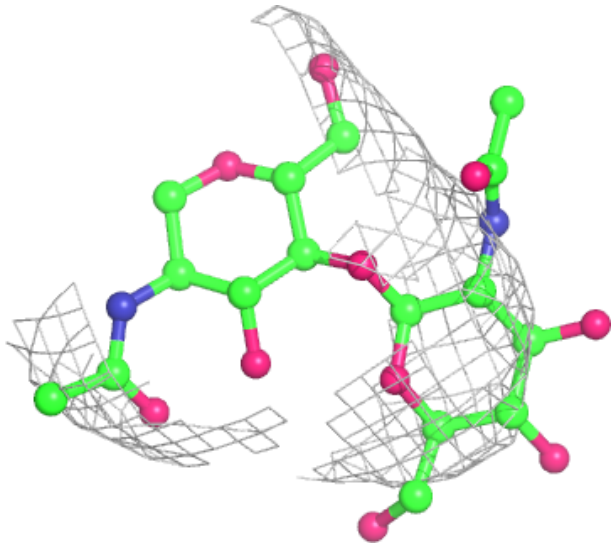


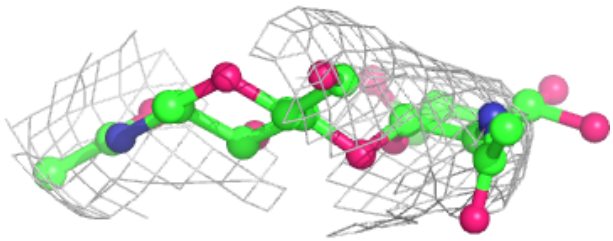


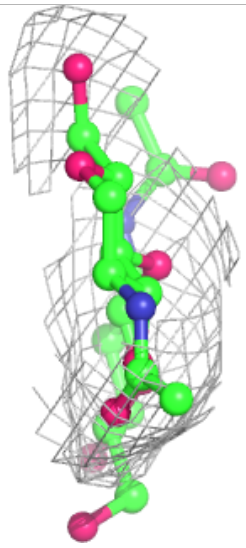


Electron density around Chain H:

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

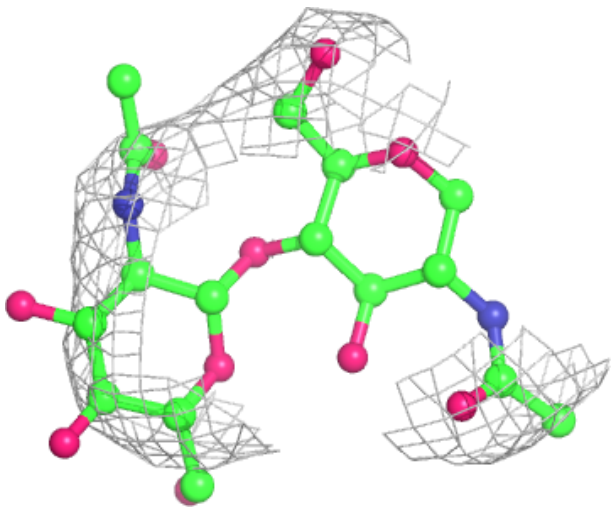


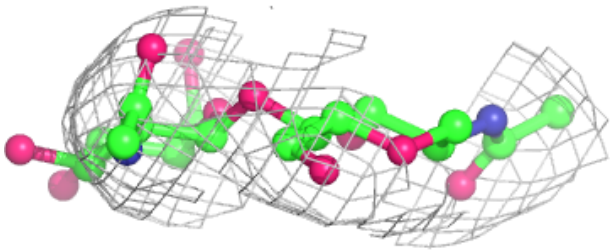


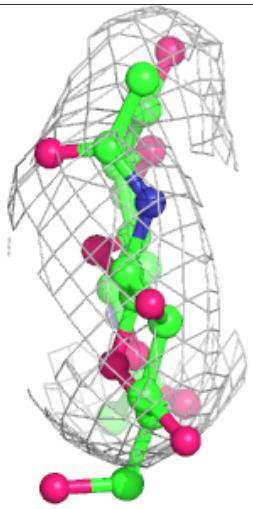


Electron density around Chain L:

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

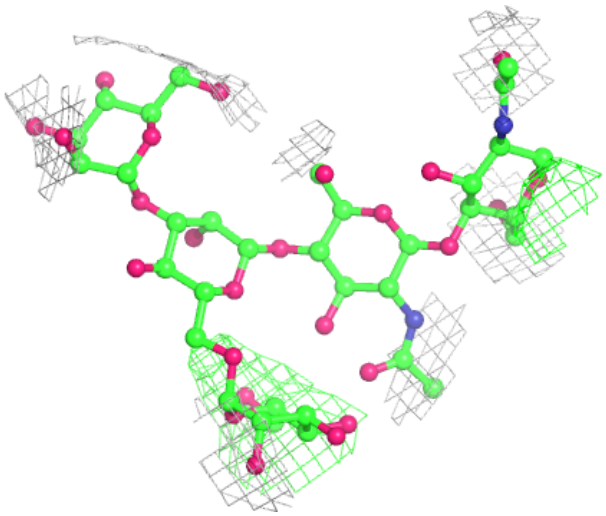


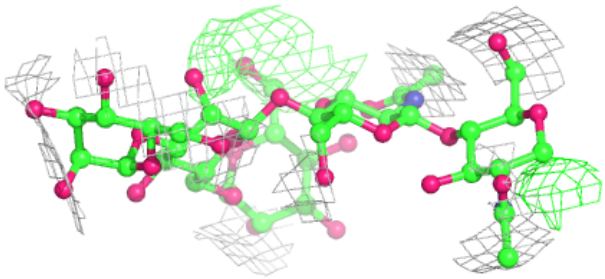


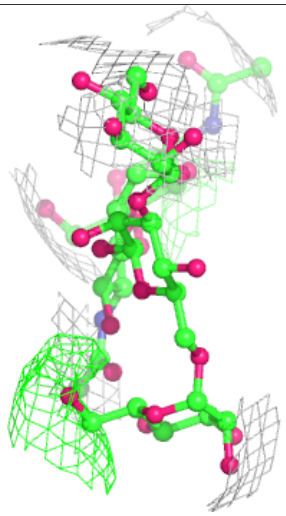


Electron density around Chain J:

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

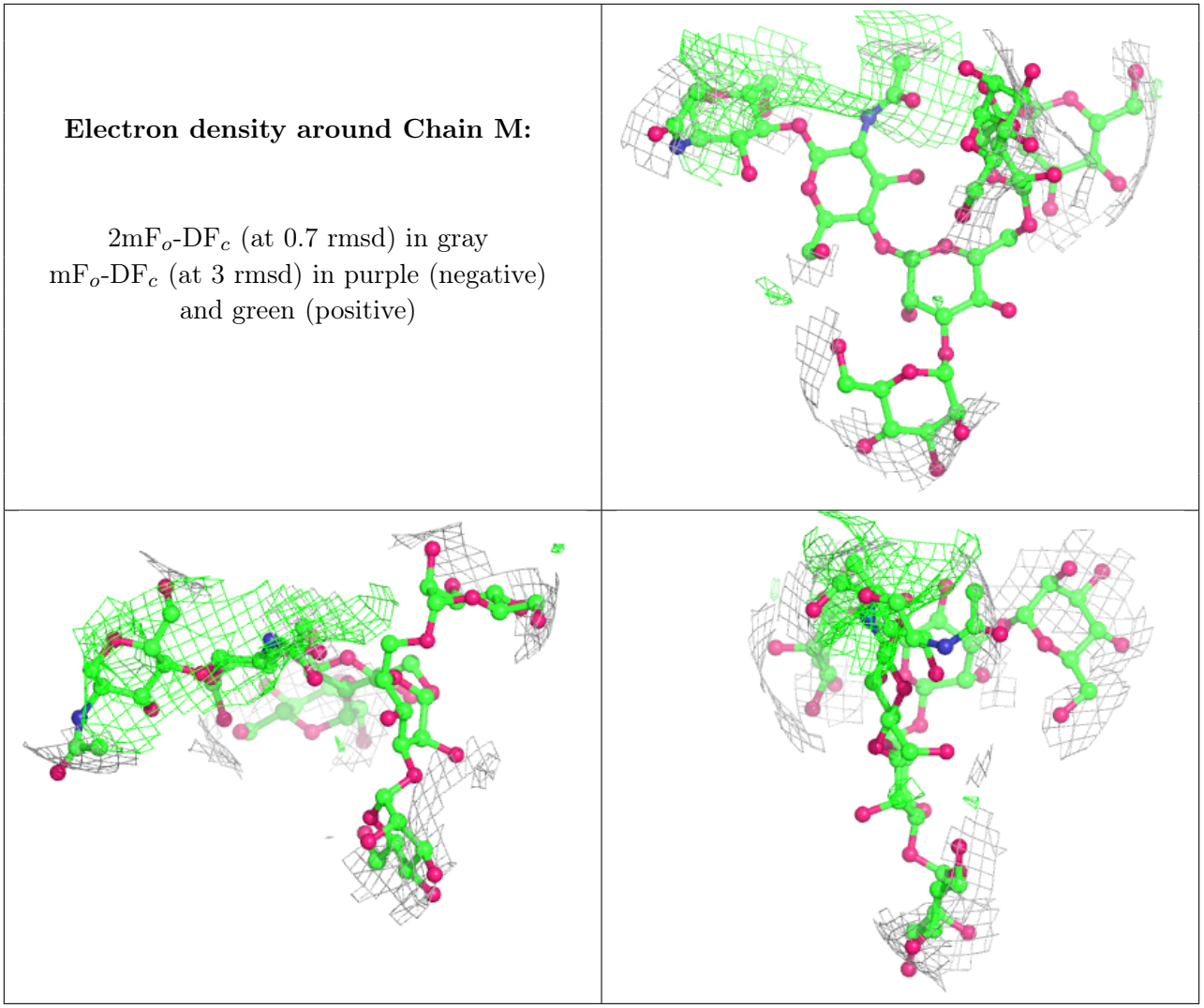






Electron density around Chain M:

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



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
8	NAG	A	703	14/15	0.69	0.15	220,302,317,319	0
8	NAG	A	702	14/15	0.72	0.22	176,262,301,329	0
8	NAG	A	701	14/15	0.74	0.16	208,284,320,323	0
8	NAG	C	703	14/15	0.77	0.10	220,307,339,365	0
8	NAG	B	702	14/15	0.86	0.11	185,265,281,284	0
8	NAG	B	703	14/15	0.88	0.11	248,293,336,338	0
8	NAG	C	701	14/15	0.89	0.14	163,236,262,270	0
8	NAG	C	702	14/15	0.90	0.23	179,214,265,270	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	B	701	14/15	0.92	0.18	167,236,267,278	0

6.5 Other polymers (i)

There are no such residues in this entry.