Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2021 – 11:32 AM GMT

PDB ID	:	7AMK
Title	:	Zebrafish RET Cadherin Like Domains 1 to 4.
Authors	:	Purkiss, A.G.; McDonald, N.Q.; Goodman, K.M.; Narowtek, A.; Knowles, P.P.
Deposited on	:	2020-10-09
Resolution	:	2.20 Å(reported)

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

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

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

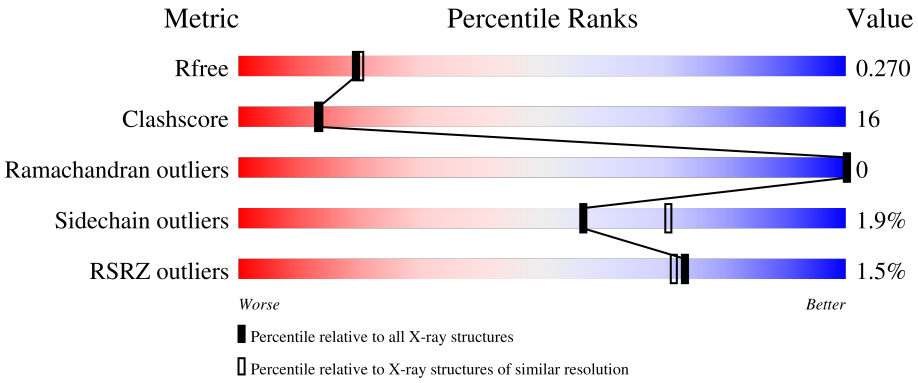
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	480	2% 74% 25%
1	B	480	74% 24%
2	C	7	14% 57% 29%
3	D	2	100%
3	E	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	100%
4	F	3	100%
4	G	3	100%
5	H	5	20% 20% 60%
6	J	4	25% 75%
7	K	5	80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PEG	A	611	-	-	X	-
12	PEG	A	612	-	-	X	-
12	PEG	A	615	-	-	X	-
12	PEG	B	607	-	-	X	-
12	PEG	B	611	-	-	X	-
3	NAG	D	2	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 8199 atoms, of which 13 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.

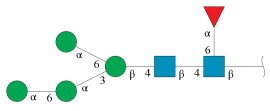
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase receptor Ret.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	2	0
			3680	2351	601	712	16			
1	B	472	Total	C	N	O	S	0	1	0
			3678	2346	604	713	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	GLN	ASN	engineered mutation	UNP A8E7C6
A	308	GLN	ASN	engineered mutation	UNP A8E7C6
A	390	GLN	ASN	engineered mutation	UNP A8E7C6
A	433	GLN	ASN	engineered mutation	UNP A8E7C6
B	259	GLN	ASN	engineered mutation	UNP A8E7C6
B	308	GLN	ASN	engineered mutation	UNP A8E7C6
B	390	GLN	ASN	engineered mutation	UNP A8E7C6
B	433	GLN	ASN	engineered mutation	UNP A8E7C6

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

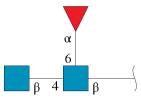


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			82	46	2	34			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

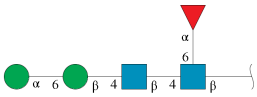
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



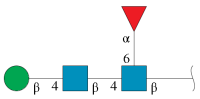
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



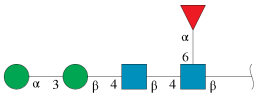
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

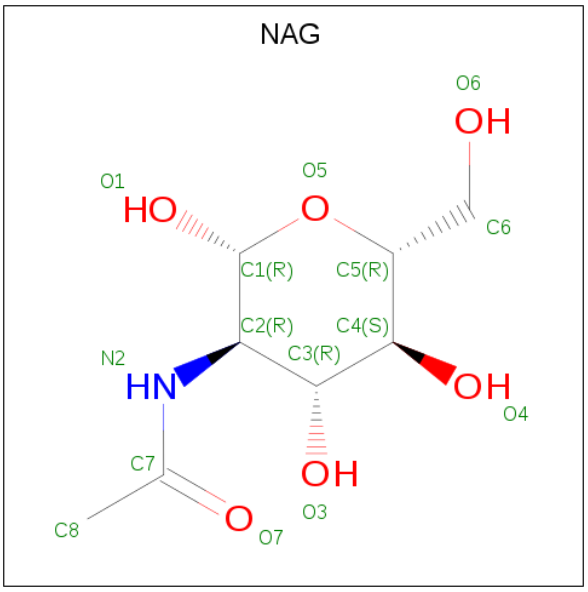


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

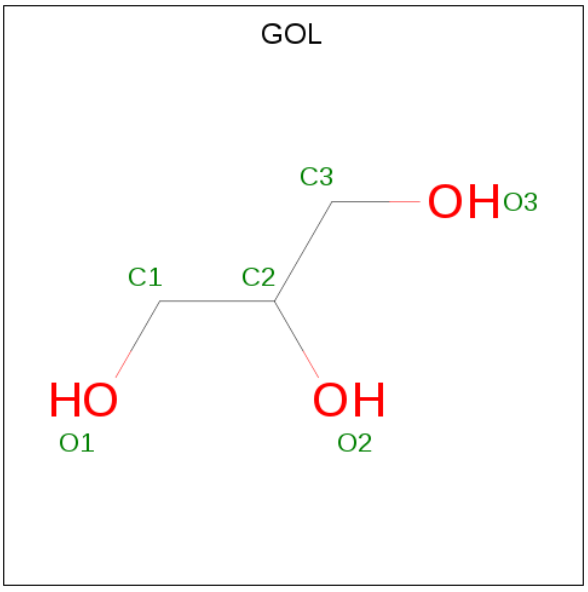
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Ca	0	0
			3	3		
8	A	3	Total	Ca	0	0
			3	3		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



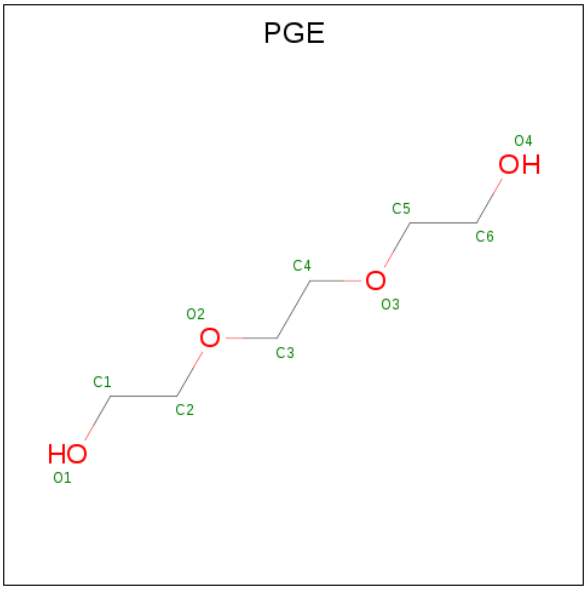
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

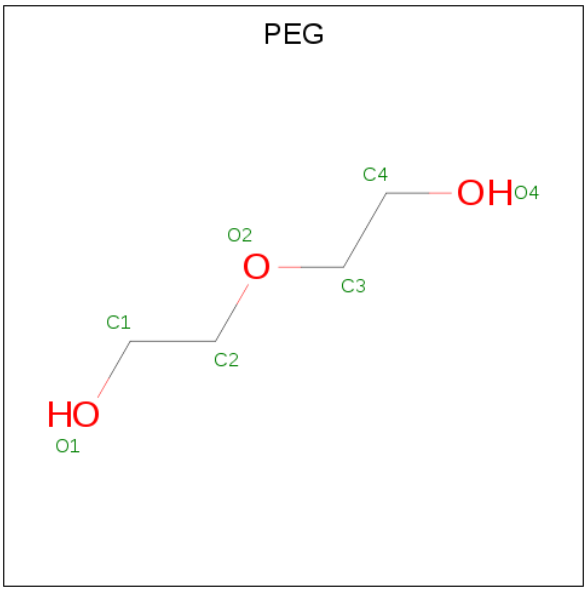
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



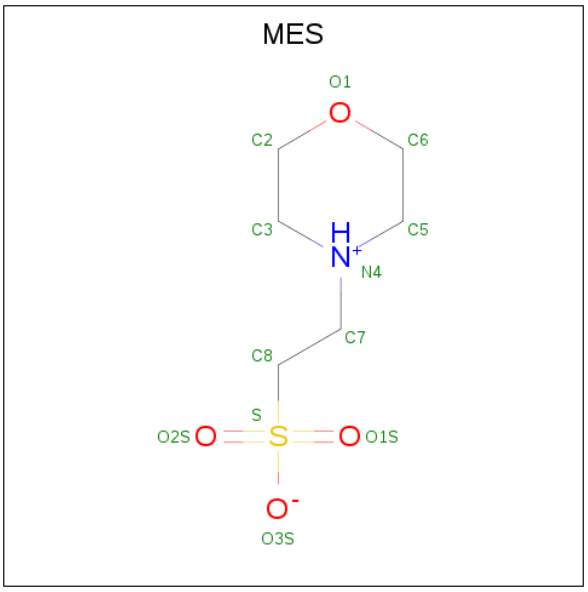
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 10 6 4	0	0
11	A	1	Total C O 10 6 4	0	0
11	B	1	Total C O 10 6 4	0	0
11	B	1	Total C O 10 6 4	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 14 is water.

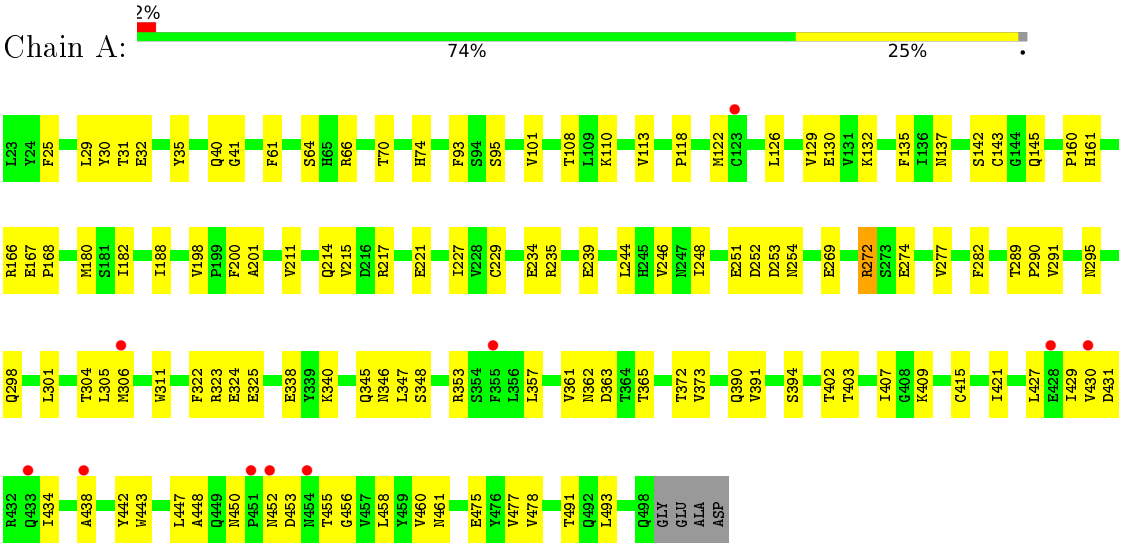
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	102	Total	O	0	0
			102	102		
14	B	117	Total	O	0	0
			117	117		

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.

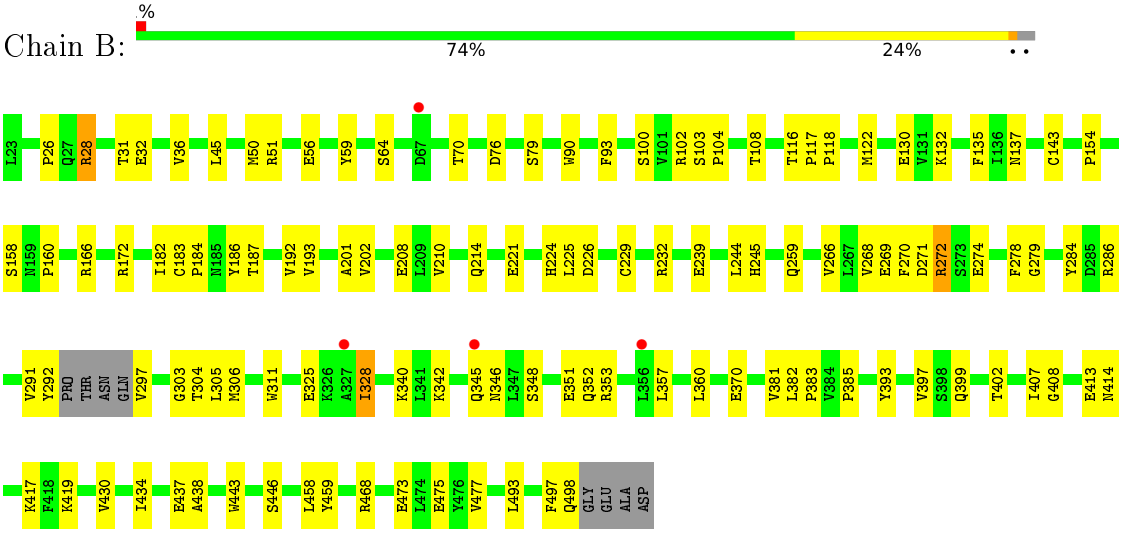
• Molecule 1: Proto-oncogene tyrosine-protein kinase receptor Ret

Chain A:



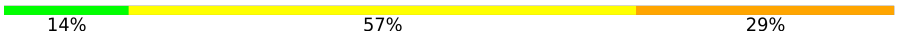
• Molecule 1: Proto-oncogene tyrosine-protein kinase receptor Ret

Chain B:



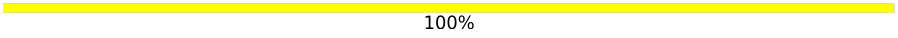
• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:

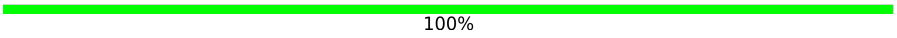


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain I:

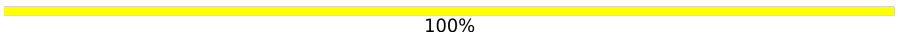


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:

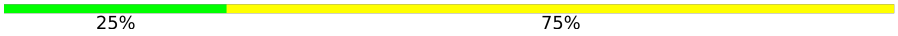


• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain J:



• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.17Å 70.50Å 105.44Å 105.41° 100.93° 100.25°	Depositor
Resolution (Å)	65.96 – 2.20 65.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (65.96-2.20) 91.3 (65.96-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.225 , 0.269 0.225 , 0.270	Depositor DCC
R_{free} test set	3097 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8199	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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: GOL, PGE, NAG, CA, BMA, FUC, MES, PEG, 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	0.42	0/3770	0.60	0/5155
1	B	0.44	0/3761	0.61	0/5134
All	All	0.43	0/7531	0.61	0/10289

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	3680	0	3466	120	1
1	B	3678	0	3501	107	0
2	C	82	0	70	10	0
3	D	28	0	25	3	0
3	E	28	0	25	5	0
3	I	28	0	25	0	0
4	F	38	0	34	0	0
4	G	38	0	32	4	0
5	H	60	0	52	8	0
6	J	49	0	43	1	0
7	K	60	0	52	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	3	0	0	0	0
8	B	3	0	0	0	0
9	A	28	0	26	1	0
9	B	14	0	13	3	0
10	A	12	0	16	1	0
10	B	12	0	16	1	0
11	A	24	0	32	4	0
11	B	20	0	28	6	0
12	A	42	0	60	33	0
12	B	28	0	40	18	0
13	B	12	13	12	1	0
14	A	102	0	0	6	0
14	B	117	0	0	5	0
All	All	8186	13	7568	251	1

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 16.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:HA	12:A:612:PEG:H12	1.26	1.17
1:B:413:GLU:HG2	12:B:611:PEG:H32	1.33	1.05
2:C:3:BMA:H3	2:C:4:MAN:H5	1.42	0.98
11:A:614:PGE:H1	11:A:614:PGE:H6	1.51	0.91
2:C:3:BMA:H3	2:C:4:MAN:C5	2.02	0.90
1:B:385:PRO:HD2	12:B:611:PEG:H21	1.52	0.89
12:A:615:PEG:H22	1:B:408:GLY:HA2	1.58	0.86
3:E:2:NAG:H3	3:E:2:NAG:H83	1.58	0.85
1:A:450:ASN:HB3	1:A:455:THR:HG23	1.62	0.82
1:A:289:THR:H	12:A:612:PEG:H42	1.43	0.82
1:A:305:LEU:HD22	1:A:357:LEU:HD11	1.61	0.81
1:B:414:ASN:HD22	12:B:611:PEG:C3	1.94	0.81
1:B:184:PRO:HG2	9:B:604:NAG:H83	1.64	0.80
1:B:414:ASN:HD22	12:B:611:PEG:H31	1.45	0.79
1:A:403:THR:HA	1:A:460:VAL:HG23	1.66	0.78
1:B:443:TRP:HA	7:K:1:NAG:C8	2.14	0.77
1:A:29[B]:LEU:HD23	1:A:130:GLU:HB3	1.67	0.77
1:B:443:TRP:HA	7:K:1:NAG:H83	1.64	0.77
1:A:291:VAL:HA	12:A:612:PEG:C1	2.13	0.76
1:A:323:ARG:NH1	1:A:338:GLU:OE2	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:TRP:CZ2	7:K:2:NAG:H5	2.21	0.75
1:A:407:ILE:HD11	1:A:460:VAL:HG12	1.68	0.75
1:B:437:GLU:HG2	1:B:468:ARG:NH2	2.03	0.73
1:B:413:GLU:HG3	12:B:607:PEG:H21	1.71	0.72
6:J:2:NAG:H4	6:J:3:BMA:O2	1.89	0.72
1:A:443:TRP:HA	4:G:1:NAG:C8	2.19	0.71
1:A:40:GLN:HG2	11:A:614:PGE:H3	1.71	0.71
1:A:298:GLN:OE1	12:A:611:PEG:H22	1.90	0.71
1:B:385:PRO:HG2	12:B:611:PEG:H42	1.74	0.70
1:A:29[B]:LEU:HD21	1:B:473:GLU:HB2	1.72	0.70
1:B:208:GLU:OE1	11:B:609:PGE:H3	1.92	0.69
1:A:200:PHE:O	12:A:613:PEG:H32	1.91	0.68
2:C:3:BMA:H2	2:C:4:MAN:H3	1.74	0.68
1:A:29[B]:LEU:HD21	1:B:473:GLU:CB	2.24	0.68
1:B:244:LEU:HB3	14:B:761:HOH:O	1.93	0.68
1:B:385:PRO:CD	12:B:611:PEG:H21	2.22	0.68
1:A:64:SER:HB2	1:A:70:THR:OG1	1.94	0.67
1:B:370:GLU:O	14:B:701:HOH:O	2.12	0.67
1:B:271:ASP:HA	1:B:419:LYS:HB2	1.77	0.67
1:B:274:GLU:HB2	1:B:345:GLN:HA	1.77	0.67
1:A:461:ASN:HD22	4:G:1:NAG:H83	1.60	0.67
1:B:413:GLU:HA	12:B:607:PEG:H32	1.75	0.67
1:A:227:ILE:HG12	1:A:244:LEU:HD21	1.76	0.67
1:B:100:SER:O	14:B:702:HOH:O	2.13	0.67
3:D:1:NAG:O3	3:D:2:NAG:O5	2.04	0.66
1:A:429:ILE:HD12	1:A:429:ILE:H	1.61	0.66
1:A:298:GLN:HB2	12:A:611:PEG:H32	1.77	0.66
1:A:443:TRP:HA	4:G:1:NAG:H82	1.77	0.66
1:A:391:VAL:HG21	1:B:221:GLU:HG2	1.78	0.65
1:A:161:HIS:ND1	11:A:610:PGE:O4	2.28	0.65
1:A:324:GLU:HB2	12:A:612:PEG:H41	1.78	0.65
5:H:1:NAG:H61	5:H:5:FUC:H3	1.79	0.65
1:A:430:VAL:HG23	1:A:431:ASP:H	1.60	0.65
12:A:616:PEG:H21	14:A:781:HOH:O	1.95	0.65
1:B:259:GLN:HB2	1:B:284:TYR:HE2	1.62	0.64
1:B:225:LEU:HB2	14:B:761:HOH:O	1.95	0.64
5:H:1:NAG:H62	5:H:2:NAG:C1	2.28	0.64
1:A:290:PRO:HA	10:A:606:GOL:H2	1.79	0.64
1:B:272:ARG:NH1	1:B:348:SER:O	2.30	0.64
1:A:272:ARG:NH1	1:A:348:SER:O	2.31	0.63
1:A:434:ILE:HG23	1:A:438:ALA:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HG12	1:A:244:LEU:CD2	2.29	0.63
1:A:365:THR:HG21	12:A:611:PEG:H41	1.80	0.63
1:B:270:PHE:CE1	12:B:611:PEG:H22	2.34	0.63
1:A:166:ARG:O	1:A:214:GLN:HG2	1.98	0.63
1:B:259:GLN:HB2	1:B:284:TYR:CE2	2.34	0.62
1:B:417:LYS:NZ	14:B:704:HOH:O	2.32	0.62
1:A:434:ILE:CG2	1:A:438:ALA:HB3	2.29	0.62
1:A:198:VAL:HG12	1:A:200:PHE:HD1	1.63	0.62
1:A:450:ASN:HB3	1:A:455:THR:CG2	2.30	0.61
1:A:289:THR:O	12:A:612:PEG:H42	2.00	0.61
1:A:295:ASN:CB	12:A:615:PEG:H31	2.30	0.61
1:A:35:TYR:OH	14:A:701:HOH:O	2.09	0.60
1:A:362:ASN:HA	1:A:372:THR:HG22	1.82	0.60
1:A:198:VAL:CG1	1:A:200:PHE:HD1	2.14	0.60
1:A:234:GLU:OE1	1:A:234:GLU:N	2.27	0.60
12:A:616:PEG:O1	4:G:1:NAG:H81	2.02	0.60
1:A:430:VAL:HG12	1:A:477:VAL:HG23	1.82	0.60
1:A:251:GLU:HA	12:A:611:PEG:H11	1.84	0.59
1:A:365:THR:HG21	12:A:611:PEG:C4	2.33	0.59
1:A:61:PHE:CD1	1:A:118:PRO:HB3	2.38	0.59
1:B:93:PHE:CZ	1:B:137:ASN:HB2	2.38	0.59
1:B:414:ASN:HB2	12:B:611:PEG:H31	1.85	0.59
1:B:31:THR:HG22	1:B:132:LYS:HB3	1.84	0.58
1:B:291:VAL:HG13	1:B:292:TYR:CD2	2.38	0.58
1:B:446:SER:HB3	1:B:459:TYR:CZ	2.39	0.58
3:D:1:NAG:O7	3:D:1:NAG:H3	2.03	0.58
1:A:322:PHE:CD1	12:A:612:PEG:H21	2.38	0.58
1:A:282:PHE:CE1	1:A:338:GLU:HG2	2.38	0.58
1:A:429:ILE:HD11	12:A:616:PEG:H41	1.84	0.58
1:B:305:LEU:HD22	1:B:357:LEU:HD11	1.84	0.58
1:A:252:ASP:H	12:A:611:PEG:C1	2.16	0.57
1:B:413:GLU:CG	12:B:611:PEG:H32	2.23	0.57
1:B:64:SER:HB2	1:B:70:THR:CG2	2.35	0.57
1:A:29[B]:LEU:CD2	1:A:130:GLU:HB3	2.33	0.57
1:B:270:PHE:H	11:B:610:PGE:H62	1.68	0.57
2:C:1:NAG:H61	2:C:2:NAG:N2	2.19	0.57
1:B:166:ARG:O	1:B:214:GLN:HG2	2.06	0.56
2:C:1:NAG:H61	2:C:2:NAG:C7	2.35	0.56
1:A:95:SER:HB2	14:A:754:HOH:O	2.05	0.56
1:B:430:VAL:HG21	1:B:475:GLU:HG2	1.87	0.55
1:A:215:VAL:HG21	1:A:248:ILE:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:CD2	1:A:357:LEU:HD11	2.33	0.55
3:E:2:NAG:H3	3:E:2:NAG:C8	2.33	0.55
1:A:391:VAL:HG21	1:B:221:GLU:CG	2.37	0.55
1:A:272:ARG:HD2	1:A:421:ILE:HD11	1.89	0.55
1:B:184:PRO:CG	9:B:604:NAG:H83	2.36	0.55
1:A:289:THR:H	12:A:612:PEG:C4	2.19	0.54
1:A:325:GLU:HG2	14:A:752:HOH:O	2.08	0.54
1:B:303:GLY:HA2	1:B:360:LEU:O	2.07	0.54
1:A:450:ASN:OD1	1:A:452:ASN:HB2	2.07	0.54
5:H:2:NAG:O7	5:H:2:NAG:C3	2.56	0.54
1:A:142:SER:HB3	1:A:145:GLN:HG3	1.89	0.53
1:B:352:GLN:HB2	1:B:383:PRO:HD3	1.90	0.53
3:E:2:NAG:C1	3:E:2:NAG:H82	2.38	0.53
1:A:453:ASP:HB2	1:A:455:THR:HG22	1.91	0.53
1:A:322:PHE:CE1	12:A:612:PEG:H21	2.44	0.53
1:B:108:THR:HG23	1:B:130:GLU:HG3	1.90	0.53
1:B:270:PHE:HE1	12:B:611:PEG:H22	1.72	0.53
1:A:458:LEU:HD21	1:A:493:LEU:HD11	1.90	0.53
1:A:427:LEU:CD2	1:A:478:VAL:HG22	2.39	0.53
1:A:93:PHE:CE2	1:A:137:ASN:HB2	2.44	0.53
1:B:458:LEU:HD21	1:B:493:LEU:HD21	1.89	0.53
1:A:324:GLU:N	12:A:612:PEG:H22	2.24	0.52
11:B:610:PGE:H2	13:B:613:MES:O2S	2.10	0.52
1:B:116:THR:HB	1:B:117:PRO:CD	2.40	0.52
1:A:274:GLU:HB3	1:A:345:GLN:HA	1.92	0.51
1:A:217:ARG:HD2	1:A:221:GLU:HG2	1.92	0.51
1:A:277:VAL:HG13	1:A:340:LYS:HB3	1.91	0.51
1:A:429:ILE:HD12	1:A:429:ILE:N	2.26	0.51
1:B:118:PRO:HA	1:B:122:MET:SD	2.51	0.51
1:A:295:ASN:H	12:A:615:PEG:H31	1.76	0.51
1:A:74:HIS:HB2	9:A:604:NAG:H82	1.92	0.51
1:A:217:ARG:HD2	1:A:217:ARG:O	2.11	0.51
1:A:301:LEU:HD23	1:A:363:ASP:HA	1.93	0.51
5:H:2:NAG:H3	5:H:2:NAG:O7	2.11	0.51
5:H:1:NAG:C6	5:H:5:FUC:H3	2.40	0.50
1:B:268:VAL:HB	1:B:381:VAL:HG22	1.93	0.50
1:A:25:PHE:CZ	1:A:113:VAL:HG12	2.47	0.50
1:B:224:HIS:ND1	1:B:245:HIS:ND1	2.59	0.50
1:A:311:TRP:CH2	1:A:353:ARG:HD2	2.47	0.50
1:B:154:PRO:HG2	10:B:606:GOL:H31	1.94	0.50
1:A:323:ARG:HE	1:B:417:LYS:NZ	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HA	1:A:132:LYS:O	2.12	0.50
1:A:407:ILE:HD11	1:A:460:VAL:CG1	2.39	0.49
1:B:158:SER:HB2	1:B:172:ARG:HH22	1.77	0.49
1:B:187:THR:OG1	1:B:232:ARG:HB3	2.13	0.48
1:A:403:THR:HA	1:A:460:VAL:CG2	2.39	0.48
1:B:272:ARG:O	1:B:346:ASN:HA	2.12	0.48
1:B:102:ARG:H	1:B:102:ARG:HG2	1.42	0.48
1:B:116:THR:HB	1:B:117:PRO:HD2	1.95	0.48
5:H:1:NAG:H61	5:H:5:FUC:H5	1.96	0.48
1:A:168:PRO:HA	1:A:211:VAL:HG13	1.96	0.48
1:A:409:LYS:HA	1:A:456:GLY:O	2.13	0.48
1:B:184:PRO:HG2	9:B:604:NAG:C8	2.40	0.48
1:B:397:VAL:CG2	1:B:407:ILE:HG23	2.43	0.48
1:B:458:LEU:HD21	1:B:493:LEU:CD2	2.44	0.47
1:A:447:LEU:HD23	1:A:448:ALA:N	2.29	0.47
1:B:160:PRO:CD	1:B:244:LEU:HD11	2.44	0.47
1:B:160:PRO:HD3	1:B:244:LEU:HD11	1.96	0.47
1:B:311:TRP:CZ3	1:B:353:ARG:HD2	2.49	0.47
1:A:180:MET:HG2	1:A:188:ILE:HD12	1.96	0.47
1:B:93:PHE:CE1	5:H:1:NAG:H82	2.49	0.47
5:H:1:NAG:H61	5:H:5:FUC:C3	2.44	0.47
1:A:93:PHE:CZ	1:A:137:ASN:HB2	2.49	0.47
1:B:397:VAL:O	1:B:497:PHE:HA	2.15	0.47
1:A:442:TYR:OH	14:A:702:HOH:O	2.21	0.46
1:A:324:GLU:OE1	12:A:612:PEG:H41	2.15	0.46
1:A:289:THR:HB	12:A:612:PEG:H31	1.97	0.46
1:B:430:VAL:HG22	1:B:477:VAL:HG23	1.98	0.46
1:A:298:GLN:HB2	12:A:611:PEG:C3	2.45	0.46
1:A:453:ASP:HB2	1:A:455:THR:CG2	2.45	0.46
1:B:304:THR:HG22	1:B:306:MET:CE	2.46	0.46
1:B:385:PRO:CG	12:B:611:PEG:H21	2.45	0.46
1:A:324:GLU:HB2	12:A:612:PEG:C4	2.43	0.46
1:B:269:GLU:O	1:B:272:ARG:HG2	2.16	0.46
1:A:227:ILE:CG1	1:A:244:LEU:HD21	2.46	0.46
1:B:201:ALA:O	1:B:210:VAL:HG22	2.16	0.46
1:A:269:GLU:HB3	14:A:770:HOH:O	2.16	0.45
1:A:298:GLN:HB2	12:A:611:PEG:H22	1.98	0.45
1:B:193:VAL:HG23	1:B:226:ASP:HB2	1.98	0.45
12:A:615:PEG:H21	1:B:407:ILE:O	2.16	0.45
1:A:61:PHE:CE1	1:A:118:PRO:HB3	2.51	0.45
1:B:158:SER:HB2	1:B:172:ARG:NH2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:CYS:O	1:B:239:GLU:HA	2.16	0.45
1:B:192:VAL:HG13	1:B:202:VAL:HG23	1.99	0.45
1:B:64:SER:HB2	1:B:70:THR:HG21	1.97	0.45
1:A:394:SER:HB2	1:B:28:ARG:HH22	1.81	0.45
1:A:41:GLY:CA	11:A:614:PGE:H32	2.47	0.45
1:B:143:CYS:HB2	1:B:182:ILE:O	2.18	0.44
1:B:266:VAL:HG13	1:B:278:PHE:HB3	1.97	0.44
1:A:101:VAL:O	1:A:101:VAL:HG12	2.18	0.44
1:A:323:ARG:HE	1:B:417:LYS:HZ1	1.66	0.44
1:A:229:CYS:O	1:A:239:GLU:HA	2.17	0.44
1:B:51:ARG:HD2	1:B:56:GLU:O	2.16	0.44
1:A:253:ASP:OD1	1:A:254:ASN:ND2	2.50	0.44
1:B:413:GLU:CG	12:B:607:PEG:H21	2.45	0.44
2:C:1:NAG:H61	2:C:2:NAG:H82	2.00	0.44
1:A:122:MET:HB3	1:A:126:LEU:HD12	2.00	0.44
1:B:183:CYS:HB3	1:B:186:TYR:CD2	2.53	0.44
1:A:402:THR:O	1:A:460:VAL:HG21	2.18	0.43
1:A:298:GLN:HG3	12:A:611:PEG:H12	1.98	0.43
1:B:399:GLN:HG3	1:B:498:GLN:O	2.18	0.43
1:A:143:CYS:HB2	1:A:182:ILE:O	2.18	0.43
1:A:118:PRO:HA	1:A:122:MET:SD	2.58	0.43
1:A:160:PRO:HG2	1:A:246:VAL:HG22	2.01	0.43
1:B:270:PHE:H	11:B:610:PGE:C6	2.30	0.43
1:A:108:THR:HG23	1:A:130:GLU:HG3	2.00	0.43
1:A:304:THR:O	1:A:306:MET:HE3	2.19	0.43
1:A:272:ARG:O	1:A:346:ASN:HA	2.17	0.43
1:B:269:GLU:HB3	11:B:610:PGE:H62	2.01	0.43
2:C:2:NAG:O3	2:C:6:MAN:H5	2.19	0.43
3:E:2:NAG:C1	3:E:2:NAG:C8	2.97	0.43
2:C:1:NAG:C6	2:C:2:NAG:H82	2.49	0.42
1:A:325:GLU:HA	12:B:607:PEG:H12	2.01	0.42
1:A:430:VAL:HG22	1:A:475:GLU:O	2.19	0.42
1:A:201:ALA:CB	12:A:613:PEG:H22	2.49	0.42
1:B:59:TYR:HB3	1:B:118:PRO:HD3	2.01	0.42
1:B:269:GLU:HB3	11:B:610:PGE:C6	2.49	0.42
1:B:393:TYR:HB2	1:B:493:LEU:HD12	2.00	0.42
1:A:31:THR:O	1:A:32:GLU:HG2	2.20	0.42
3:D:1:NAG:O7	3:D:1:NAG:C3	2.67	0.42
1:A:30:TYR:CE1	1:A:129:VAL:HG11	2.55	0.42
1:B:297:VAL:HG12	1:B:297:VAL:O	2.19	0.42
1:A:25:PHE:CZ	1:A:129:VAL:HG23	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ILE:HG12	1:B:438:ALA:HB3	2.01	0.42
1:B:270:PHE:CZ	12:B:611:PEG:H22	2.54	0.42
2:C:3:BMA:H62	2:C:6:MAN:H3	2.01	0.42
1:B:325:GLU:OE1	1:B:328:ILE:HB	2.20	0.41
1:A:298:GLN:CD	12:A:611:PEG:H22	2.39	0.41
1:B:26:PRO:HD3	1:B:50:MET:HG3	2.02	0.41
1:B:31:THR:HA	1:B:132:LYS:O	2.20	0.41
2:C:3:BMA:H62	2:C:6:MAN:C3	2.50	0.41
1:A:361:VAL:HB	1:A:373:VAL:CG2	2.50	0.41
1:B:413:GLU:O	12:B:611:PEG:H41	2.21	0.41
1:A:25:PHE:CZ	1:A:113:VAL:CG1	3.03	0.41
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.21	0.41
1:B:272:ARG:NH2	1:B:382:LEU:O	2.52	0.41
1:B:414:ASN:ND2	12:B:611:PEG:H31	2.24	0.41
1:A:200:PHE:O	12:A:613:PEG:C3	2.66	0.41
1:B:305:LEU:CD2	1:B:357:LEU:HD11	2.51	0.41
1:B:103:SER:HA	1:B:104:PRO:C	2.41	0.41
1:A:64:SER:HG	1:A:110:LYS:H	1.64	0.41
1:B:36:VAL:HG11	1:B:90:TRP:CD2	2.56	0.41
3:E:2:NAG:C3	3:E:2:NAG:C8	2.97	0.41
1:B:45:LEU:C	1:B:45:LEU:HD12	2.42	0.40
1:A:430:VAL:HG23	1:A:431:ASP:N	2.33	0.40
12:A:615:PEG:H32	12:A:615:PEG:H12	1.81	0.40
1:B:279:GLY:O	1:B:340:LYS:HA	2.21	0.40
1:B:297:VAL:CG1	1:B:297:VAL:O	2.68	0.40
1:B:76:ASP:HB3	1:B:79:SER:OG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:NH2	1:A:491:THR:OG1[1_666]	2.14	0.06

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	476/480 (99%)	462 (97%)	14 (3%)	0	100	100
1	B	469/480 (98%)	459 (98%)	10 (2%)	0	100	100
All	All	945/960 (98%)	921 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	398/441 (90%)	391 (98%)	7 (2%)	59	72
1	B	404/441 (92%)	396 (98%)	8 (2%)	55	69
All	All	802/882 (91%)	787 (98%)	15 (2%)	57	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	135	PHE
1	A	167	GLU
1	A	272	ARG
1	A	347	LEU
1	A	390	GLN
1	A	415	CYS
1	B	28	ARG
1	B	32	GLU
1	B	135	PHE
1	B	272	ARG
1	B	286	ARG
1	B	328	ILE
1	B	342	LYS
1	B	402	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	414	ASN

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

33 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	C	1	1,2	14,14,15	0.41	0	17,19,21	0.43	0
2	NAG	C	2	2	14,14,15	0.34	0	17,19,21	0.45	0
2	BMA	C	3	2	11,11,12	0.88	0	15,15,17	0.84	0
2	MAN	C	4	2	11,11,12	1.19	0	15,15,17	1.53	2 (13%)
2	MAN	C	5	2	11,11,12	0.98	2 (18%)	15,15,17	1.05	0
2	MAN	C	6	2	11,11,12	0.93	0	15,15,17	1.16	1 (6%)
2	FUC	C	7	2	10,10,11	0.83	0	14,14,16	0.94	0
3	NAG	D	1	1,3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	D	2	3	14,14,15	0.44	0	17,19,21	0.51	0
3	NAG	E	1	1,3	14,14,15	0.33	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.56	0
4	NAG	F	1	1,4	14,14,15	0.40	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.34	0
4	FUC	F	3	4	10,10,11	0.88	0	14,14,16	0.84	0
4	NAG	G	1	1,4	14,14,15	0.28	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	2	4	14,14,15	0.20	0	17,19,21	0.60	1 (5%)
4	FUC	G	3	4	10,10,11	1.09	0	14,14,16	0.84	1 (7%)
5	NAG	H	1	1,5	14,14,15	0.58	0	17,19,21	0.88	1 (5%)
5	NAG	H	2	5	14,14,15	0.16	0	17,19,21	0.77	1 (5%)
5	BMA	H	3	5	11,11,12	1.14	1 (9%)	15,15,17	1.10	0
5	MAN	H	4	5	11,11,12	0.99	0	15,15,17	0.92	0
5	FUC	H	5	5	10,10,11	1.94	3 (30%)	14,14,16	1.45	3 (21%)
3	NAG	I	1	1,3	14,14,15	0.64	0	17,19,21	0.59	0
3	NAG	I	2	3	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	J	1	1,6	14,14,15	0.27	0	17,19,21	0.53	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.48	0
6	BMA	J	3	6	11,11,12	0.93	0	15,15,17	0.93	0
6	FUC	J	4	6	10,10,11	1.39	2 (20%)	14,14,16	1.21	1 (7%)
7	NAG	K	1	1,7	14,14,15	0.26	0	17,19,21	0.69	1 (5%)
7	NAG	K	2	7	14,14,15	0.27	0	17,19,21	0.51	0
7	BMA	K	3	7	11,11,12	0.69	0	15,15,17	0.85	1 (6%)
7	MAN	K	4	7	11,11,12	1.35	2 (18%)	15,15,17	1.29	2 (13%)
7	FUC	K	5	7	10,10,11	1.65	2 (20%)	14,14,16	0.99	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	FUC	C	7	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	F	3	4	-	-	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	FUC	H	5	5	-	-	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	FUC	J	4	6	-	-	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	1/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	FUC	K	5	7	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	5	FUC	C1-C2	4.05	1.61	1.52
7	K	5	FUC	C2-C3	3.62	1.57	1.52
5	H	5	FUC	C2-C3	3.06	1.57	1.52
6	J	4	FUC	C2-C3	2.52	1.56	1.52
5	H	3	BMA	C2-C3	2.47	1.56	1.52
7	K	5	FUC	O5-C5	2.31	1.48	1.43
5	H	5	FUC	O2-C2	2.31	1.48	1.43
7	K	4	MAN	C4-C3	2.30	1.58	1.52
6	J	4	FUC	C4-C5	2.27	1.57	1.52
2	C	5	MAN	C2-C3	2.16	1.55	1.52
2	C	5	MAN	C1-C2	2.02	1.56	1.52
7	K	4	MAN	C4-C5	2.01	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	4.93	118.88	112.19
2	C	6	MAN	O2-C2-C3	-3.74	102.64	110.14
5	H	5	FUC	O2-C2-C1	2.92	115.12	109.15
6	J	4	FUC	O5-C5-C4	2.92	114.75	109.52
5	H	1	NAG	C1-O5-C5	2.84	116.04	112.19
7	K	4	MAN	C1-O5-C5	2.77	115.95	112.19
7	K	4	MAN	O2-C2-C3	-2.61	104.91	110.14
5	H	5	FUC	C1-C2-C3	2.52	112.76	109.67
2	C	4	MAN	O2-C2-C3	-2.48	105.17	110.14
7	K	3	BMA	O2-C2-C3	-2.36	105.41	110.14
7	K	1	NAG	C1-O5-C5	2.23	115.22	112.19
5	H	5	FUC	C1-O5-C5	2.10	117.55	112.78
4	G	3	FUC	O2-C2-C1	2.08	113.40	109.15
5	H	2	NAG	C2-N2-C7	2.05	125.82	122.90
4	G	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

16 monomers are involved in 34 short contacts:

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

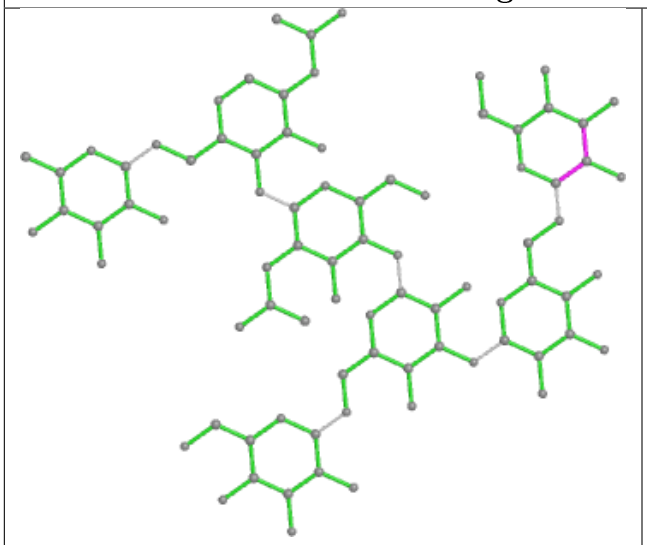
Continued on next page...

Continued from previous page...

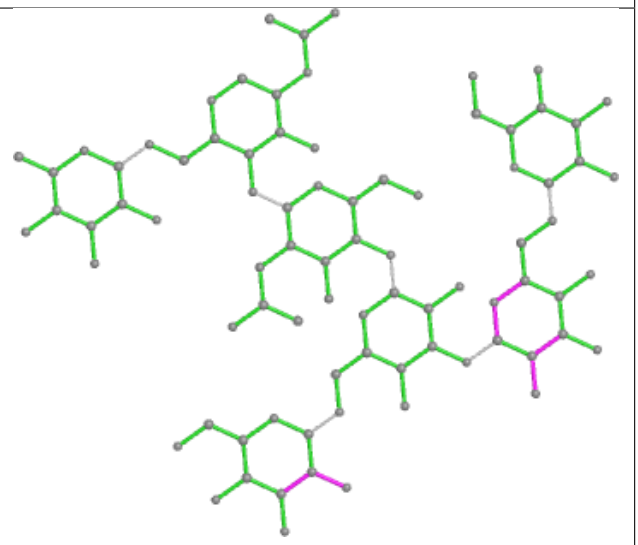
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	5	0

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

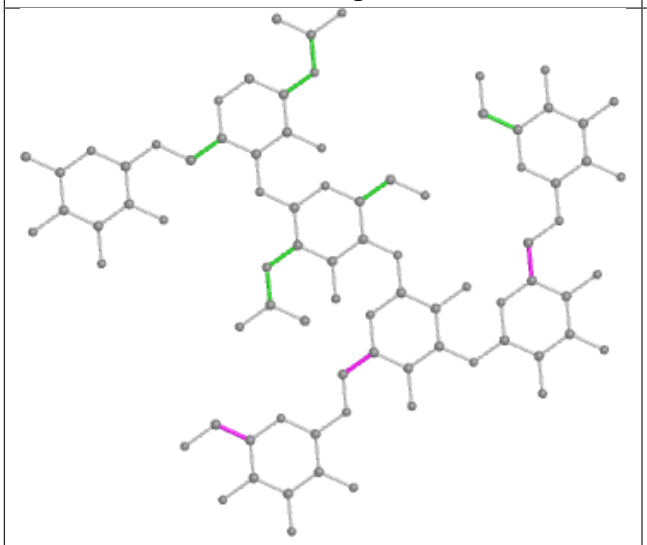
Oligosaccharide Chain C



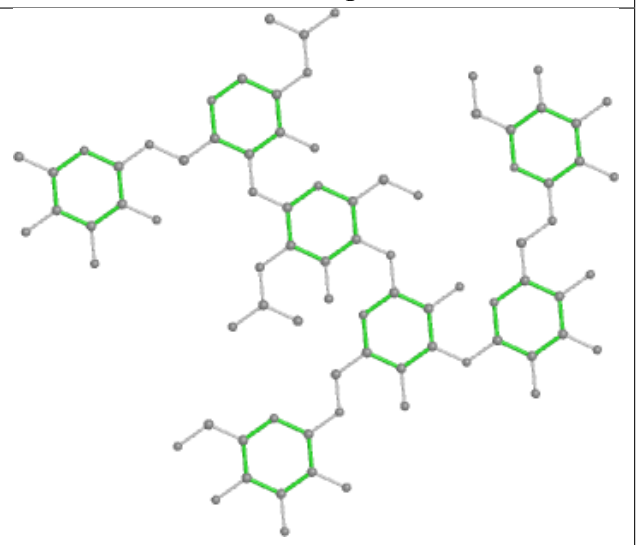
Bond lengths



Bond angles

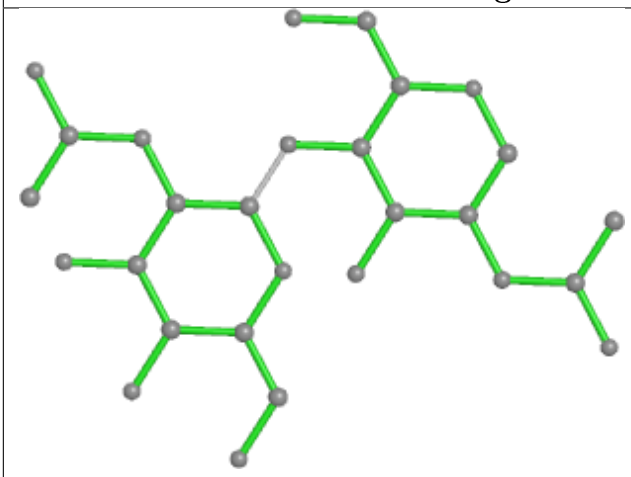


Torsions

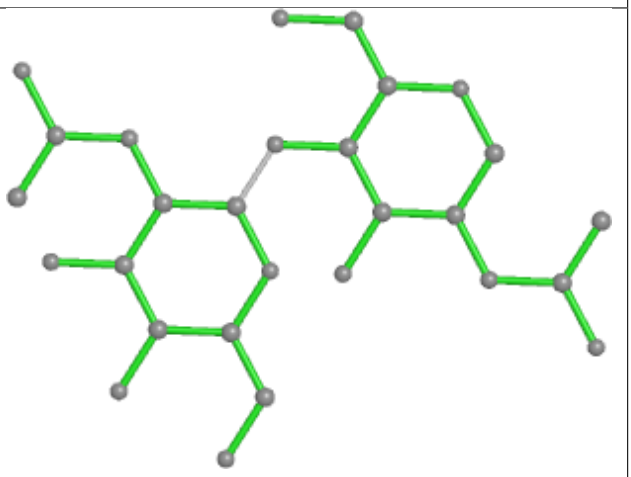


Rings

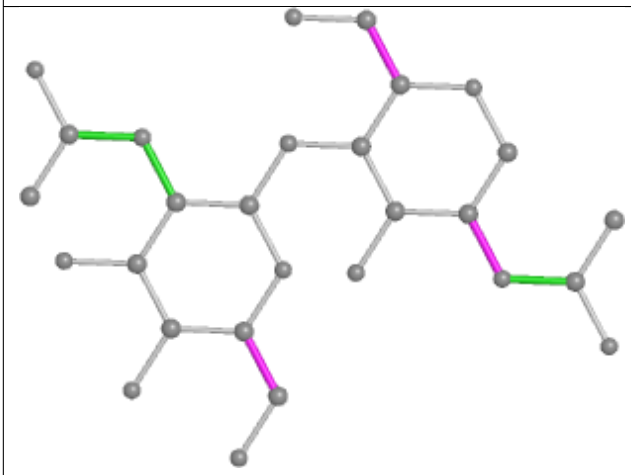
Oligosaccharide Chain D



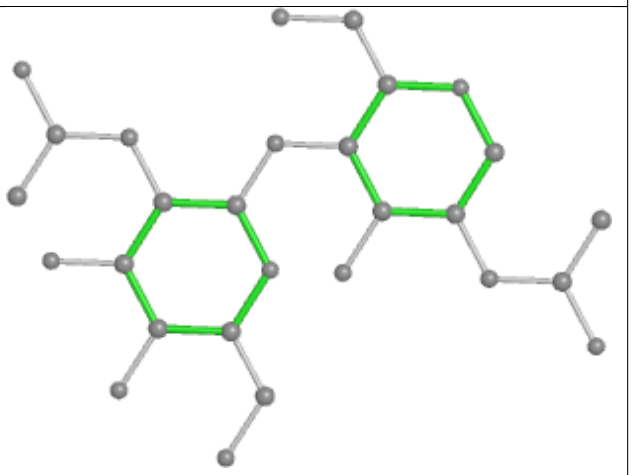
Bond lengths



Bond angles

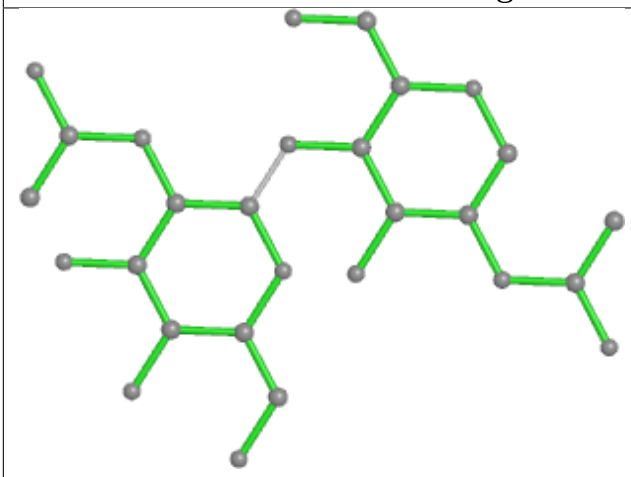


Torsions

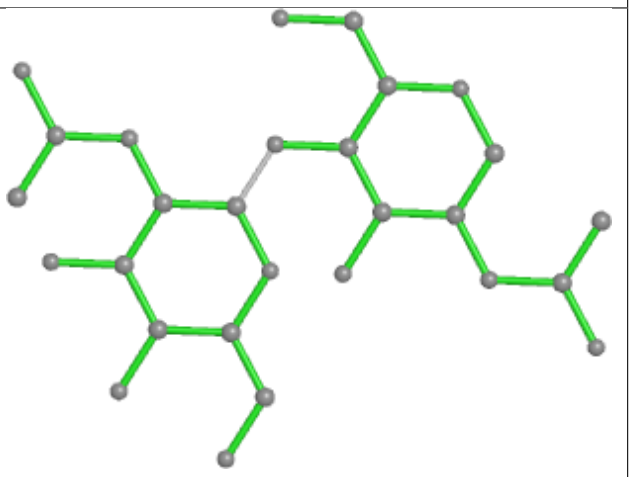


Rings

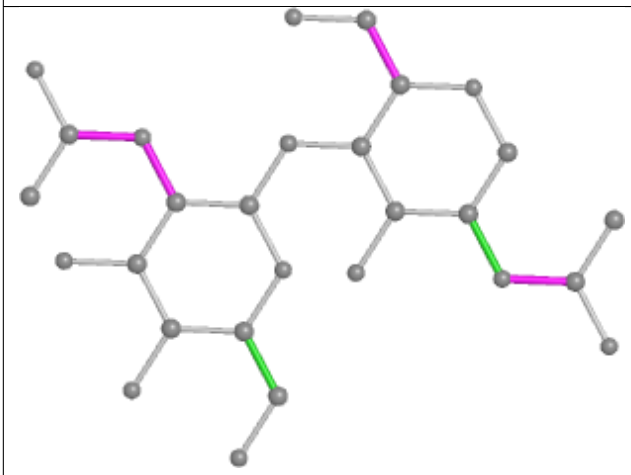
Oligosaccharide Chain E



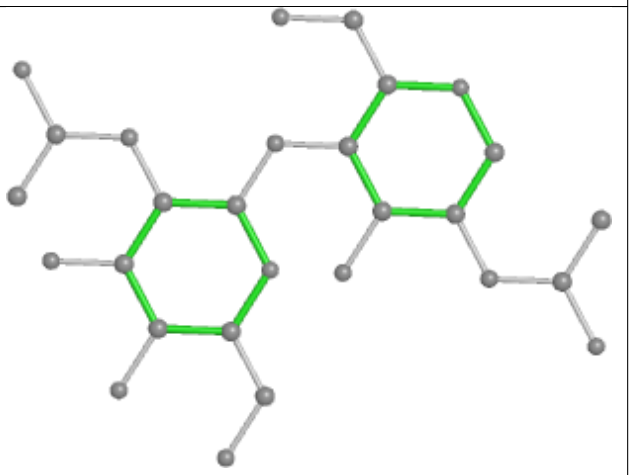
Bond lengths



Bond angles

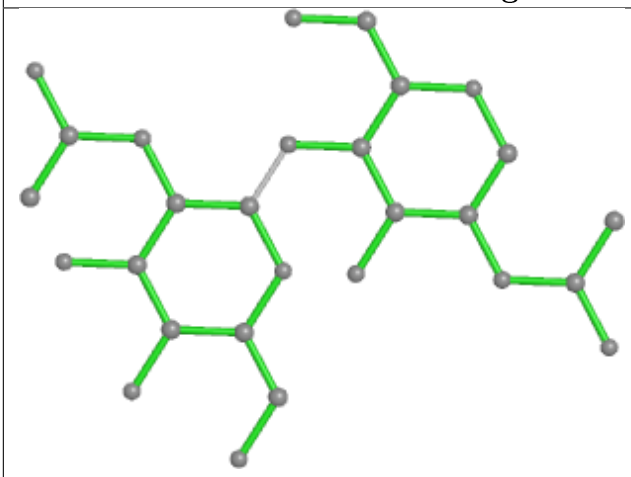


Torsions

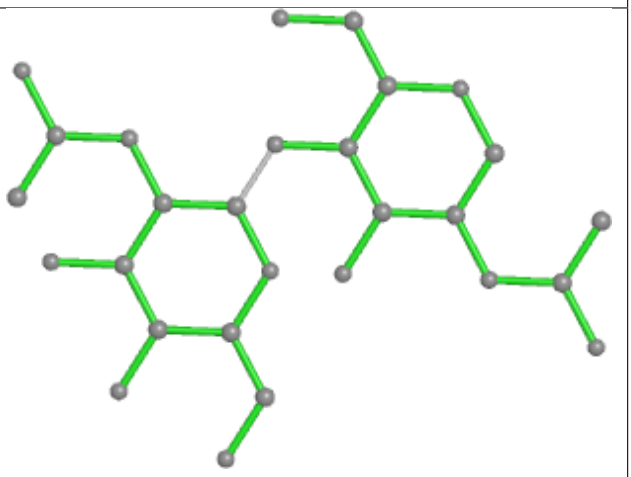


Rings

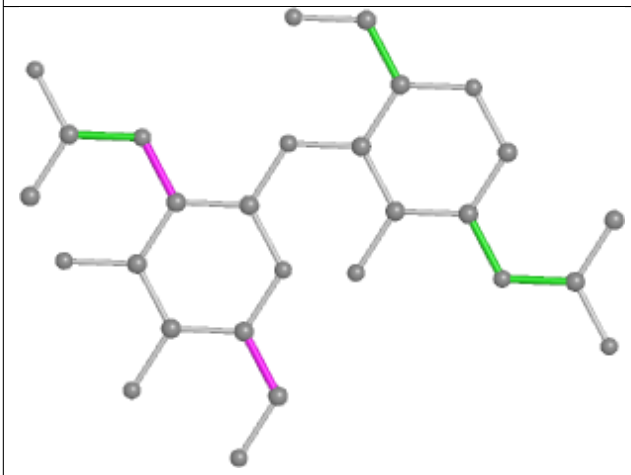
Oligosaccharide Chain I



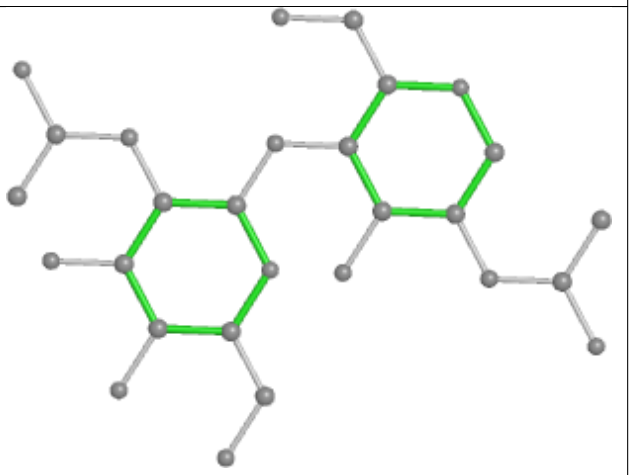
Bond lengths



Bond angles

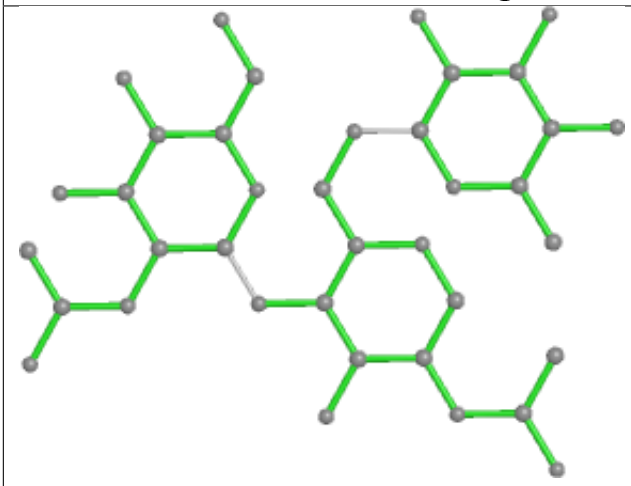


Torsions

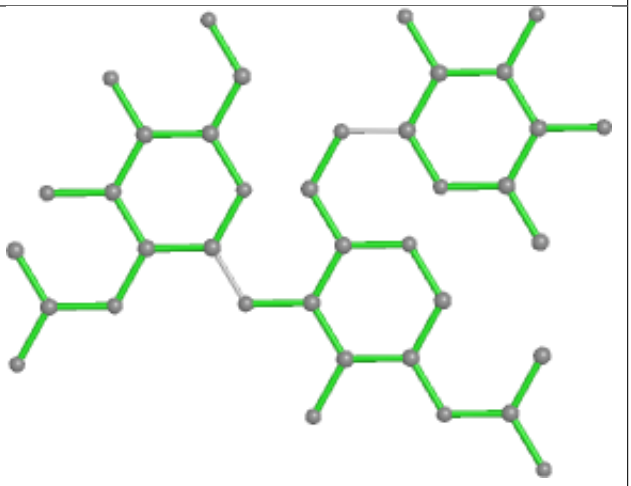


Rings

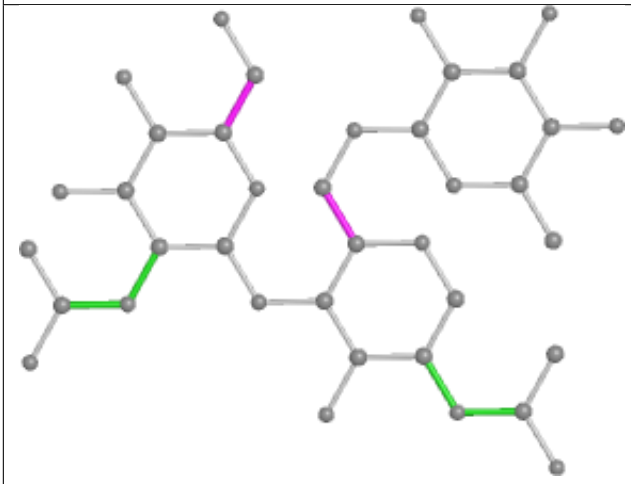
Oligosaccharide Chain F



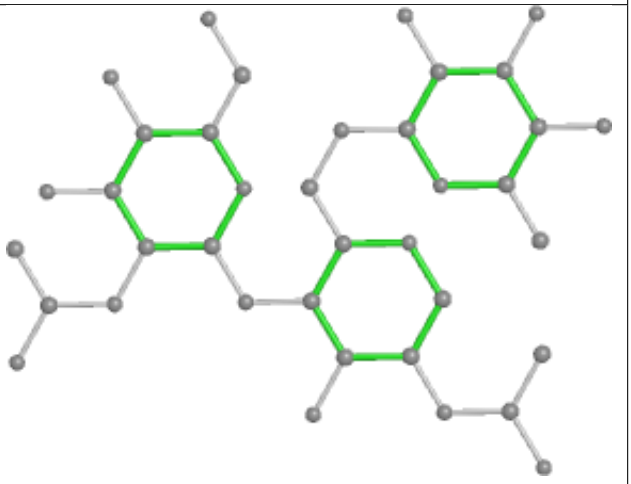
Bond lengths



Bond angles

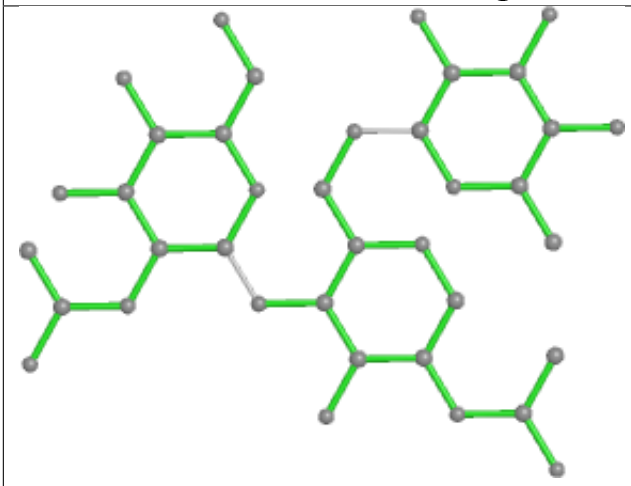


Torsions

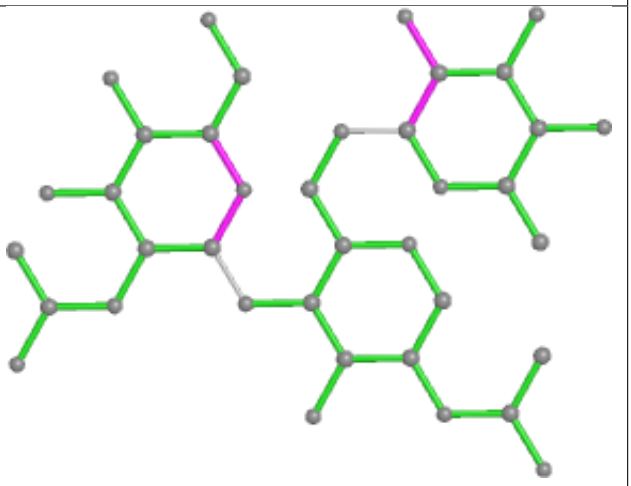


Rings

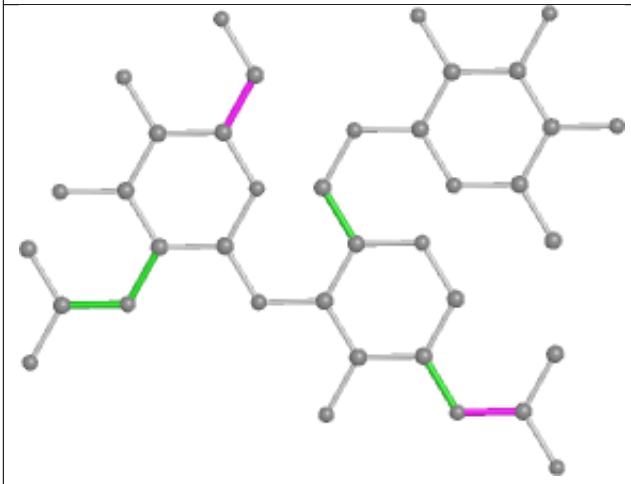
Oligosaccharide Chain G



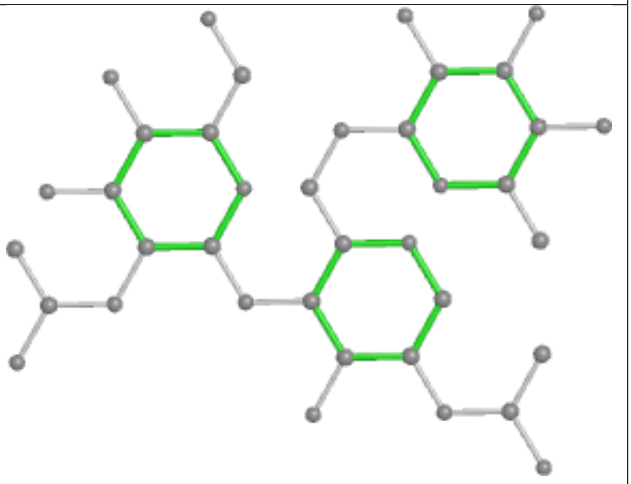
Bond lengths



Bond angles

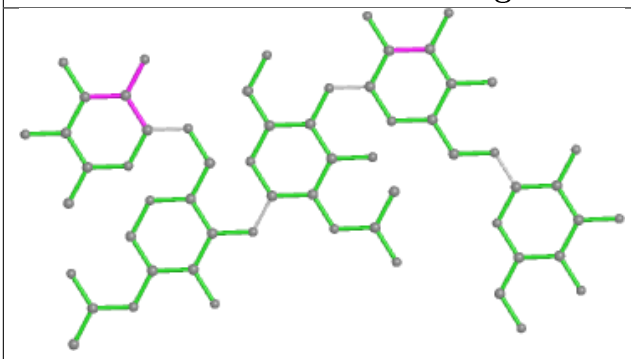


Torsions

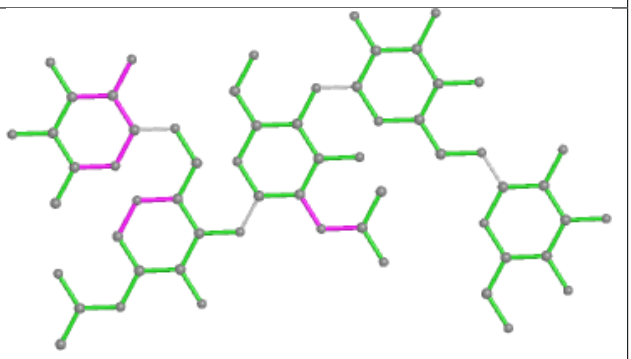


Rings

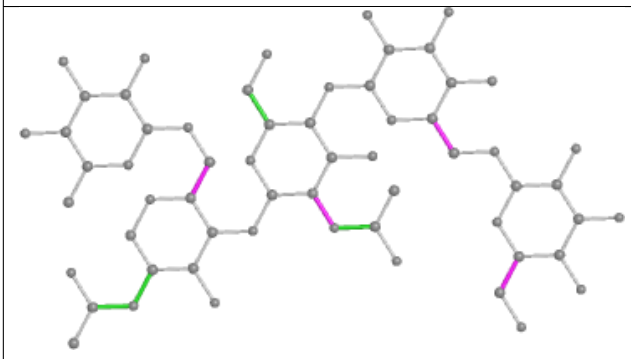
Oligosaccharide Chain H



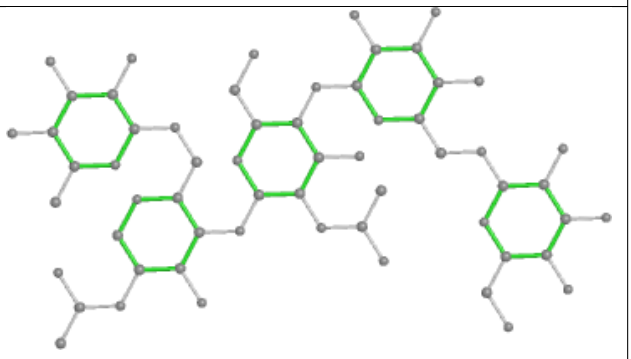
Bond lengths



Bond angles

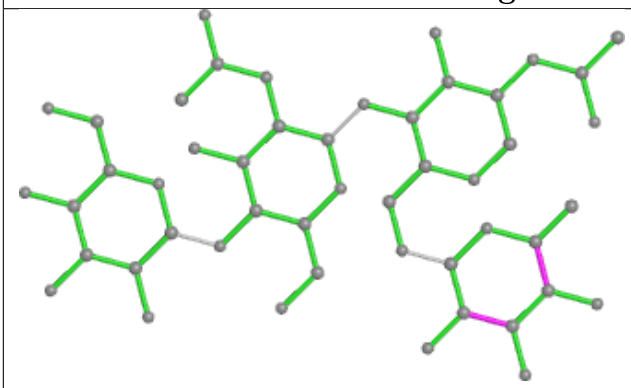


Torsions

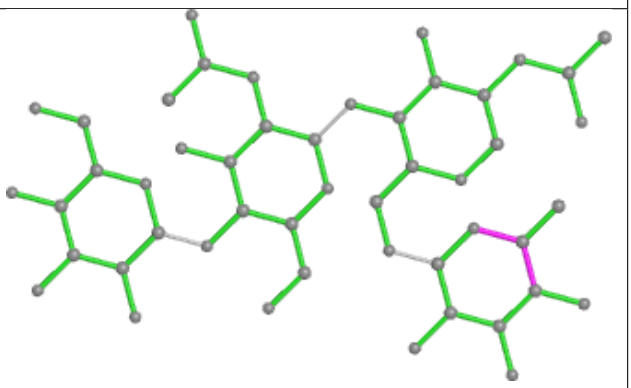


Rings

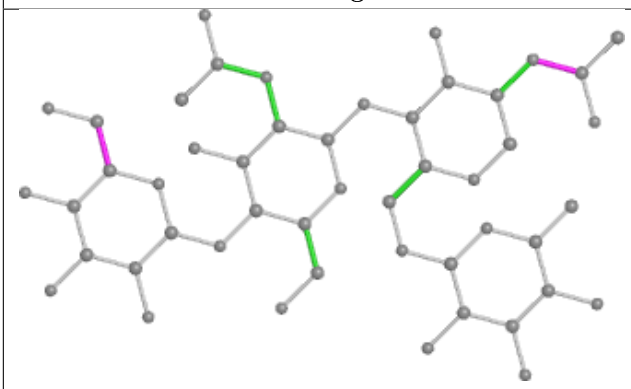
Oligosaccharide Chain J



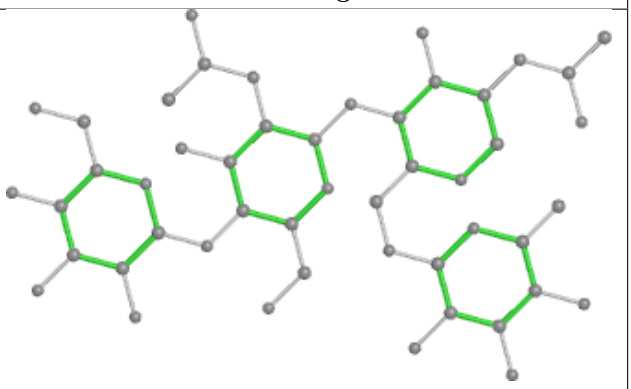
Bond lengths



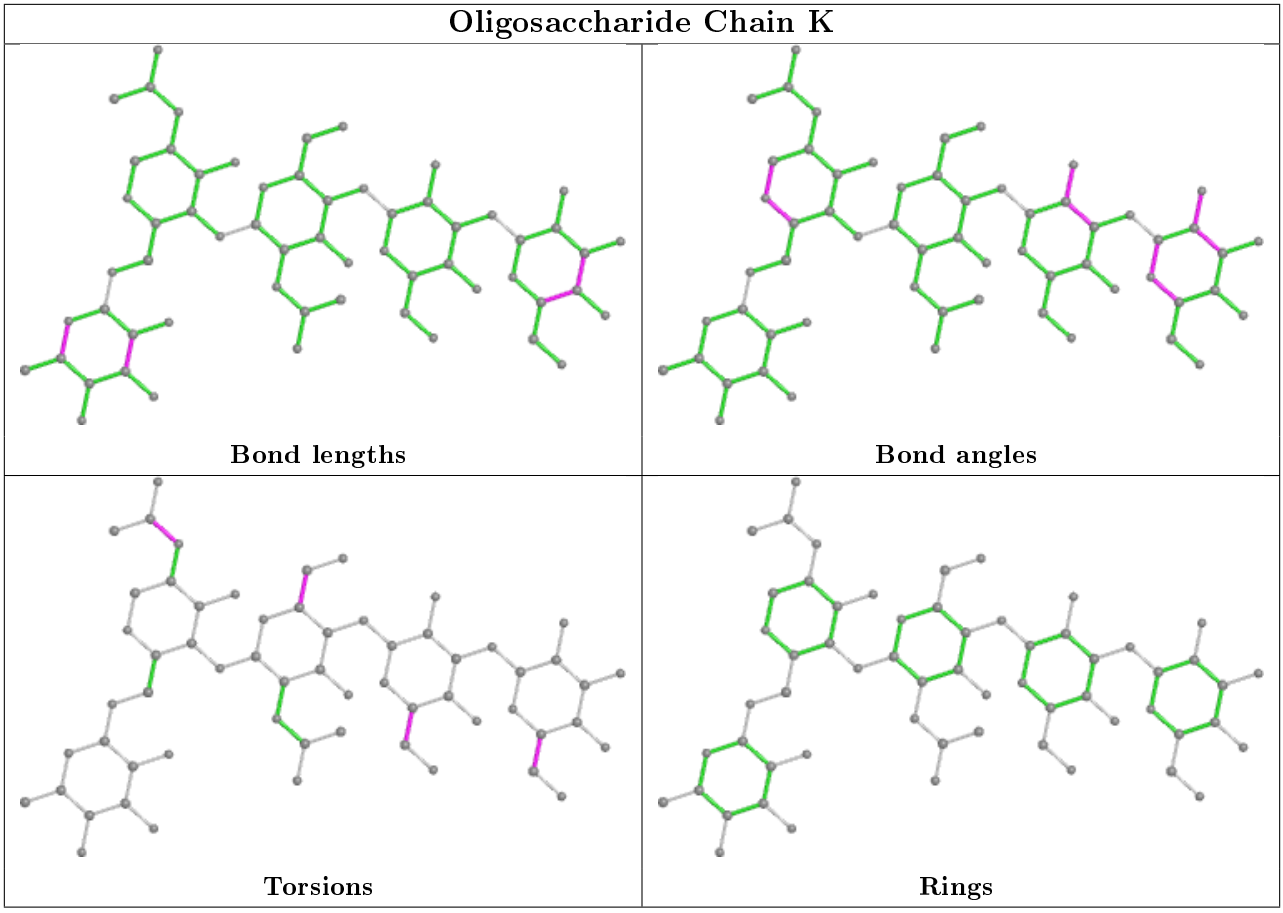
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
12	PEG	A	613	-	6,6,6	0.62	0	5,5,5	0.47	0
9	NAG	A	605	1	14,14,15	0.45	0	17,19,21	0.44	0
10	GOL	B	605	-	5,5,5	0.84	0	5,5,5	0.98	0
11	PGE	A	610	-	9,9,9	0.61	0	8,8,8	0.31	0
10	GOL	A	607	-	5,5,5	1.07	0	5,5,5	0.86	0
12	PEG	A	616	-	6,6,6	0.47	0	5,5,5	0.35	0
13	MES	B	613	-	12,12,12	2.01	1 (8%)	14,16,16	2.24	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PEG	A	615	-	6,6,6	0.50	0	5,5,5	0.34	0
10	GOL	A	606	-	5,5,5	0.97	0	5,5,5	0.91	0
12	PEG	B	608	-	6,6,6	0.49	0	5,5,5	0.43	0
9	NAG	B	604	1	14,14,15	0.37	0	17,19,21	0.60	0
11	PGE	B	610	-	9,9,9	0.56	0	8,8,8	0.37	0
12	PEG	A	612	-	6,6,6	0.47	0	5,5,5	0.60	0
12	PEG	A	611	-	6,6,6	0.55	0	5,5,5	0.27	0
12	PEG	B	607	-	6,6,6	0.71	0	5,5,5	0.59	0
11	PGE	A	614	-	9,9,9	0.61	0	8,8,8	0.26	0
9	NAG	A	604	1	14,14,15	0.35	0	17,19,21	0.66	0
12	PEG	B	611	-	6,6,6	0.42	0	5,5,5	0.62	0
10	GOL	B	606	-	5,5,5	0.99	0	5,5,5	0.82	0
12	PEG	A	609	-	6,6,6	0.52	0	5,5,5	0.35	0
12	PEG	B	612	-	6,6,6	0.52	0	5,5,5	0.22	0
11	PGE	B	609	-	9,9,9	0.64	0	8,8,8	0.30	0
11	PGE	A	608	-	3,3,9	0.62	0	2,2,8	0.15	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
12	PEG	A	613	-	-	3/4/4/4	-
9	NAG	A	605	1	-	2/6/23/26	0/1/1/1
10	GOL	B	605	-	-	3/4/4/4	-
11	PGE	A	610	-	-	1/7/7/7	-
10	GOL	A	607	-	-	2/4/4/4	-
12	PEG	A	616	-	-	1/4/4/4	-
13	MES	B	613	-	-	1/6/14/14	0/1/1/1
12	PEG	A	615	-	-	2/4/4/4	-
10	GOL	A	606	-	-	2/4/4/4	-
12	PEG	B	608	-	-	1/4/4/4	-
9	NAG	B	604	1	-	1/6/23/26	0/1/1/1
11	PGE	B	610	-	-	4/7/7/7	-
12	PEG	A	612	-	-	2/4/4/4	-
12	PEG	A	611	-	-	1/4/4/4	-
12	PEG	B	607	-	-	2/4/4/4	-
11	PGE	A	614	-	-	6/7/7/7	-
9	NAG	A	604	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEG	B	611	-	-	3/4/4/4	-
10	GOL	B	606	-	-	4/4/4/4	-
12	PEG	A	609	-	-	2/4/4/4	-
12	PEG	B	612	-	-	1/4/4/4	-
11	PGE	B	609	-	-	4/7/7/7	-
11	PGE	A	608	-	-	1/1/1/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	613	MES	C8-S	-6.62	1.68	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	613	MES	O1S-S-C8	4.86	112.77	106.92
13	B	613	MES	C6-C5-N4	-3.65	104.57	110.10
13	B	613	MES	C5-N4-C3	3.11	115.82	108.83
13	B	613	MES	O3S-S-C8	3.03	110.66	105.77
13	B	613	MES	C7-N4-C5	2.23	116.93	111.23

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	610	PGE	C4-C3-O2-C2
12	B	612	PEG	O2-C3-C4-O4
11	A	614	PGE	O2-C3-C4-O3
11	B	610	PGE	O3-C5-C6-O4
12	B	611	PEG	O2-C3-C4-O4
10	B	605	GOL	O1-C1-C2-C3
10	B	605	GOL	C1-C2-C3-O3
10	A	607	GOL	O1-C1-C2-C3
10	B	606	GOL	O1-C1-C2-C3
10	B	606	GOL	C1-C2-C3-O3
9	A	604	NAG	C4-C5-C6-O6
12	A	613	PEG	O1-C1-C2-O2
11	A	608	PGE	O2-C3-C4-O3
12	A	612	PEG	O1-C1-C2-O2
12	A	611	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	614	PGE	O1-C1-C2-O2
10	A	607	GOL	O1-C1-C2-O2
11	A	614	PGE	O3-C5-C6-O4
11	B	609	PGE	O1-C1-C2-O2
9	B	604	NAG	C3-C2-N2-C7
12	B	607	PEG	O2-C3-C4-O4
9	A	605	NAG	C4-C5-C6-O6
9	A	604	NAG	O5-C5-C6-O6
11	A	614	PGE	C3-C4-O3-C5
12	A	609	PEG	C4-C3-O2-C2
12	A	613	PEG	C4-C3-O2-C2
11	A	614	PGE	C4-C3-O2-C2
9	A	605	NAG	O5-C5-C6-O6
10	B	606	GOL	O1-C1-C2-O2
11	B	609	PGE	C4-C3-O2-C2
12	A	616	PEG	C4-C3-O2-C2
11	A	610	PGE	C1-C2-O2-C3
13	B	613	MES	C7-C8-S-O2S
11	B	609	PGE	C6-C5-O3-C4
12	A	613	PEG	C1-C2-O2-C3
12	B	611	PEG	O1-C1-C2-O2
10	B	605	GOL	O2-C2-C3-O3
10	B	606	GOL	O2-C2-C3-O3
11	B	609	PGE	C3-C4-O3-C5
12	B	611	PEG	C4-C3-O2-C2
12	A	609	PEG	C1-C2-O2-C3
11	B	610	PGE	C6-C5-O3-C4
12	A	615	PEG	C1-C2-O2-C3
11	A	614	PGE	C1-C2-O2-C3
10	A	606	GOL	C1-C2-C3-O3
12	A	612	PEG	C1-C2-O2-C3
10	A	606	GOL	O2-C2-C3-O3
12	B	607	PEG	C1-C2-O2-C3
11	B	610	PGE	O2-C3-C4-O3
12	A	615	PEG	C4-C3-O2-C2
12	B	608	PEG	O2-C3-C4-O4

There are no ring outliers.

16 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	613	PEG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	610	PGE	1	0
12	A	616	PEG	3	0
13	B	613	MES	1	0
12	A	615	PEG	5	0
10	A	606	GOL	1	0
9	B	604	NAG	3	0
11	B	610	PGE	5	0
12	A	612	PEG	12	0
12	A	611	PEG	10	0
12	B	607	PEG	4	0
11	A	614	PGE	3	0
9	A	604	NAG	1	0
12	B	611	PEG	14	0
10	B	606	GOL	1	0
11	B	609	PGE	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	476/480 (99%)	0.11	10 (2%) 63 61	13, 38, 69, 99	1 (0%)
1	B	472/480 (98%)	-0.04	4 (0%) 86 85	18, 34, 57, 84	0
All	All	948/960 (98%)	0.04	14 (1%) 73 72	13, 36, 62, 99	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	ALA	3.7
1	A	430	VAL	3.3
1	A	452	ASN	2.8
1	A	355	PHE	2.8
1	B	356	LEU	2.3
1	A	451	PRO	2.3
1	B	345	GLN	2.2
1	A	306	MET	2.2
1	B	327	ALA	2.2
1	A	123	CYS	2.1
1	A	433	GLN	2.1
1	A	428	GLU	2.1
1	B	67	ASP	2.0
1	A	454	ASN	2.0

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

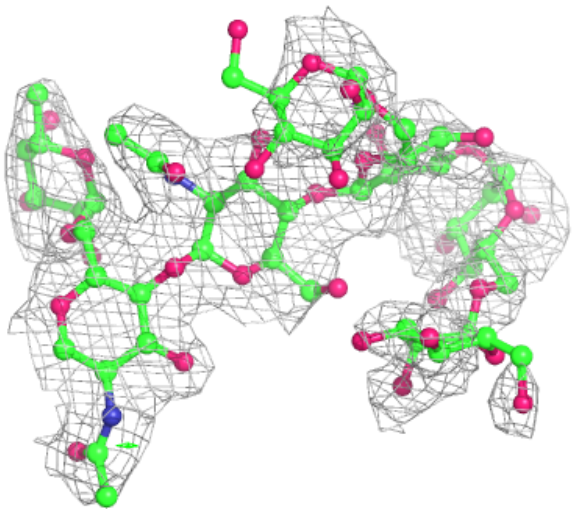
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

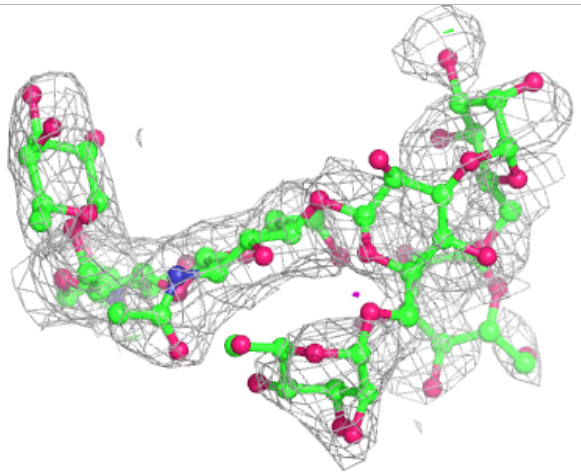
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	J	3	11/12	0.29	0.34	92,104,107,108	0
2	MAN	C	4	11/12	0.36	0.27	89,106,111,114	0
4	FUC	G	3	10/11	0.48	0.24	90,94,100,103	0
2	MAN	C	5	11/12	0.50	0.35	82,94,103,111	0
3	NAG	D	2	14/15	0.52	0.44	95,113,117,120	0
2	BMA	C	3	11/12	0.57	0.26	88,97,104,107	0
5	MAN	H	4	11/12	0.58	0.22	73,85,92,93	0
5	BMA	H	3	11/12	0.60	0.24	64,81,89,92	0
7	MAN	K	4	11/12	0.61	0.19	50,60,66,68	0
3	NAG	D	1	14/15	0.63	0.36	102,112,119,123	0
4	NAG	F	2	14/15	0.67	0.36	82,90,98,99	0
4	NAG	G	2	14/15	0.71	0.23	66,82,89,90	0
7	FUC	K	5	10/11	0.74	0.21	45,51,60,67	0
4	NAG	G	1	14/15	0.78	0.19	58,68,77,81	0
3	NAG	E	1	14/15	0.80	0.15	34,47,59,63	0
3	NAG	E	2	14/15	0.80	0.23	54,69,79,79	0
2	MAN	C	6	11/12	0.80	0.35	89,95,101,107	0
5	NAG	H	2	14/15	0.80	0.17	68,79,87,91	0
6	NAG	J	2	14/15	0.81	0.31	74,88,98,102	0
4	NAG	F	1	14/15	0.83	0.27	65,73,86,87	0
5	NAG	H	1	14/15	0.83	0.18	40,51,59,61	0
7	BMA	K	3	11/12	0.84	0.12	54,57,62,63	0
3	NAG	I	2	14/15	0.84	0.21	68,79,85,92	0
6	NAG	J	1	14/15	0.86	0.23	47,59,67,76	0
5	FUC	H	5	10/11	0.87	0.21	38,48,55,55	0
2	FUC	C	7	10/11	0.87	0.18	63,73,80,87	0
7	NAG	K	1	14/15	0.88	0.12	30,39,51,52	0
3	NAG	I	1	14/15	0.89	0.12	42,53,68,70	0
6	FUC	J	4	10/11	0.90	0.25	49,57,62,66	0
2	NAG	C	1	14/15	0.91	0.12	45,55,62,69	0
2	NAG	C	2	14/15	0.91	0.14	62,73,86,91	0
7	NAG	K	2	14/15	0.94	0.14	39,44,59,60	0
4	FUC	F	3	10/11	0.94	0.31	50,68,74,76	0

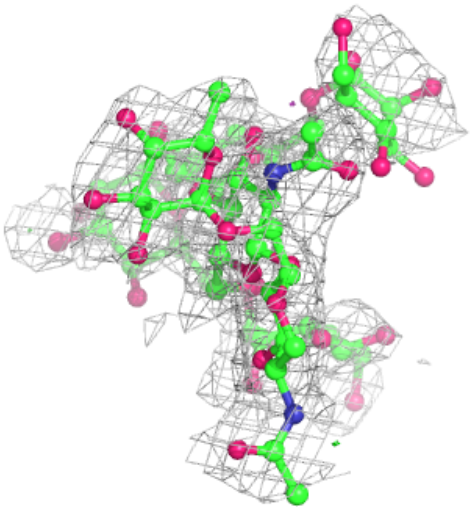
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

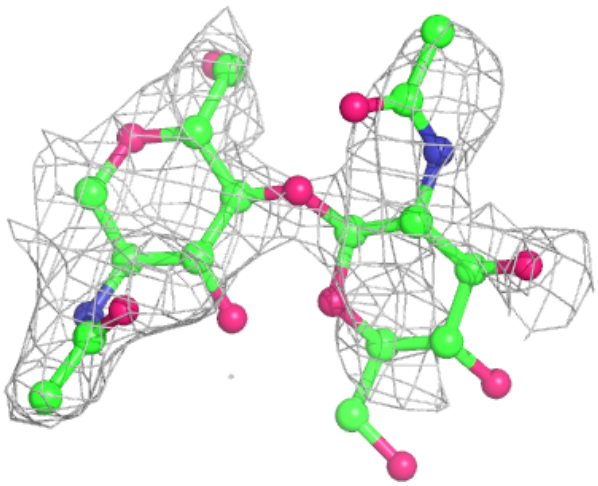


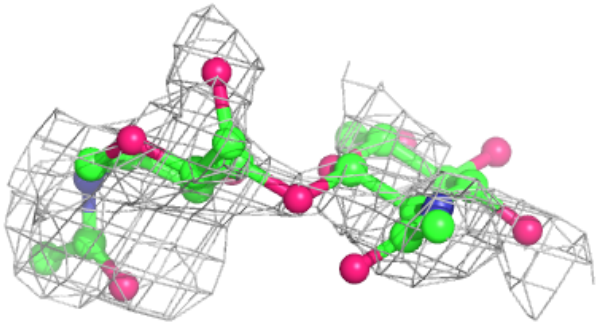


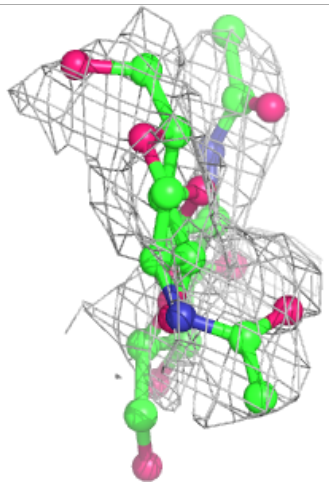


Electron density around Chain D:

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

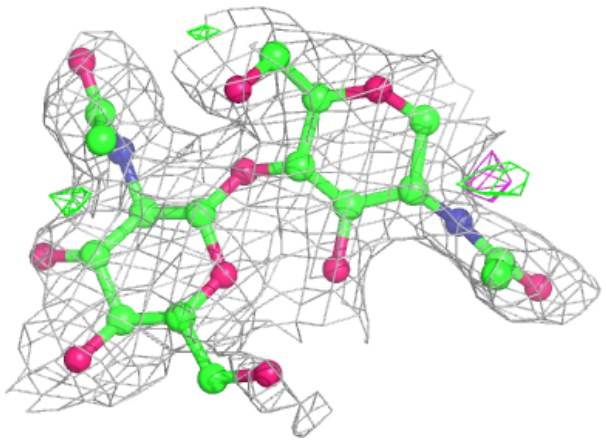


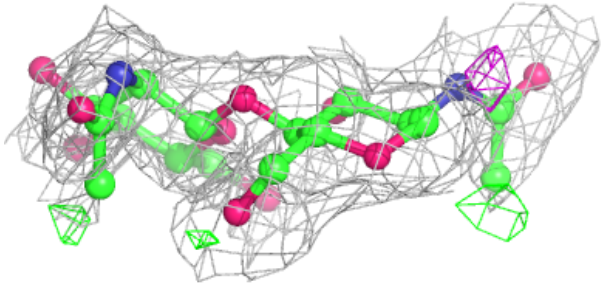


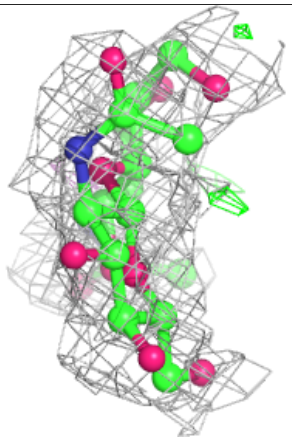


Electron density around Chain E:

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

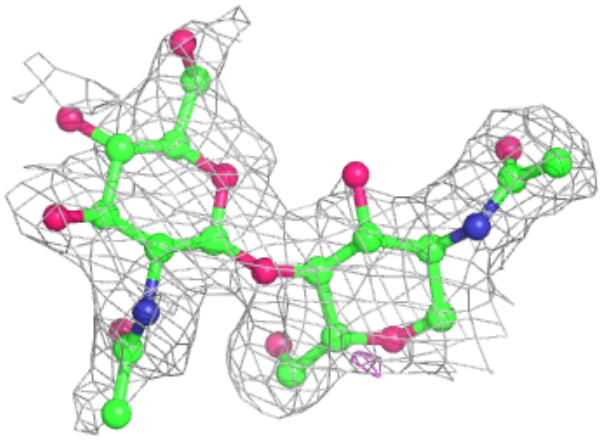


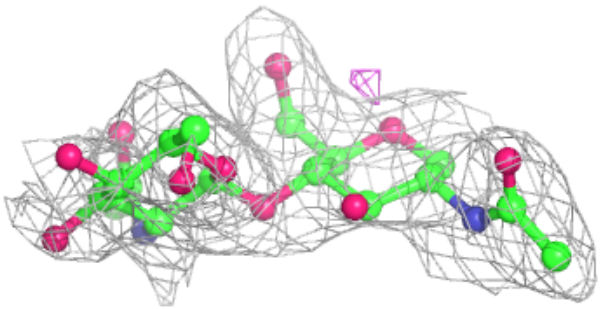


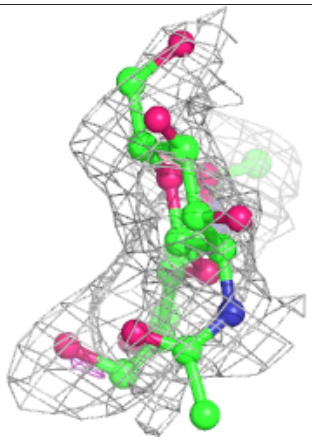


Electron density around Chain I:

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

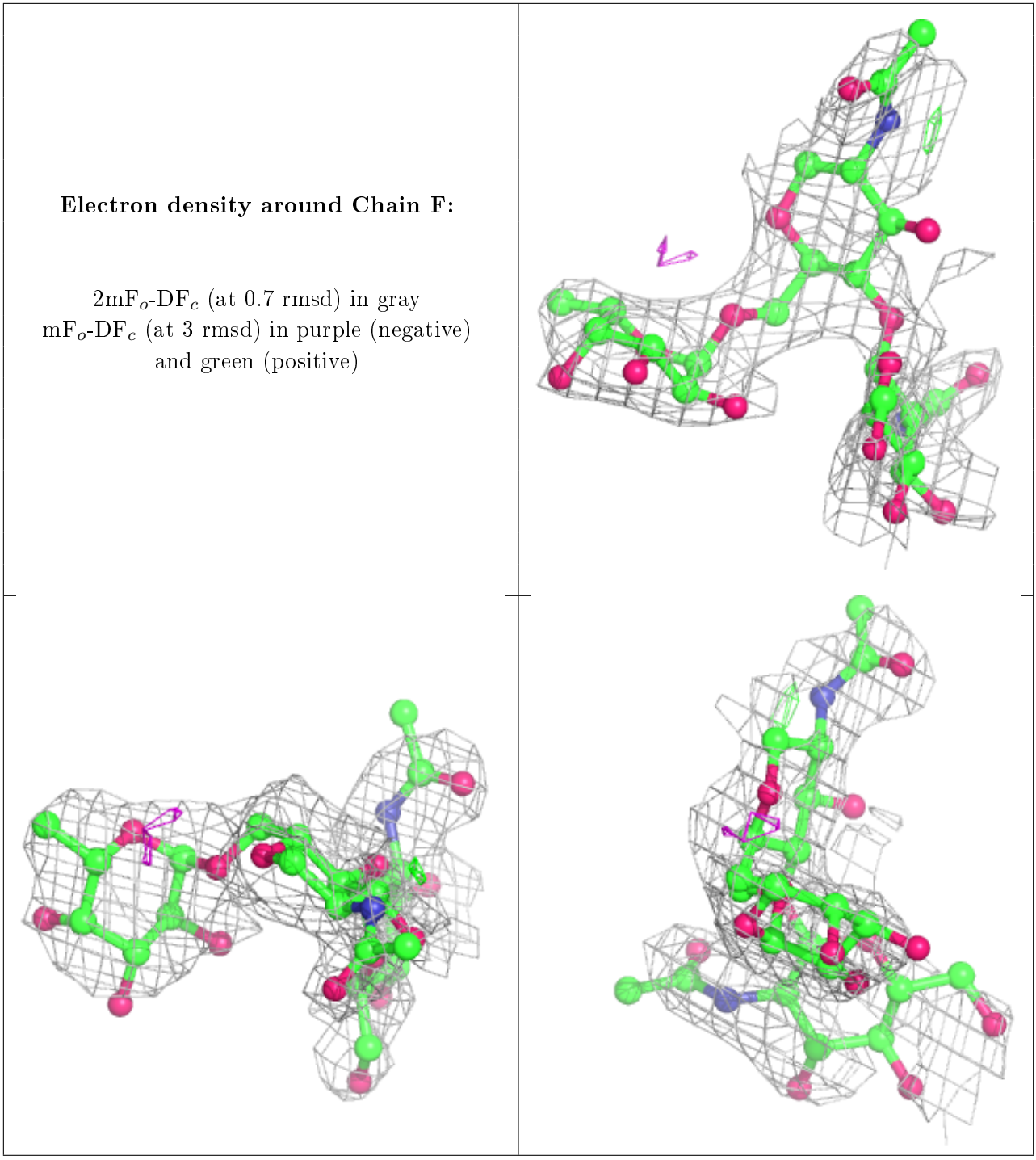






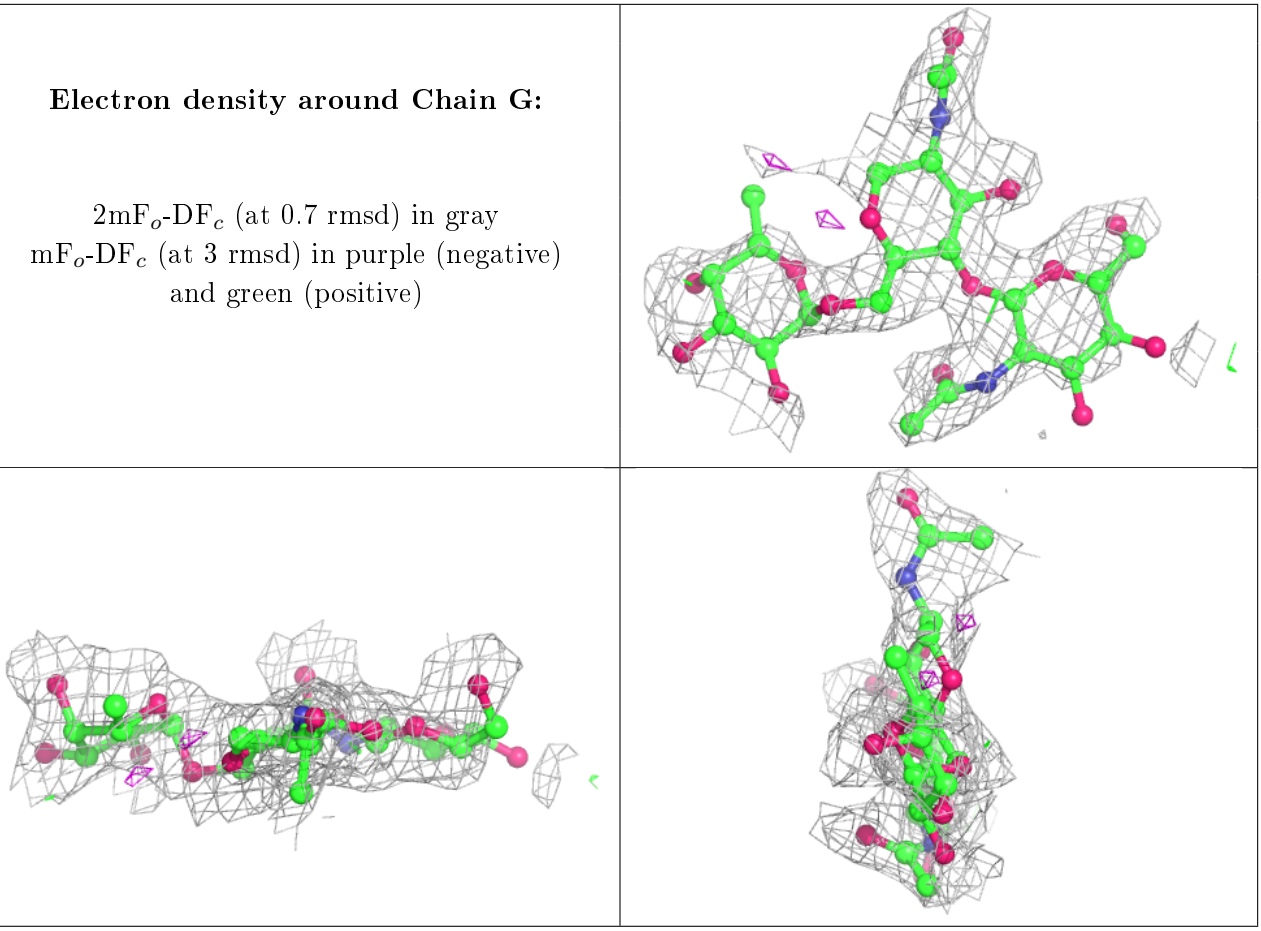
Electron density around Chain F:

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



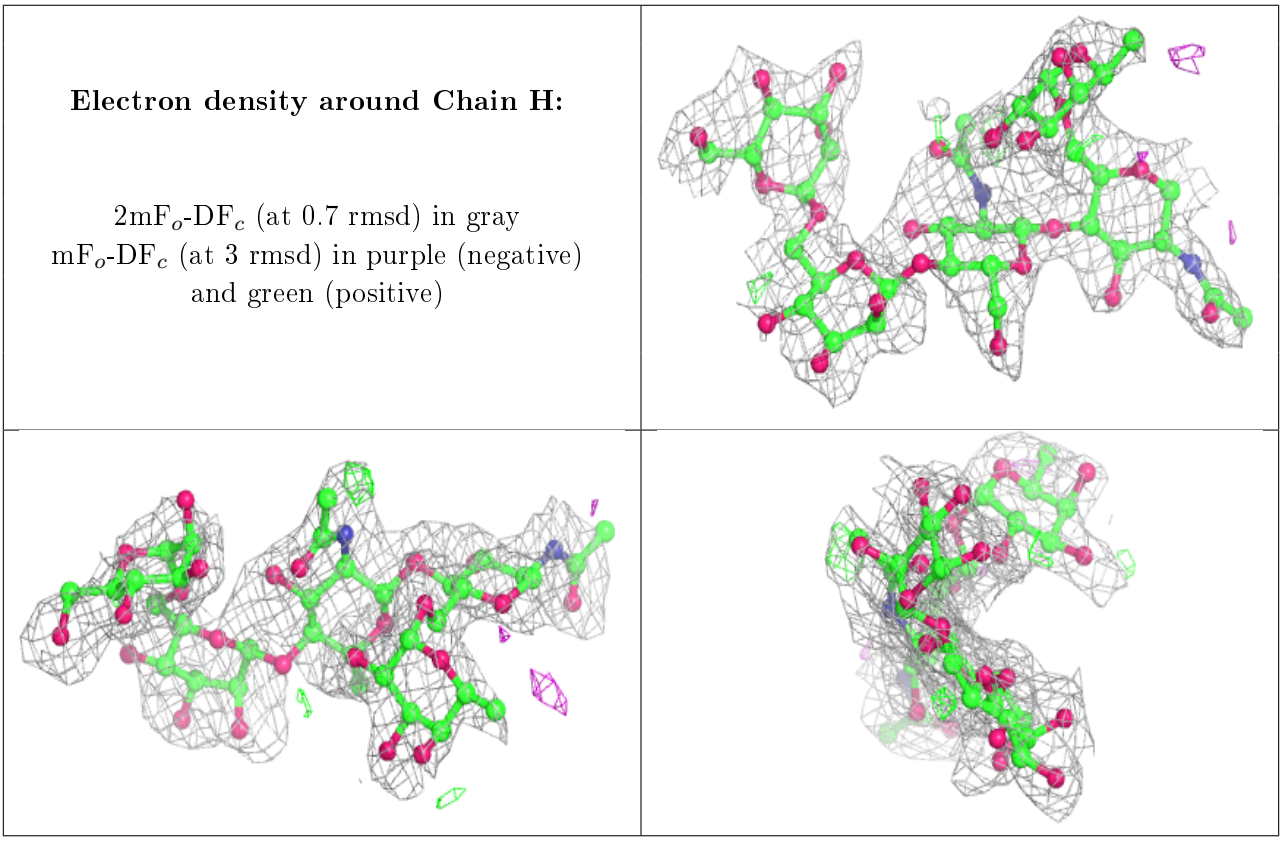
Electron density around Chain G:

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



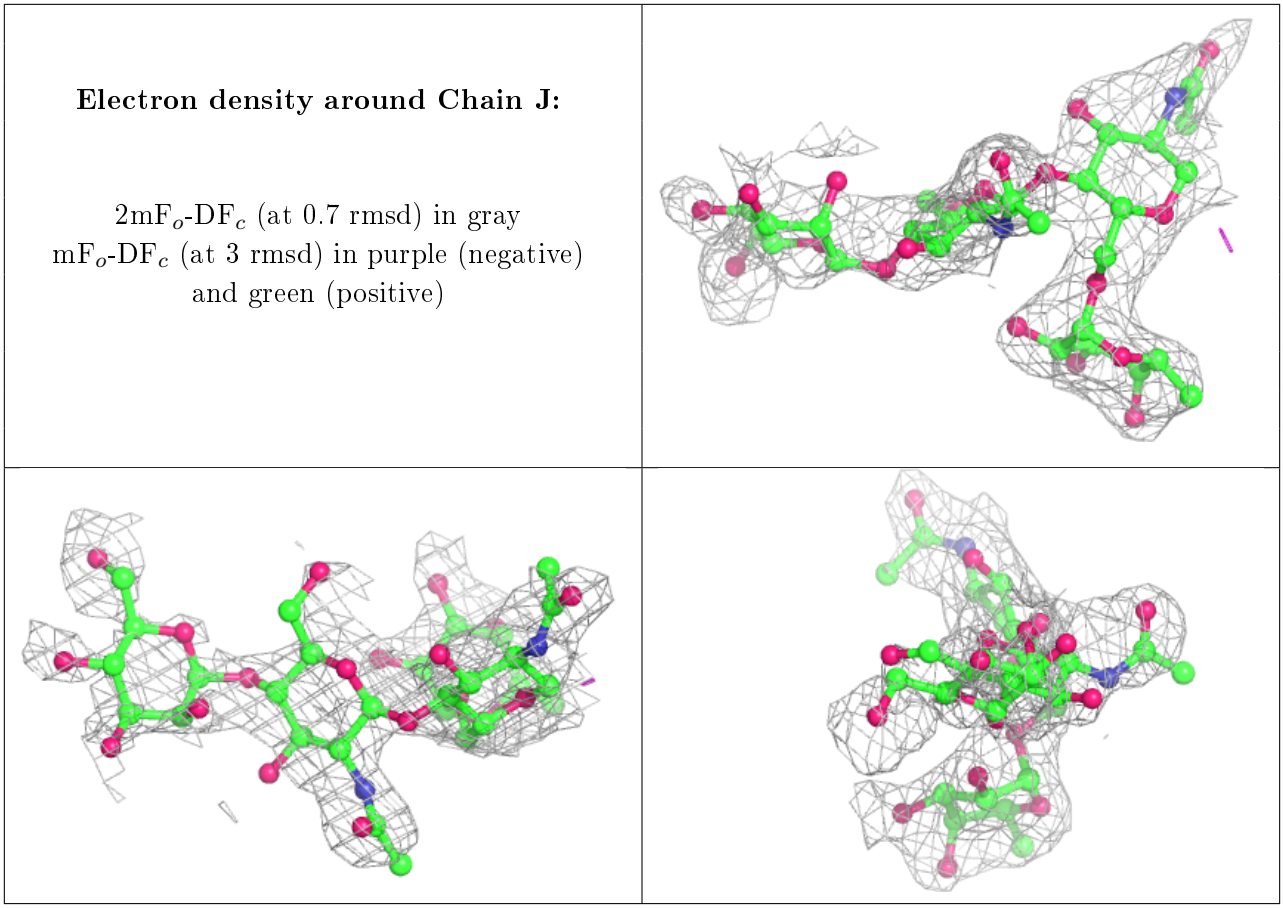
Electron density around Chain H:

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



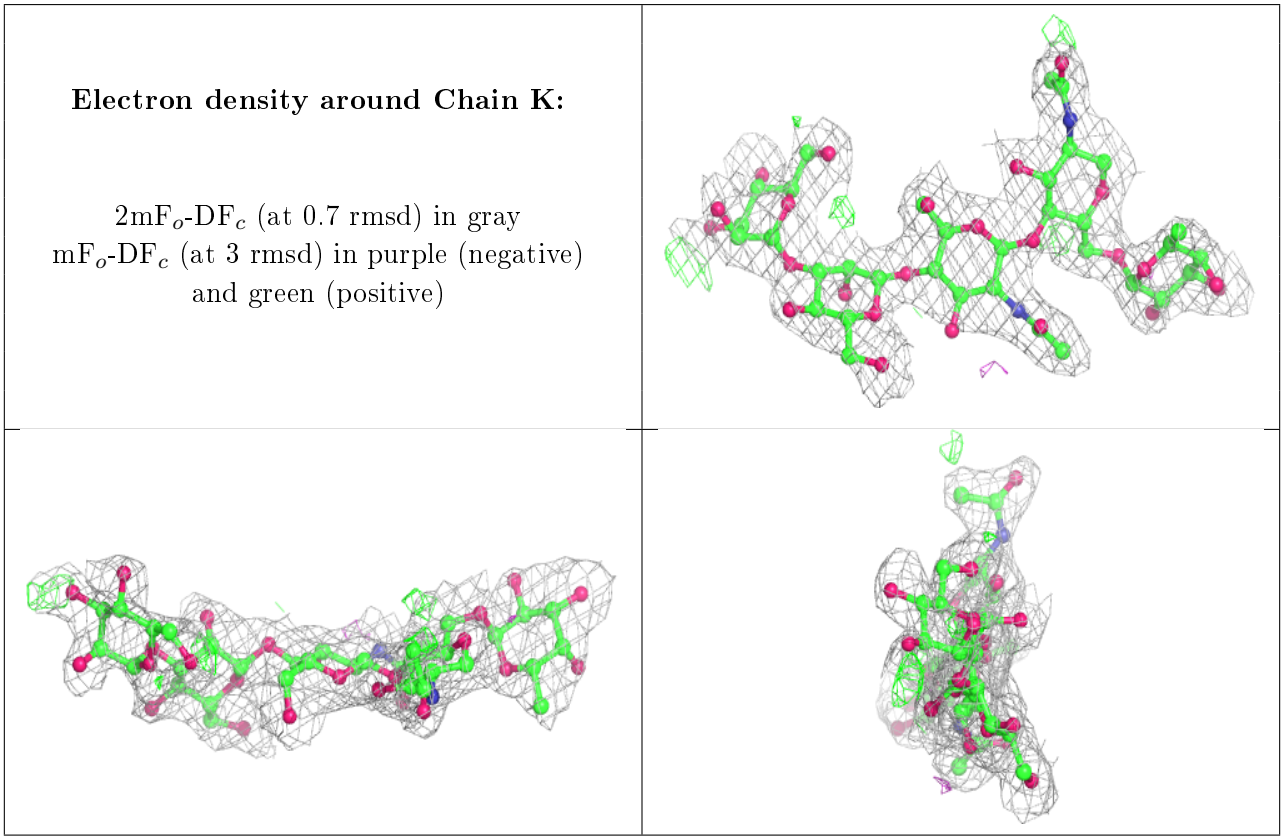
Electron density around Chain J:

$2mF_o$-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 K:

$2mF_o$-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
9	NAG	B	604	14/15	0.63	0.29	60,75,82,90	0
9	NAG	A	604	14/15	0.63	0.28	54,74,91,97	0
9	NAG	A	605	14/15	0.68	0.23	57,74,79,93	0
10	GOL	A	607	6/6	0.69	0.18	43,52,56,59	0
11	PGE	A	614	10/10	0.75	0.18	49,53,58,60	0
10	GOL	B	605	6/6	0.78	0.18	42,45,52,53	0
11	PGE	B	609	10/10	0.79	0.29	38,47,51,62	0
12	PEG	B	612	7/7	0.80	0.17	45,46,51,51	0
12	PEG	A	616	7/7	0.81	0.20	58,58,60,63	0
10	GOL	B	606	6/6	0.83	0.23	40,45,49,52	0
13	MES	B	613	12/12	0.84	0.19	36,51,58,69	25
12	PEG	A	615	7/7	0.84	0.23	43,48,50,54	0
12	PEG	B	611	7/7	0.88	0.36	26,31,39,41	0
11	PGE	A	610	10/10	0.88	0.22	34,40,54,61	0
12	PEG	A	609	7/7	0.89	0.11	31,40,47,50	0
12	PEG	B	608	7/7	0.89	0.14	29,41,43,45	0
10	GOL	A	606	6/6	0.89	0.19	29,39,42,42	0
12	PEG	A	612	7/7	0.91	0.25	25,30,32,34	0
12	PEG	B	607	7/7	0.91	0.24	28,34,37,38	0
12	PEG	A	613	7/7	0.91	0.18	18,36,45,45	0
11	PGE	B	610	10/10	0.92	0.28	31,50,58,65	0
11	PGE	A	608	4/10	0.92	0.12	31,35,38,42	0
12	PEG	A	611	7/7	0.93	0.14	35,36,47,57	0
8	CA	B	603	1/1	0.99	0.10	22,22,22,22	0
8	CA	A	602	1/1	0.99	0.10	17,17,17,17	0
8	CA	A	601	1/1	0.99	0.11	22,22,22,22	0
8	CA	B	602	1/1	0.99	0.12	22,22,22,22	0
8	CA	A	603	1/1	1.00	0.09	13,13,13,13	0
8	CA	B	601	1/1	1.00	0.11	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.