Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 11:27 AM EDT

PDB ID	:	6EG1
Title	:	Crystal structure of Dpr2 Ig1-Ig2 in complex with DIP-Theta Ig1-Ig3
Authors	:	Cosmanescu, F.; Patel, S.; Shapiro, L.
Deposited on	:	2018-08-17
Resolution	:	2.95 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:

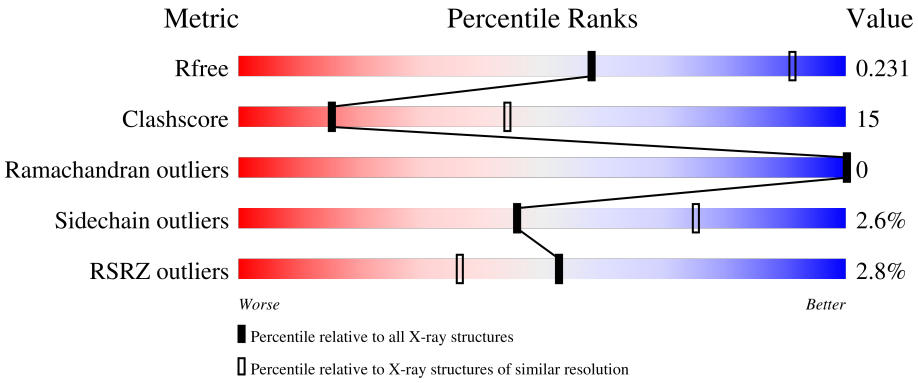
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	231	3% 74% 21% 5%
1	C	231	5% 66% 27% • 5%
2	B	302	% 68% 28% • •
2	D	302	3% 69% 28% • •
3	E	3	100%

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Mol	Chain	Length	Quality of chain
3	I	3	33% 67%
3	J	3	33% 33% 33%
3	K	3	100%
3	N	3	67% 33%
4	F	5	60% 40%
4	L	5	40% 60%
5	G	4	75% 25%
5	M	4	100%
6	H	2	100%
7	O	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	D	505	-	-	-	X
3	NAG	E	2	-	-	-	X
3	NAG	J	2	-	-	-	X
3	FUC	J	3	-	-	-	X
3	NAG	K	2	-	-	-	X
3	FUC	N	3	-	-	-	X
7	NAG	O	1	-	-	-	X
7	NAG	O	2	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 8685 atoms, of which 20 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 Defective proboscis extension response 2, isoform F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1724	1091	301	324	8			
1	C	219	Total	C	N	O	S	0	0	0
			1701	1075	298	320	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	-	expression tag	UNP Q59DZ4
A	102	SER	-	expression tag	UNP Q59DZ4
A	324	HIS	-	expression tag	UNP Q59DZ4
A	325	HIS	-	expression tag	UNP Q59DZ4
A	326	HIS	-	expression tag	UNP Q59DZ4
A	327	HIS	-	expression tag	UNP Q59DZ4
A	328	HIS	-	expression tag	UNP Q59DZ4
A	329	HIS	-	expression tag	UNP Q59DZ4
A	330	HIS	-	expression tag	UNP Q59DZ4
A	331	HIS	-	expression tag	UNP Q59DZ4
C	101	GLY	-	expression tag	UNP Q59DZ4
C	102	SER	-	expression tag	UNP Q59DZ4
C	324	HIS	-	expression tag	UNP Q59DZ4
C	325	HIS	-	expression tag	UNP Q59DZ4
C	326	HIS	-	expression tag	UNP Q59DZ4
C	327	HIS	-	expression tag	UNP Q59DZ4
C	328	HIS	-	expression tag	UNP Q59DZ4
C	329	HIS	-	expression tag	UNP Q59DZ4
C	330	HIS	-	expression tag	UNP Q59DZ4
C	331	HIS	-	expression tag	UNP Q59DZ4

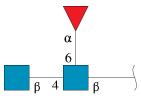
- Molecule 2 is a protein called Dpr-interacting protein theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	295	Total	C	N	O	S	0	0	0
			2327	1485	396	431	15			
2	D	295	Total	C	N	O	S	0	1	0
			2333	1489	397	432	15			

There are 12 discrepancies between the modelled and reference sequences:

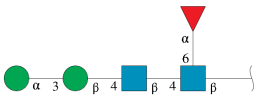
Chain	Residue	Modelled	Actual	Comment	Reference
B	424	HIS	-	expression tag	UNP Q9VMN6
B	425	HIS	-	expression tag	UNP Q9VMN6
B	426	HIS	-	expression tag	UNP Q9VMN6
B	427	HIS	-	expression tag	UNP Q9VMN6
B	428	HIS	-	expression tag	UNP Q9VMN6
B	429	HIS	-	expression tag	UNP Q9VMN6
D	424	HIS	-	expression tag	UNP Q9VMN6
D	425	HIS	-	expression tag	UNP Q9VMN6
D	426	HIS	-	expression tag	UNP Q9VMN6
D	427	HIS	-	expression tag	UNP Q9VMN6
D	428	HIS	-	expression tag	UNP Q9VMN6
D	429	HIS	-	expression tag	UNP Q9VMN6

- Molecule 3 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.



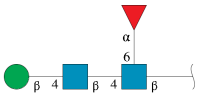
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	N	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 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
4	F	5	Total	C	N	O	0	0	0
			60	34	2	24			
4	L	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 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
5	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

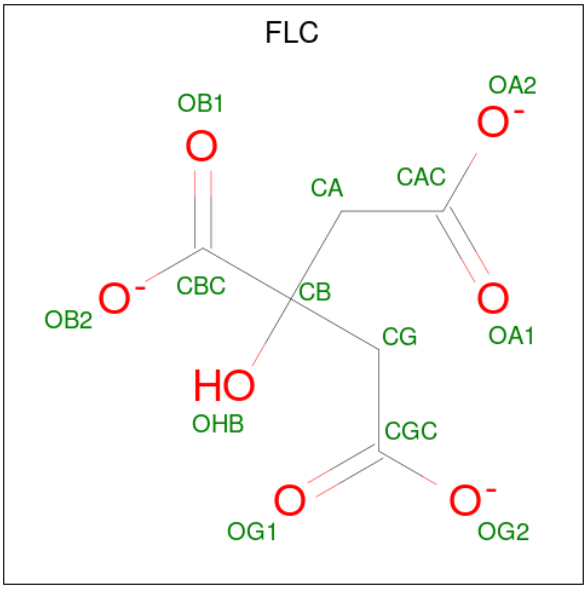
- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

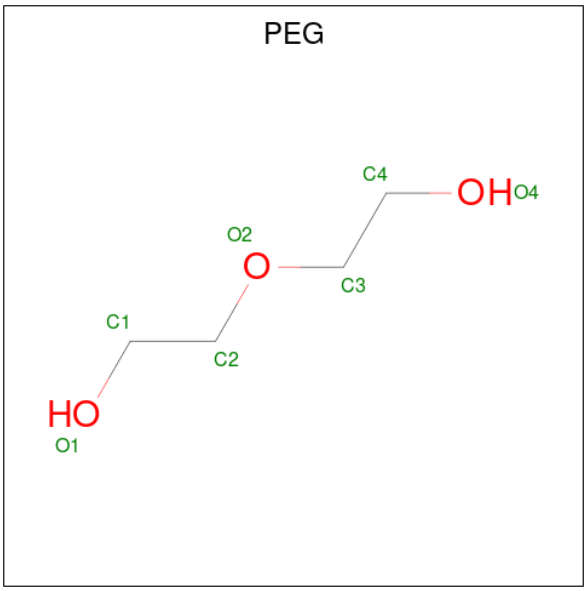
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	O	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



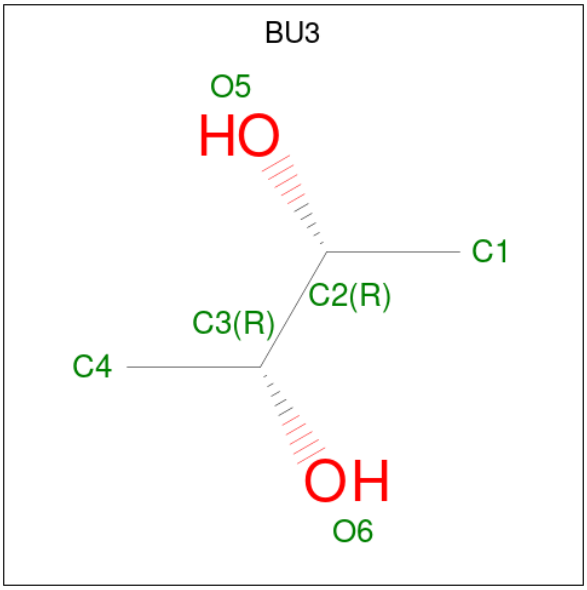
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 13 6 7	0	0
8	C	1	Total C O 13 6 7	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



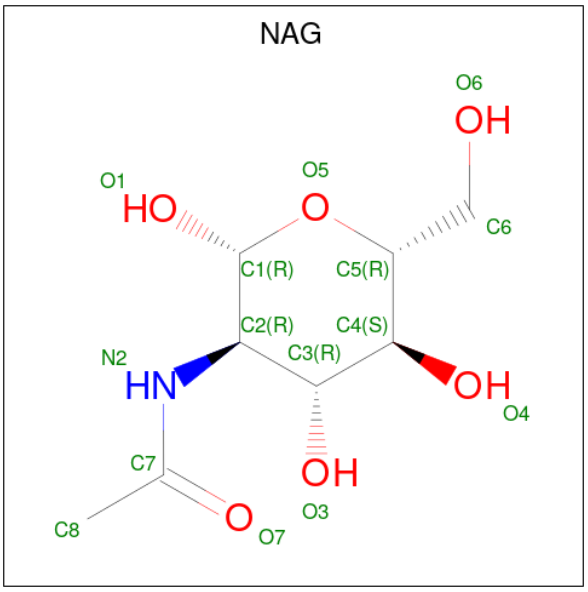
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0

- Molecule 10 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C H O 16 4 10 2	0	0
10	C	1	Total C H O 16 4 10 2	0	0

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



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

- Molecule 12 is water.

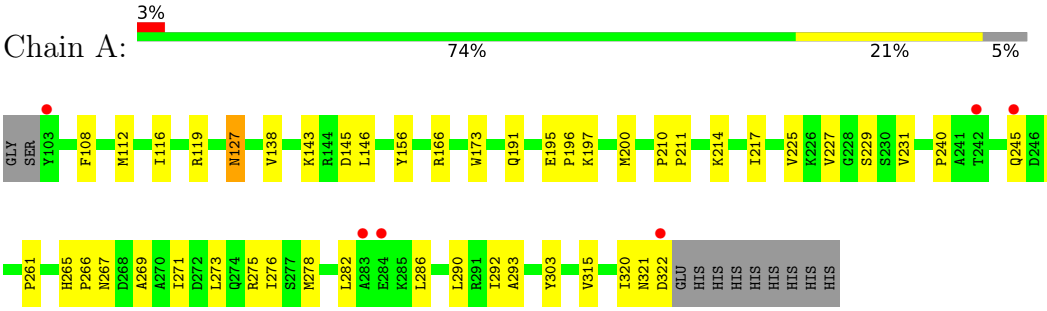
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	12	Total O 12 12	0	0
12	B	16	Total O 16 16	0	0
12	C	10	Total O 10 10	0	0
12	D	16	Total O 16 16	0	0

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.

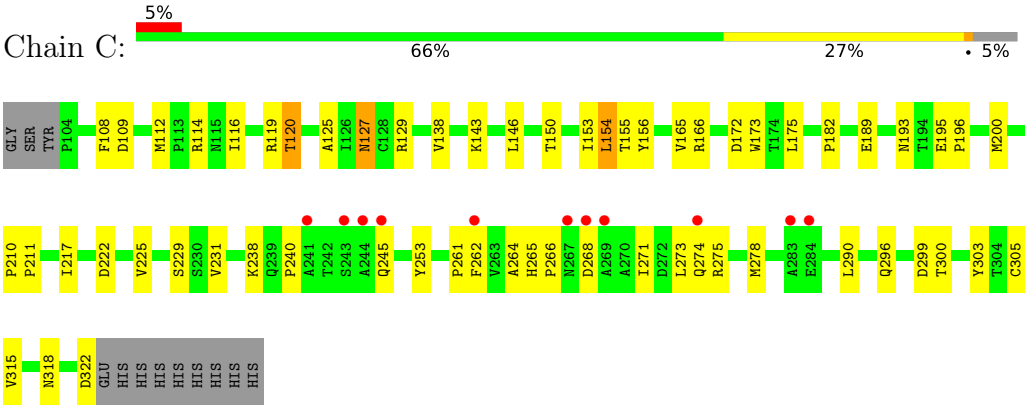
• Molecule 1: Defective proboscis extension response 2, isoform F

Chain A:



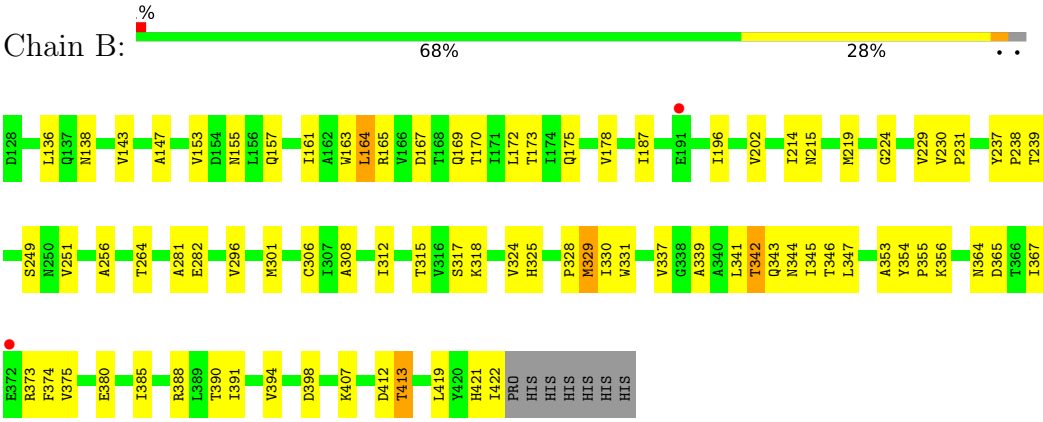
• Molecule 1: Defective proboscis extension response 2, isoform F

Chain C:



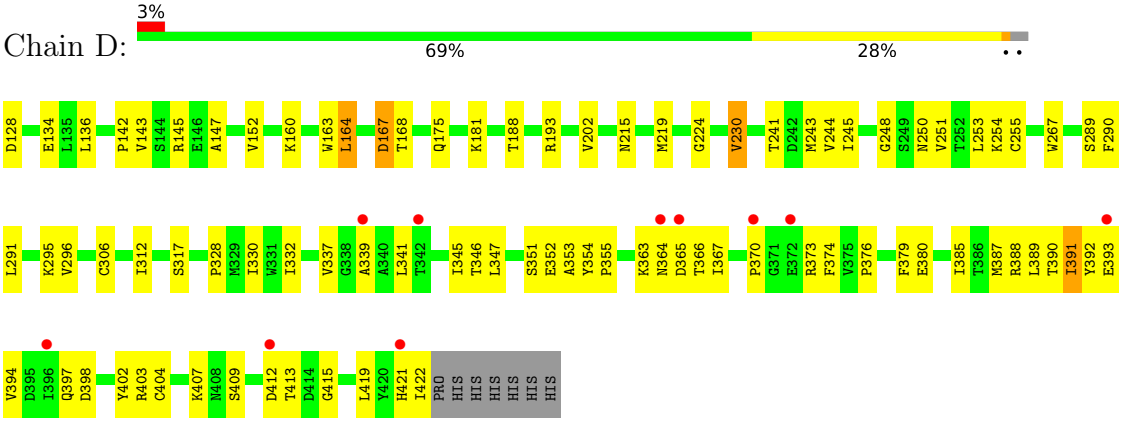
• Molecule 2: Dpr-interacting protein theta

Chain B:



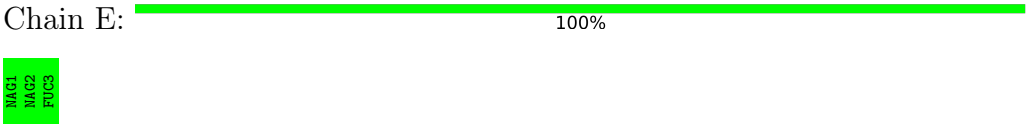
• Molecule 2: Dpr-interacting protein theta

Chain D:



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

Chain E:

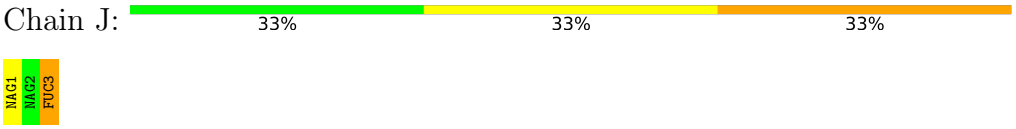


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

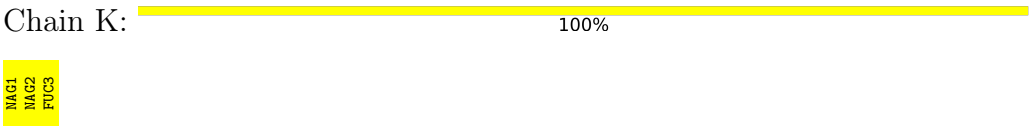
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:



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

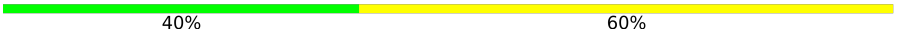
Chain N:

• Molecule 4: 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 F:

• Molecule 4: 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 L:

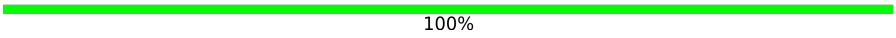


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

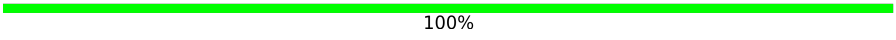
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



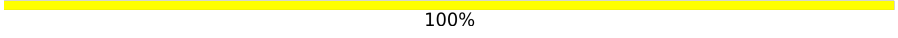
• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.77Å 120.91Å 144.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.95 19.96 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.95) 99.6 (19.96-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.93Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.178 , 0.231 0.178 , 0.231	Depositor DCC
R_{free} test set	1978 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8685	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: NAG, FUC, FLC, MAN, PEG, BU3, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/1769	0.48	0/2418
1	C	0.27	0/1739	0.48	0/2375
2	B	0.26	0/2378	0.46	0/3241
2	D	0.26	0/2387	0.47	0/3253
All	All	0.26	0/8273	0.47	0/11287

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	1724	0	1726	40	0
1	C	1701	0	1704	61	0
2	B	2327	0	2343	76	0
2	D	2333	0	2351	79	0
3	E	38	0	34	0	0
3	I	38	0	34	1	0
3	J	38	0	34	1	0
3	K	38	0	34	2	0
3	N	38	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	60	0	52	1	0
4	L	60	0	52	1	0
5	G	49	0	43	2	0
5	M	49	0	43	0	0
6	H	24	0	22	0	0
7	O	28	0	25	2	0
8	C	26	0	10	3	0
9	C	7	0	10	0	0
9	D	7	0	10	0	0
10	C	12	20	20	2	0
11	D	14	0	13	1	0
12	A	12	0	0	1	0
12	B	16	0	0	1	0
12	C	10	0	0	0	0
12	D	16	0	0	0	0
All	All	8665	20	8594	257	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 15.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:HG21	2:B:318:LYS:HD3	1.63	0.81
2:D:363:LYS:O	2:D:366:THR:HG22	1.82	0.79
2:B:143:VAL:CG2	2:B:230:VAL:HG22	2.13	0.79
2:D:407:LYS:HG3	2:D:412:ASP:HB3	1.66	0.77
1:C:154:LEU:HD23	1:C:154:LEU:H	1.50	0.76
2:D:370:PRO:HB3	2:D:376:PRO:HD2	1.67	0.75
1:C:264:ALA:HB1	1:C:268:ASP:OD2	1.86	0.75
1:C:273:LEU:HD12	1:C:273:LEU:H	1.52	0.74
2:D:332:ILE:HD11	2:D:415:GLY:HA3	1.68	0.74
2:B:143:VAL:HG21	2:B:230:VAL:HG22	1.69	0.74
1:A:225:VAL:CG2	1:A:229:SER:HB2	2.19	0.73
2:D:394:VAL:HG23	2:D:398:ASP:HB2	1.71	0.72
1:C:271:ILE:H	1:C:271:ILE:HD12	1.55	0.71
2:B:343:GLN:O	2:B:394:VAL:HG23	1.90	0.71
1:C:119:ARG:HH12	1:C:210:PRO:HD2	1.54	0.70
2:D:391:ILE:HD13	2:D:391:ILE:H	1.58	0.67
2:D:346:THR:OG1	2:D:390:THR:HG22	1.94	0.67
2:D:373:ARG:NH2	2:D:398:ASP:OD2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LEU:HA	2:B:172:LEU:HG	1.77	0.66
1:A:112:MET:CE	1:A:127[A]:ASN:HB2	2.26	0.66
1:A:278:MET:HG3	1:A:290:LEU:HD12	1.78	0.66
1:C:108:PHE:HB3	1:C:200:MET:HE2	1.78	0.65
2:B:229:VAL:HB	2:B:312:ILE:HG12	1.77	0.65
1:C:265:HIS:N	1:C:266:PRO:HA	2.10	0.65
2:D:160:LYS:HG2	2:D:175[B]:GLN:CG	2.25	0.65
2:D:339:ALA:HA	2:D:422:ILE:HD11	1.77	0.64
1:A:247:ILE:HD12	1:A:286:LEU:HD22	1.80	0.64
2:D:341:LEU:HD21	2:D:421:HIS:NE2	2.13	0.64
1:A:227:VAL:HG23	1:A:320:ILE:O	1.98	0.64
1:C:120:THR:CG2	1:C:182:PRO:HD3	2.28	0.63
1:A:217:ILE:HG21	1:A:315:VAL:HG21	1.79	0.63
1:C:275:ARG:NH2	1:C:299:ASP:OD2	2.31	0.63
2:B:341:LEU:O	2:B:342:THR:HG22	1.99	0.63
1:A:195:GLU:OE2	1:A:196:PRO:HA	1.99	0.62
2:B:245:ILE:HG12	2:B:251:VAL:HB	1.80	0.62
1:C:275:ARG:HH21	1:C:296:GLN:HG2	1.64	0.62
1:C:312:ALA:HB3	4:L:2:NAG:H81	1.81	0.62
1:C:273:LEU:O	1:C:274:GLN:HG2	1.99	0.62
2:B:308:ALA:O	2:B:315:THR:HG23	2.01	0.61
1:A:247:ILE:HG13	1:A:282:LEU:HD11	1.84	0.60
1:C:225:VAL:CG1	1:C:229:SER:HB2	2.32	0.60
1:C:238:LYS:NZ	8:C:409:FLC:HG1	2.16	0.60
1:C:217:ILE:HG21	1:C:315:VAL:HG21	1.84	0.59
1:C:225:VAL:HG21	1:C:231:VAL:HG22	1.84	0.59
2:D:160:LYS:HG2	2:D:175[B]:GLN:HG3	1.84	0.59
1:C:108:PHE:HB3	1:C:200:MET:CE	2.32	0.59
2:D:367:ILE:H	2:D:367:ILE:HD12	1.68	0.59
1:A:143:LYS:HG3	2:B:169:GLN:OE1	2.03	0.59
2:D:245:ILE:HD11	2:D:296:VAL:HG21	1.85	0.59
2:B:244:VAL:C	2:B:245:ILE:HD12	2.24	0.58
1:C:217:ILE:HD12	1:C:315:VAL:HG23	1.86	0.58
2:D:363:LYS:HZ2	2:D:398:ASP:HA	1.68	0.58
2:B:153:VAL:HG21	2:B:161:ILE:CD1	2.33	0.58
2:D:328:PRO:HA	2:D:353:ALA:HB2	1.85	0.58
1:C:305:CYS:O	1:C:307:PRO:HD3	2.04	0.58
2:B:147:ALA:HB2	2:B:202:VAL:HG11	1.85	0.58
2:B:337:VAL:O	2:B:419:LEU:HA	2.04	0.58
2:D:354:TYR:HA	2:D:355:PRO:C	2.24	0.58
1:A:112:MET:HE2	1:A:127[A]:ASN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG21	10:C:413:BU3:H42	1.84	0.58
2:B:138:ASN:HD22	5:G:1:NAG:H83	1.68	0.58
1:C:193:ASN:O	2:D:181:LYS:HG2	2.04	0.57
1:C:116:ILE:N	1:C:116:ILE:HD12	2.19	0.57
2:D:243:MET:HE1	2:D:253:LEU:HD23	1.86	0.57
2:B:330:ILE:HG13	2:B:413:THR:CG2	2.34	0.57
2:B:407:LYS:HG3	2:B:412:ASP:HB3	1.86	0.57
2:B:173:THR:HG22	2:B:178:VAL:HA	1.87	0.56
2:D:142:PRO:HG2	2:D:145:ARG:HG3	1.87	0.56
1:C:300:THR:HG23	1:C:318:ASN:HA	1.86	0.56
2:D:391:ILE:O	2:D:391:ILE:HG12	2.05	0.56
2:B:136:LEU:HD23	2:B:224:GLY:N	2.20	0.56
3:N:2:NAG:O3	3:N:2:NAG:H82	2.05	0.56
2:B:153:VAL:HG21	2:B:161:ILE:HD11	1.88	0.56
3:J:1:NAG:H62	3:J:3:FUC:O2	2.05	0.55
2:B:354:TYR:HA	2:B:355:PRO:C	2.25	0.55
1:C:120:THR:HG21	1:C:182:PRO:HD3	1.88	0.55
2:D:374:PHE:CD1	2:D:391:ILE:HG22	2.41	0.55
2:D:394:VAL:HG23	2:D:398:ASP:CB	2.36	0.55
2:D:392:TYR:CD1	7:O:1:NAG:H62	2.42	0.55
2:D:402:TYR:O	2:D:403:ARG:HG3	2.07	0.55
1:C:156:TYR:CE2	2:D:215:ASN:HB3	2.42	0.54
1:C:211:PRO:CB	1:C:240:PRO:HG2	2.38	0.54
2:B:341:LEU:HD22	2:B:341:LEU:H	1.73	0.54
2:B:346:THR:CG2	2:B:390:THR:HG23	2.38	0.54
2:B:161:ILE:CD1	2:B:214:ILE:HG12	2.38	0.54
2:D:245:ILE:HD13	2:D:251:VAL:HB	1.89	0.54
1:A:156:TYR:CZ	2:B:215:ASN:HB3	2.42	0.53
1:A:217:ILE:HD12	1:A:315:VAL:HG23	1.90	0.53
1:C:165:VAL:HG21	10:C:413:BU3:C4	2.39	0.53
2:D:134:GLU:HG2	2:D:152:VAL:HG21	1.89	0.53
2:D:330:ILE:HD13	2:D:351:SER:HB3	1.88	0.53
1:A:261:PRO:HD3	1:A:273:LEU:HD21	1.89	0.53
1:A:278:MET:CG	1:A:290:LEU:HD12	2.39	0.53
1:C:278:MET:HG2	1:C:290:LEU:HD12	1.89	0.53
2:D:164:LEU:N	2:D:164:LEU:HD23	2.24	0.52
1:C:245:GLN:OE1	1:C:245:GLN:HA	2.09	0.52
2:D:374:PHE:HD1	2:D:391:ILE:HG22	1.74	0.52
2:D:363:LYS:NZ	2:D:398:ASP:HA	2.24	0.52
2:B:325:HIS:CD2	2:B:355:PRO:HD3	2.45	0.52
2:B:367:ILE:HG13	2:B:368:ILE:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:CG	1:C:200:MET:HE2	2.44	0.51
1:C:146:LEU:N	1:C:146:LEU:HD12	2.25	0.51
2:D:367:ILE:HD12	2:D:367:ILE:N	2.26	0.51
2:B:249:SER:O	2:B:296:VAL:HG23	2.11	0.51
2:D:363:LYS:HD2	2:D:402:TYR:CE1	2.46	0.51
2:D:145:ARG:O	2:D:202:VAL:HG23	2.11	0.50
2:D:330:ILE:HD13	2:D:351:SER:CB	2.41	0.50
2:D:394:VAL:CG2	2:D:398:ASP:HB2	2.40	0.50
1:A:217:ILE:HG21	1:A:315:VAL:CG2	2.42	0.50
1:C:225:VAL:HG13	1:C:229:SER:HB2	1.94	0.50
1:C:112:MET:CE	1:C:127:ASN:HB3	2.42	0.49
1:A:116:ILE:N	1:A:116:ILE:HD12	2.26	0.49
2:D:255:CYS:O	2:D:289:SER:HB2	2.12	0.49
2:B:243:MET:HA	2:B:243:MET:CE	2.43	0.49
2:B:375:VAL:HG23	2:B:390:THR:HB	1.93	0.49
2:B:238:PRO:HD2	2:B:256:ALA:HB3	1.95	0.49
2:B:346:THR:HG22	2:B:390:THR:HG23	1.95	0.49
1:C:271:ILE:O	1:C:273:LEU:HD12	2.12	0.49
2:D:255:CYS:HB2	2:D:267:TRP:CZ2	2.46	0.49
1:A:321:ASN:O	1:A:322:ASP:HB2	2.12	0.49
2:B:374:PHE:HD1	2:B:391:ILE:HG12	1.77	0.49
2:D:241:THR:O	2:D:243:MET:HG3	2.13	0.48
2:B:339:ALA:C	2:B:422:ILE:HD13	2.33	0.48
1:C:156:TYR:CZ	2:D:215:ASN:HB3	2.48	0.48
2:D:147:ALA:HB2	2:D:202:VAL:HG21	1.95	0.48
1:C:108:PHE:CB	1:C:200:MET:HE2	2.42	0.48
1:C:153:ILE:HD12	1:C:154:LEU:N	2.28	0.48
2:D:345:ILE:HG23	2:D:391:ILE:HD11	1.95	0.48
2:D:254:LYS:HG2	2:D:290:PHE:CD2	2.49	0.48
1:C:143:LYS:HZ1	1:C:189:GLU:CD	2.18	0.48
1:C:264:ALA:CB	1:C:268:ASP:OD2	2.57	0.48
2:B:341:LEU:HD22	2:B:341:LEU:N	2.29	0.47
1:A:217:ILE:CD1	1:A:315:VAL:HG23	2.45	0.47
1:A:275:ARG:HB3	1:A:293:ALA:O	2.13	0.47
2:D:387:MET:SD	2:D:404:CYS:HB2	2.55	0.47
2:B:373:ARG:NH2	2:B:398:ASP:OD2	2.48	0.47
2:B:375:VAL:CG2	2:B:390:THR:HB	2.45	0.47
2:D:143:VAL:HG21	2:D:230:VAL:HB	1.95	0.47
1:A:211:PRO:CB	1:A:240:PRO:HG2	2.44	0.47
2:B:356:LYS:HD3	2:B:380:GLU:OE1	2.15	0.47
2:B:164:LEU:HD23	2:B:164:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:ARG:HH12	2:D:397:GLN:HE21	1.63	0.47
1:A:108:PHE:CG	1:A:200:MET:HE2	2.49	0.46
1:A:276:ILE:HG12	1:A:292:ILE:HG12	1.97	0.46
2:D:152:VAL:HA	2:D:193:ARG:O	2.15	0.46
2:D:330:ILE:CD1	2:D:351:SER:HB3	2.45	0.46
1:C:166:ARG:HD3	1:C:173:TRP:CH2	2.49	0.46
2:B:375:VAL:HG23	2:B:375:VAL:O	2.15	0.46
1:C:138:VAL:HG21	1:C:173:TRP:CD1	2.50	0.46
1:A:247:ILE:CD1	1:A:286:LEU:HD22	2.44	0.46
1:C:238:LYS:HZ1	8:C:409:FLC:HA2	1.79	0.46
2:B:238:PRO:HD2	2:B:256:ALA:CB	2.45	0.46
2:D:248:GLY:O	2:D:295:LYS:HA	2.16	0.46
1:A:108:PHE:HB3	1:A:200:MET:CE	2.46	0.46
2:B:371:GLY:C	2:B:373:ARG:H	2.20	0.46
1:A:247:ILE:HG21	1:A:282:LEU:HD12	1.96	0.46
2:B:374:PHE:CD1	2:B:391:ILE:HG12	2.51	0.46
2:D:175[B]:GLN:OE1	2:D:175[B]:GLN:HA	2.16	0.46
2:D:380:GLU:HG2	2:D:385:ILE:HG12	1.96	0.45
2:B:175:GLN:HA	2:B:175:GLN:OE1	2.17	0.45
2:D:379:PHE:HE2	2:D:388:ARG:HD2	1.82	0.45
1:C:150:THR:HG22	1:C:155:THR:HA	1.99	0.45
2:D:306:CYS:O	2:D:317:SER:HA	2.16	0.45
1:A:245:GLN:CD	1:A:245:GLN:H	2.20	0.45
2:B:325:HIS:CG	2:B:355:PRO:HD3	2.51	0.45
1:C:127:ASN:HD21	1:C:172:ASP:HB3	1.80	0.45
3:I:1:NAG:H62	3:I:3:FUC:H2	1.60	0.45
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.80	0.45
1:C:253:TYR:O	1:C:303:TYR:HA	2.17	0.45
2:B:346:THR:HG22	2:B:390:THR:OG1	2.17	0.45
2:B:281:ALA:O	2:B:282:GLU:HG2	2.17	0.45
2:D:136:LEU:HD23	2:D:224:GLY:N	2.32	0.45
1:C:120:THR:HG22	1:C:182:PRO:HD3	1.97	0.44
2:D:312:ILE:N	2:D:312:ILE:HD12	2.30	0.44
2:B:243:MET:HA	2:B:243:MET:HE2	1.98	0.44
1:C:119:ARG:NH1	1:C:210:PRO:HD2	2.28	0.44
1:C:210:PRO:HB2	1:C:211:PRO:CD	2.47	0.44
2:D:254:LYS:HG2	2:D:290:PHE:HD2	1.82	0.44
1:A:108:PHE:HB3	1:A:200:MET:HE2	1.98	0.44
2:D:244:VAL:HG13	2:D:244:VAL:O	2.18	0.44
2:D:341:LEU:N	2:D:341:LEU:HD22	2.33	0.44
1:A:254:ARG:NH2	1:A:271:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:VAL:O	2:D:419:LEU:HD12	2.18	0.43
1:C:271:ILE:HD12	1:C:271:ILE:N	2.29	0.43
2:D:160:LYS:HB3	2:D:175[B]:GLN:HG2	2.00	0.43
2:D:250:ASN:ND2	11:D:505:NAG:H83	2.34	0.43
1:C:205:ASN:HD22	3:K:3:FUC:H63	1.83	0.43
7:O:1:NAG:H61	7:O:2:NAG:C7	2.48	0.43
1:A:119:ARG:HH12	1:A:210:PRO:HD2	1.84	0.43
1:A:253:TYR:O	1:A:303:TYR:HA	2.19	0.43
2:B:239:THR:CG2	2:B:318:LYS:HD3	2.43	0.43
2:D:364:ASN:O	2:D:365:ASP:HB2	2.19	0.43
1:C:238:LYS:HZ1	8:C:409:FLC:HG1	1.84	0.43
1:C:114:ARG:NH2	1:C:200:MET:HG2	2.34	0.43
2:D:245:ILE:HD11	2:D:296:VAL:CG2	2.47	0.43
2:B:369:VAL:HG13	2:B:370:PRO:HD2	2.00	0.42
1:A:112:MET:CE	1:A:127[B]:ASN:HB3	2.49	0.42
3:K:1:NAG:H61	3:K:2:NAG:C7	2.48	0.42
2:B:138:ASN:ND2	5:G:1:NAG:H83	2.31	0.42
2:B:155:ASN:O	2:B:157:GLN:HG3	2.19	0.42
2:B:380:GLU:HG2	2:B:385:ILE:HG12	2.01	0.42
2:D:347:LEU:HD12	2:D:347:LEU:N	2.34	0.42
1:A:145:ASP:O	1:A:146:LEU:HB2	2.20	0.42
2:B:306:CYS:O	2:B:317:SER:HA	2.19	0.42
2:B:337:VAL:O	2:B:419:LEU:HD12	2.18	0.42
2:D:253:LEU:HD12	2:D:291:LEU:HD23	2.01	0.42
2:D:254:LYS:HD3	2:D:290:PHE:HE2	1.85	0.42
1:A:265:HIS:HA	1:A:266:PRO:HA	1.65	0.42
2:B:165:ARG:HD3	12:B:606:HOH:O	2.19	0.42
2:D:167:ASP:OD2	2:D:168:THR:HG23	2.20	0.42
2:B:328:PRO:HA	2:B:353:ALA:HB2	2.01	0.42
2:B:346:THR:HG22	2:B:390:THR:CB	2.50	0.42
1:C:120:THR:HG23	1:C:206:VAL:HG12	2.01	0.42
1:C:195:GLU:HA	1:C:196:PRO:HA	1.79	0.42
2:D:341:LEU:HD21	2:D:421:HIS:CE1	2.54	0.42
2:B:346:THR:HG22	2:B:390:THR:HA	2.01	0.42
1:C:125:ALA:HA	1:C:175:LEU:O	2.20	0.42
1:C:322:ASP:OD1	1:C:322:ASP:N	2.53	0.42
1:A:166:ARG:HD3	1:A:173:TRP:CH2	2.55	0.42
2:B:143:VAL:HG23	2:B:229:VAL:O	2.20	0.42
2:B:187:ILE:HD12	2:B:196:ILE:O	2.20	0.42
2:B:312:ILE:HD12	2:B:312:ILE:N	2.35	0.42
2:B:364:ASN:O	2:B:365:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:PRO:HA	2:D:352:GLU:O	2.19	0.42
1:A:225:VAL:HG11	1:A:231:VAL:HG21	2.02	0.41
2:B:164:LEU:HB2	2:B:170:THR:O	2.21	0.41
2:B:231:PRO:HA	2:B:312:ILE:HG22	2.02	0.41
2:B:136:LEU:HD11	2:B:163:TRP:HH2	1.85	0.41
2:B:244:VAL:O	2:B:245:ILE:HD12	2.19	0.41
2:B:345:ILE:HD12	2:B:345:ILE:HA	1.90	0.41
1:A:267:ASN:OD1	1:A:269:ALA:N	2.52	0.41
2:B:329:MET:HE2	2:B:331:TRP:CH2	2.55	0.41
1:C:109:ASP:HB3	1:C:129:ARG:HB3	2.02	0.41
2:D:181:LYS:HA	2:D:181:LYS:HD2	1.83	0.41
2:D:392:TYR:C	2:D:393:GLU:HG3	2.40	0.41
1:A:211:PRO:HB2	1:A:240:PRO:HG2	2.03	0.41
2:B:342:THR:O	2:B:342:THR:HG23	2.19	0.41
2:B:356:LYS:HD3	2:B:380:GLU:CD	2.41	0.41
2:D:330:ILE:HG12	2:D:413:THR:CG2	2.51	0.41
2:B:343:GLN:HG2	2:B:344:ASN:N	2.36	0.41
2:B:347:LEU:O	2:B:388:ARG:HA	2.21	0.41
1:C:209:THR:HA	1:C:210:PRO:HA	1.91	0.41
2:D:136:LEU:HD11	2:D:163:TRP:HH2	1.86	0.41
4:F:1:NAG:O7	4:F:1:NAG:H3	2.20	0.41
1:C:182:PRO:HG3	1:C:208:VAL:CG1	2.51	0.41
2:D:328:PRO:CA	2:D:353:ALA:HB2	2.49	0.41
2:D:346:THR:HA	2:D:389:LEU:O	2.20	0.41
1:A:138:VAL:HA	1:A:191:GLN:O	2.20	0.41
2:D:339:ALA:HA	2:D:422:ILE:CD1	2.48	0.41
2:B:301:MET:HB2	2:B:324:VAL:HG23	2.04	0.40
2:D:345:ILE:CG2	2:D:391:ILE:HD11	2.50	0.40
1:C:261:PRO:O	1:C:262:PHE:HB2	2.21	0.40
2:D:341:LEU:HA	2:D:394:VAL:O	2.21	0.40
2:B:173:THR:HG22	2:B:178:VAL:HG22	2.02	0.40
2:B:421:HIS:HD2	2:B:422:ILE:H	1.69	0.40
1:A:214:LYS:HE3	12:A:504:HOH:O	2.21	0.40
1:C:210:PRO:HB2	1:C:211:PRO:HD2	2.02	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	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
1	C	217/231 (94%)	206 (95%)	11 (5%)	0	100	100
2	B	293/302 (97%)	269 (92%)	24 (8%)	0	100	100
2	D	294/302 (97%)	273 (93%)	21 (7%)	0	100	100
All	All	1024/1066 (96%)	958 (94%)	66 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	192/200 (96%)	189 (98%)	3 (2%)	62	84
1	C	189/200 (94%)	185 (98%)	4 (2%)	53	80
2	B	260/267 (97%)	251 (96%)	9 (4%)	36	68
2	D	261/267 (98%)	253 (97%)	8 (3%)	40	71
All	All	902/934 (97%)	878 (97%)	24 (3%)	46	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127[A]	ASN
1	A	127[B]	ASN

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Mol	Chain	Res	Type
1	A	197	LYS
2	B	164	LEU
2	B	167	ASP
2	B	219	MET
2	B	237	TYR
2	B	243	MET
2	B	264	THR
2	B	329	MET
2	B	342	THR
2	B	413	THR
1	C	120	THR
1	C	127	ASN
1	C	154	LEU
1	C	222	ASP
2	D	128	ASP
2	D	164	LEU
2	D	167	ASP
2	D	188	THR
2	D	219	MET
2	D	230	VAL
2	D	391	ILE
2	D	409	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	421	HIS
2	D	222	GLN
2	D	325	HIS
2	D	397	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)

37 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	FUC	E	3	3	10,10,11	0.82	0	14,14,16	0.82	0
4	NAG	F	1	1,4	14,14,15	0.49	0	17,19,21	0.71	0
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.55	0
4	BMA	F	3	4	11,11,12	0.61	0	15,15,17	0.74	0
4	MAN	F	4	4	11,11,12	0.73	0	15,15,17	0.93	2 (13%)
4	FUC	F	5	4	10,10,11	0.71	0	14,14,16	0.92	0
5	NAG	G	1	2,5	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	G	2	5	14,14,15	0.28	0	17,19,21	0.58	0
5	BMA	G	3	5	11,11,12	0.52	0	15,15,17	0.71	0
5	FUC	G	4	5	10,10,11	0.63	0	14,14,16	0.74	0
6	NAG	H	1	2,6	14,14,15	0.28	0	17,19,21	0.44	0
6	FUC	H	2	6	10,10,11	0.87	0	14,14,16	0.86	0
3	NAG	I	1	3,2	14,14,15	0.32	0	17,19,21	0.45	0
3	NAG	I	2	3	14,14,15	0.32	0	17,19,21	0.42	0
3	FUC	I	3	3	10,10,11	0.70	0	14,14,16	0.76	0
3	NAG	J	1	3,2	14,14,15	0.27	0	17,19,21	0.39	0
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	FUC	J	3	3	10,10,11	0.97	1 (10%)	14,14,16	1.05	1 (7%)
3	NAG	K	1	1,3	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.47	0
3	FUC	K	3	3	10,10,11	0.83	0	14,14,16	0.85	0
4	NAG	L	1	1,4	14,14,15	0.50	0	17,19,21	0.68	0
4	NAG	L	2	4	14,14,15	0.19	0	17,19,21	0.65	0
4	BMA	L	3	4	11,11,12	0.68	0	15,15,17	0.91	0
4	MAN	L	4	4	11,11,12	0.94	1 (9%)	15,15,17	0.86	1 (6%)
4	FUC	L	5	4	10,10,11	1.10	1 (10%)	14,14,16	0.91	1 (7%)
5	NAG	M	1	2,5	14,14,15	0.54	0	17,19,21	0.47	0
5	NAG	M	2	5	14,14,15	0.41	0	17,19,21	0.43	0
5	BMA	M	3	5	11,11,12	0.58	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FUC	M	4	5	10,10,11	0.67	0	14,14,16	0.86	0
3	NAG	N	1	3,2	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	N	2	3	14,14,15	0.29	0	17,19,21	0.44	0
3	FUC	N	3	3	10,10,11	0.75	0	14,14,16	0.79	0
7	NAG	O	1	2,7	14,14,15	0.31	0	17,19,21	0.52	0
7	NAG	O	2	7	14,14,15	0.28	0	17,19,21	0.50	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	FUC	M	4	5	-	-	0/1/1/1
3	NAG	N	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	FUC	N	3	3	-	-	0/1/1/1
7	NAG	O	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	5	FUC	C1-C2	2.62	1.58	1.52
3	J	3	FUC	C1-C2	2.51	1.57	1.52
4	L	4	MAN	O5-C1	-2.51	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	3	FUC	O2-C2-C1	2.43	114.12	109.15
4	L	5	FUC	O2-C2-C1	2.24	113.73	109.15
4	L	4	MAN	O2-C2-C3	-2.22	105.70	110.14
4	F	4	MAN	C1-O5-C5	2.19	115.16	112.19
4	F	4	MAN	O2-C2-C3	-2.15	105.83	110.14

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6

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

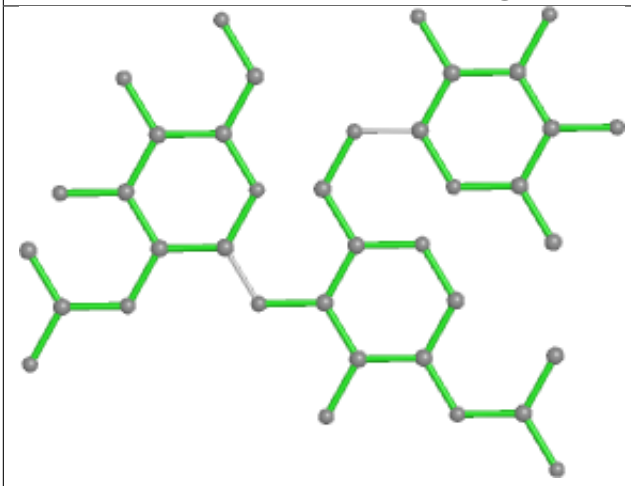
There are no ring outliers.

13 monomers are involved in 11 short contacts:

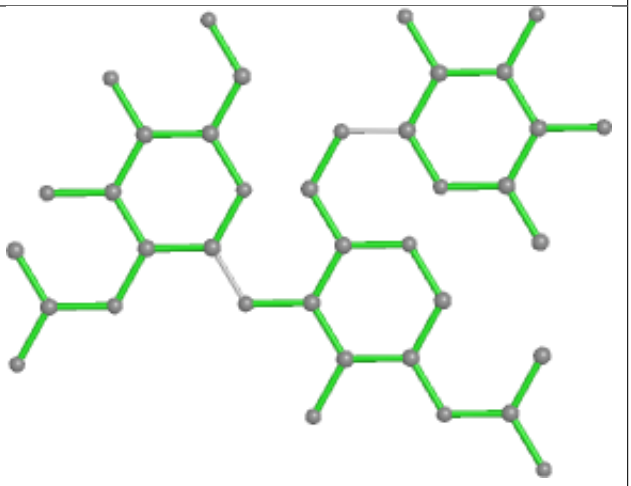
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	2	0
3	K	1	NAG	1	0
4	F	1	NAG	1	0
3	J	3	FUC	1	0
3	I	3	FUC	1	0
3	I	1	NAG	1	0
7	O	1	NAG	2	0
7	O	2	NAG	1	0
3	K	2	NAG	1	0
4	L	2	NAG	1	0
3	J	1	NAG	1	0
3	K	3	FUC	1	0
3	N	2	NAG	1	0

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

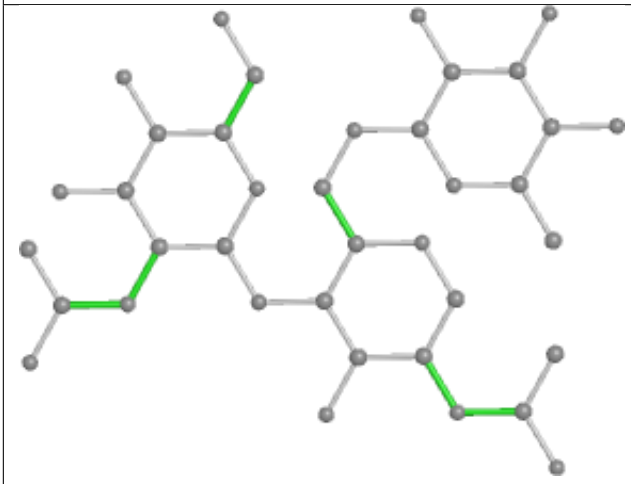
Oligosaccharide Chain E



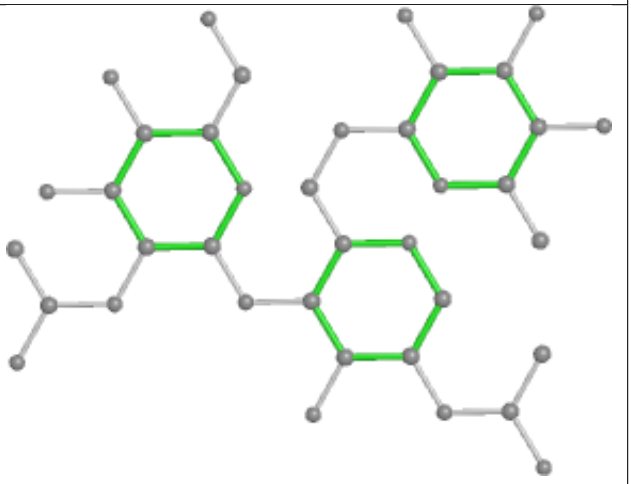
Bond lengths



Bond angles

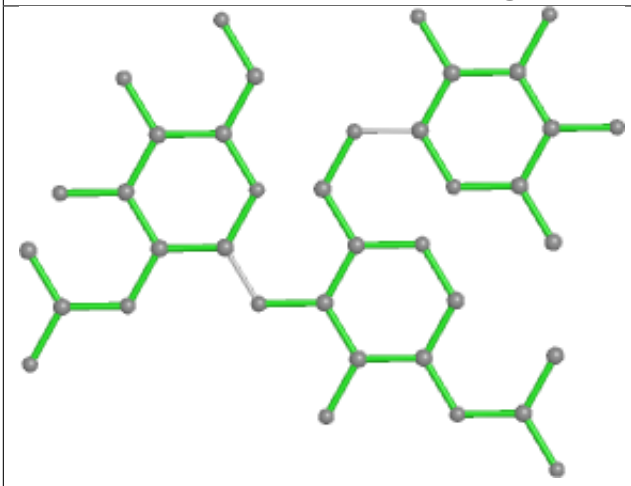


Torsions

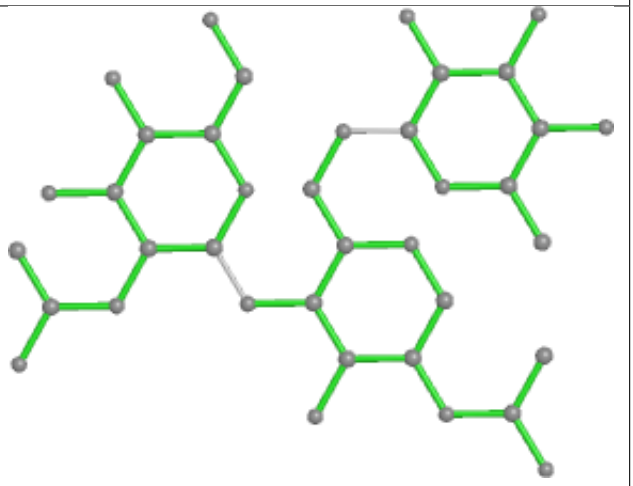


Rings

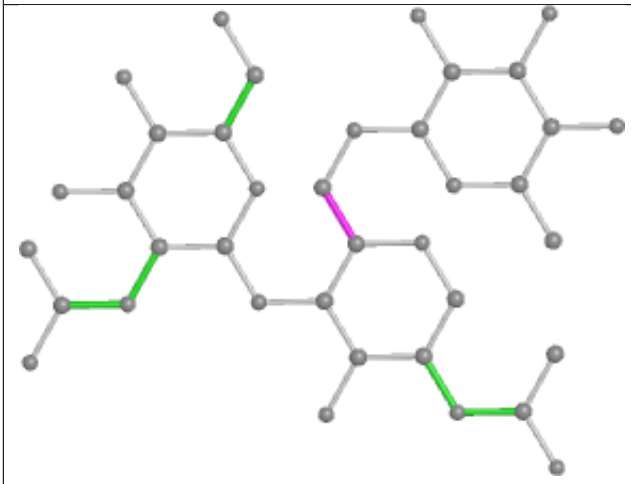
Oligosaccharide Chain I



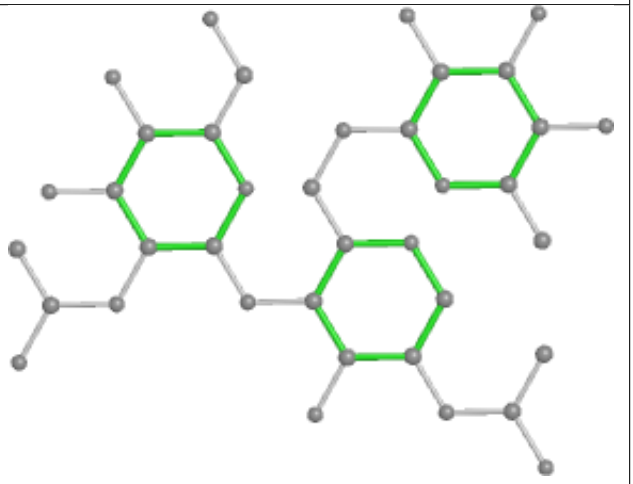
Bond lengths



Bond angles

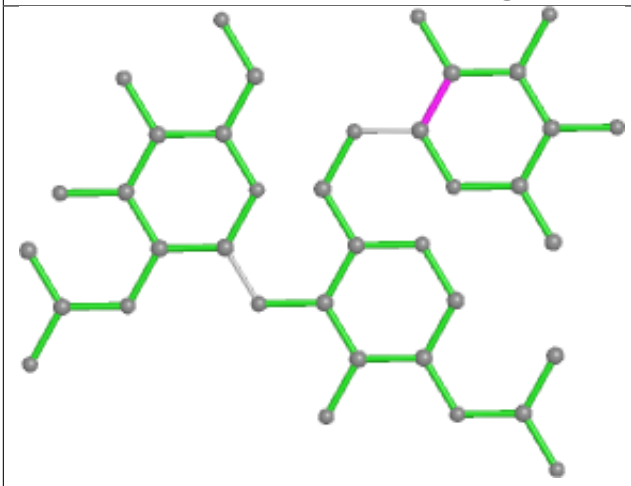


Torsions

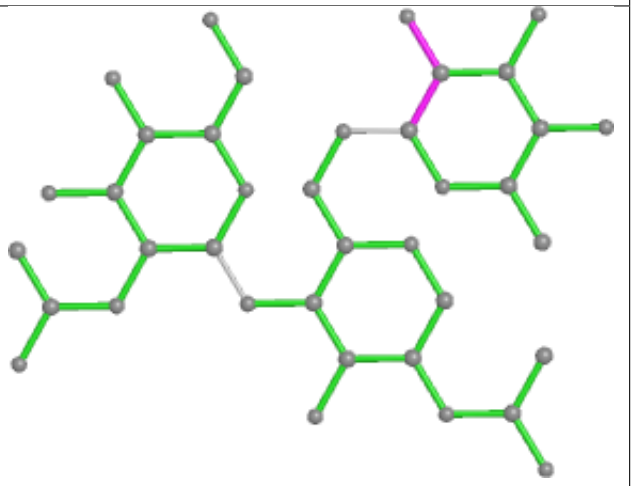


Rings

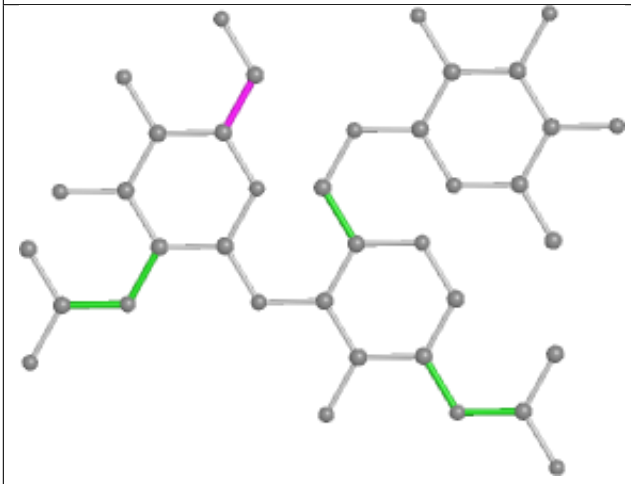
Oligosaccharide Chain J



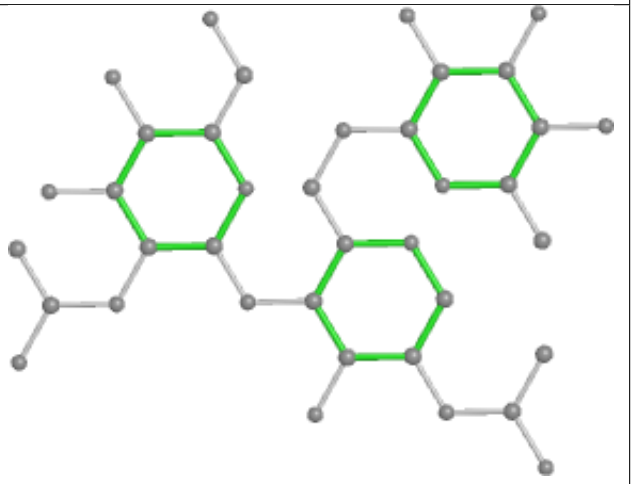
Bond lengths



Bond angles

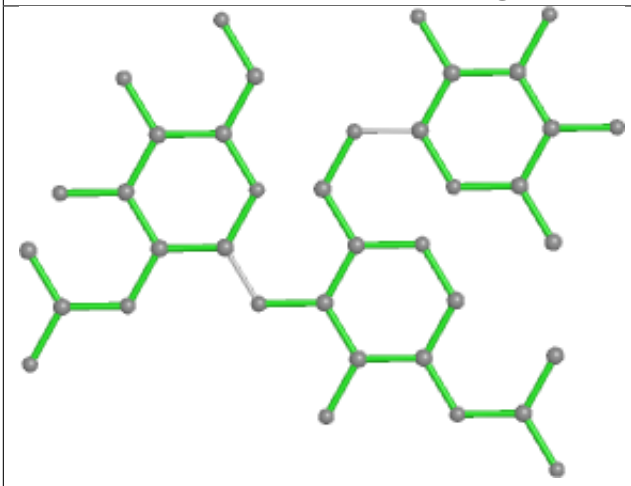


Torsions

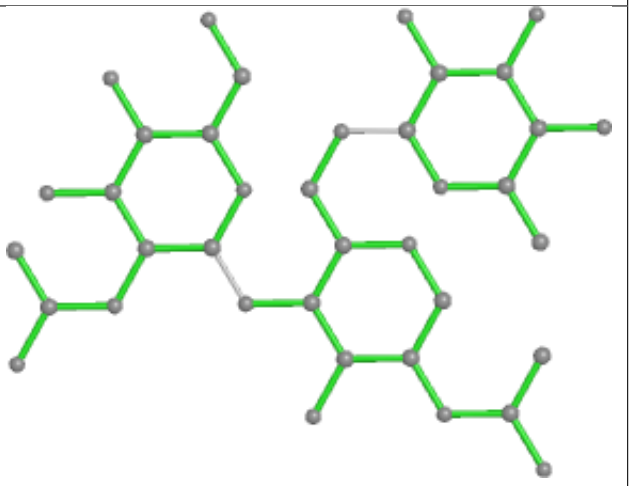


Rings

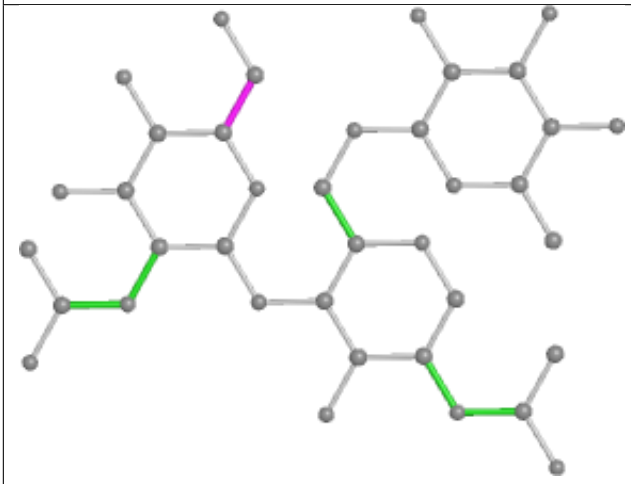
Oligosaccharide Chain K



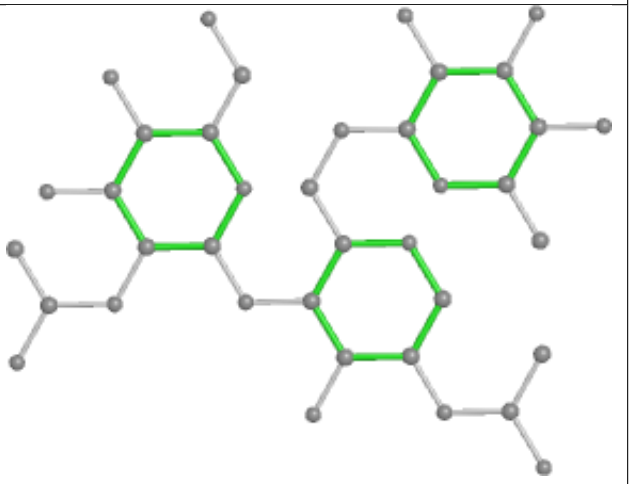
Bond lengths



Bond angles

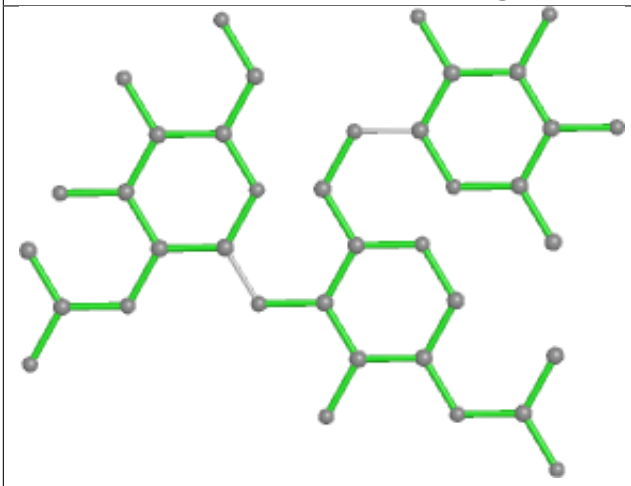


Torsions

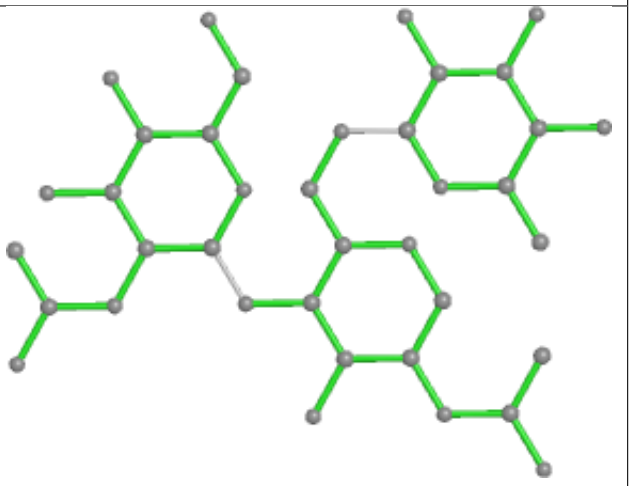


Rings

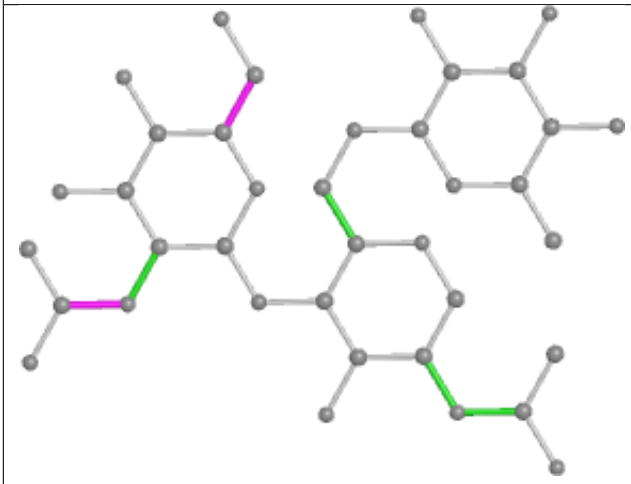
Oligosaccharide Chain N



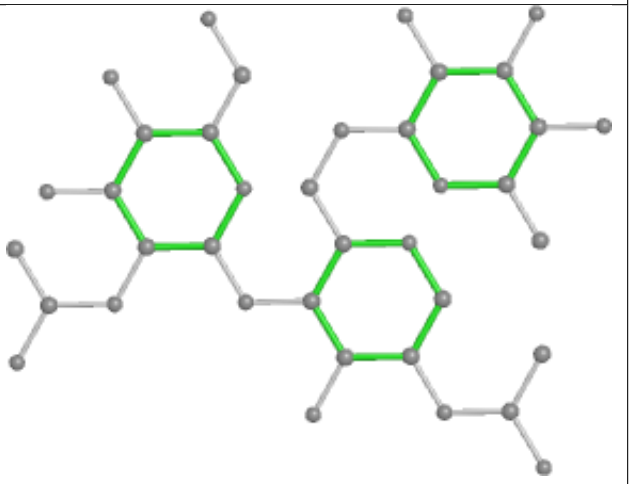
Bond lengths



Bond angles

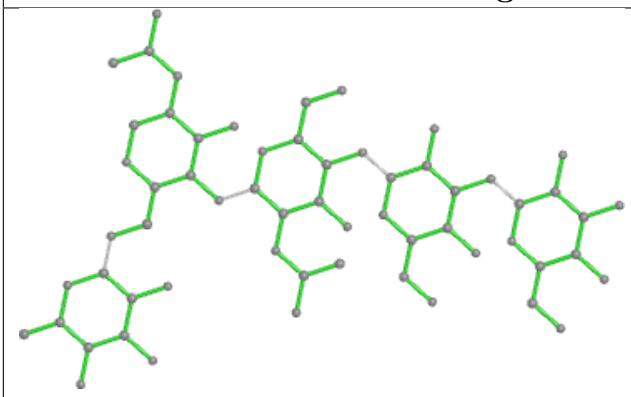


Torsions

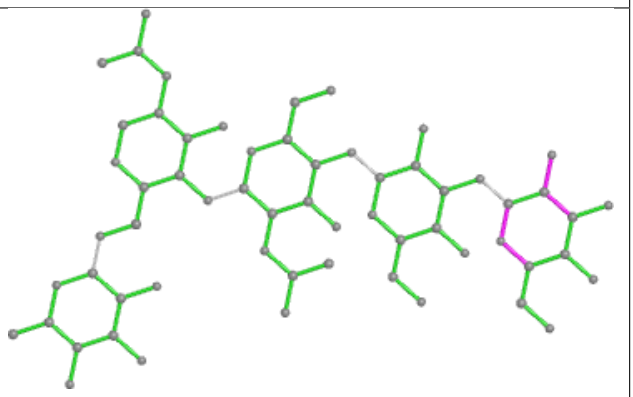


Rings

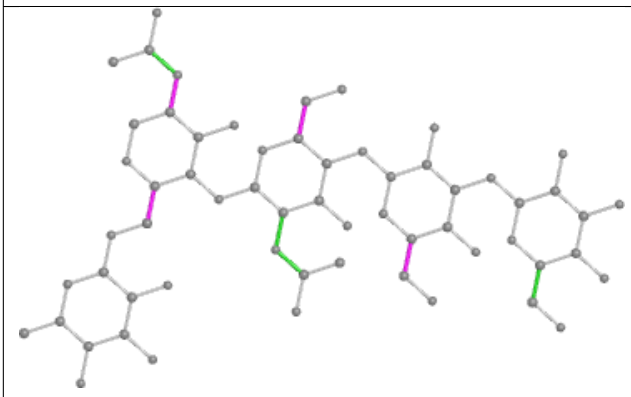
Oligosaccharide Chain F



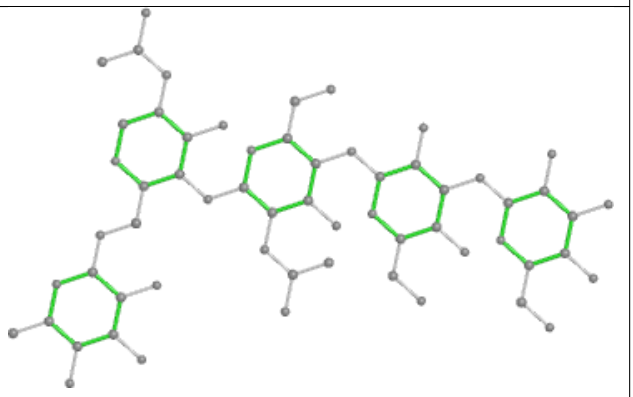
Bond lengths



Bond angles

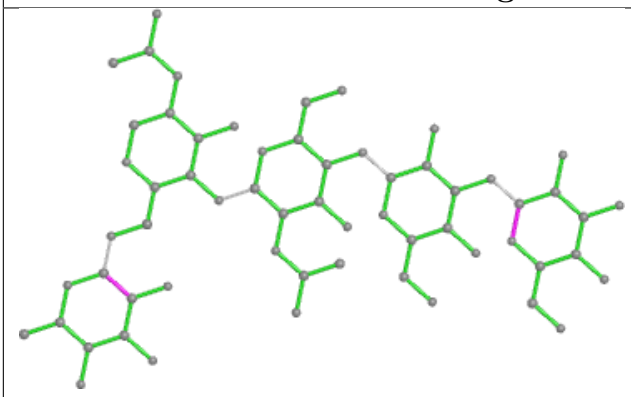


Torsions

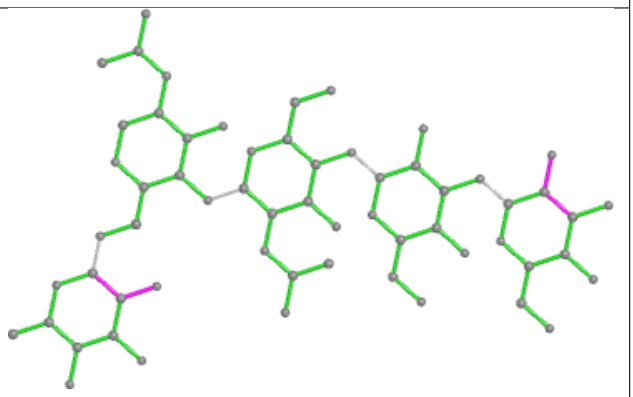


Rings

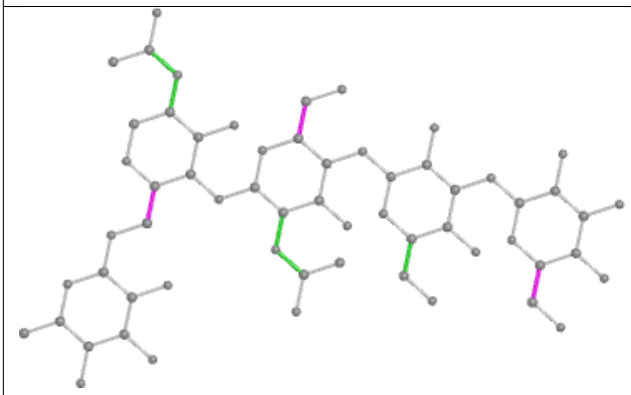
Oligosaccharide Chain L



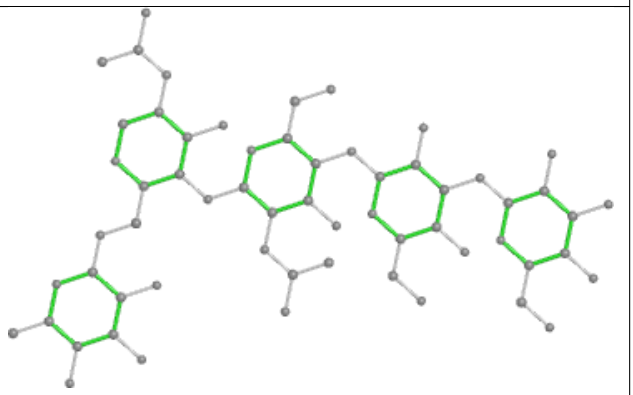
Bond lengths



Bond angles

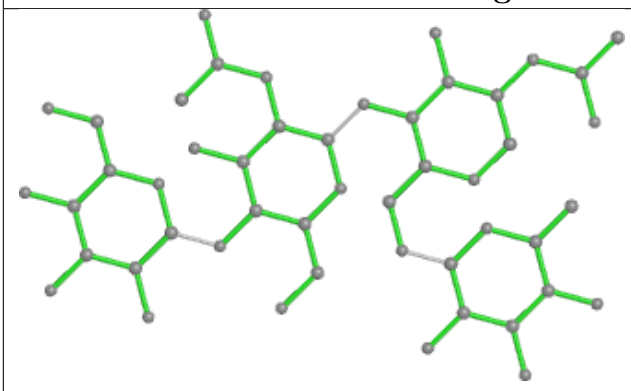


Torsions

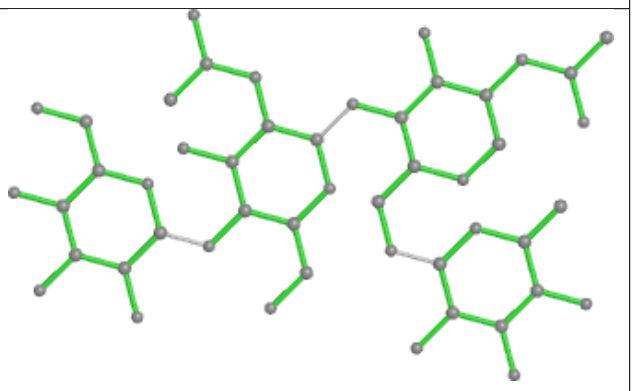


Rings

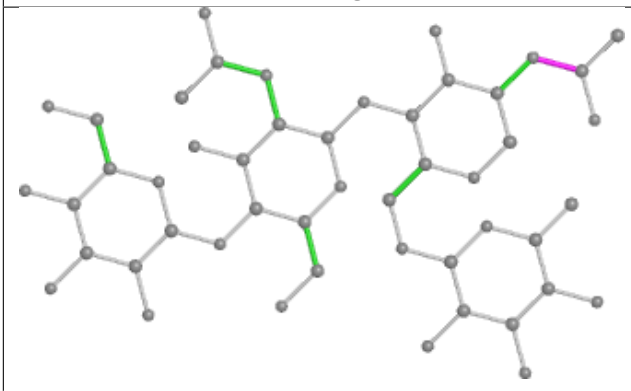
Oligosaccharide Chain G



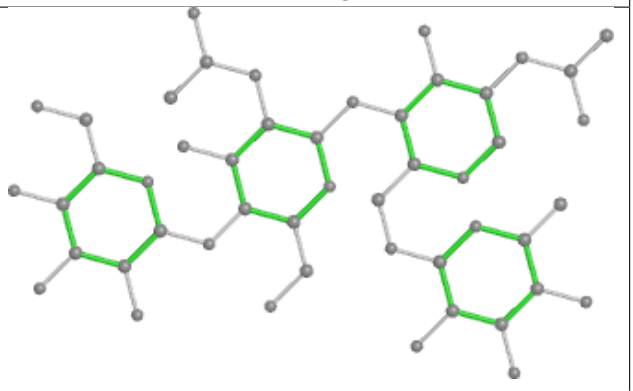
Bond lengths



Bond angles

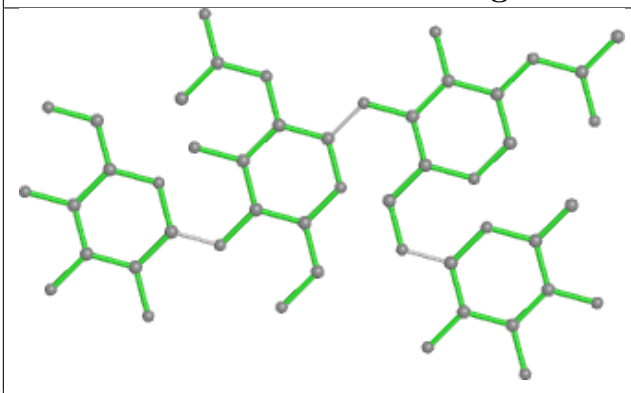


Torsions

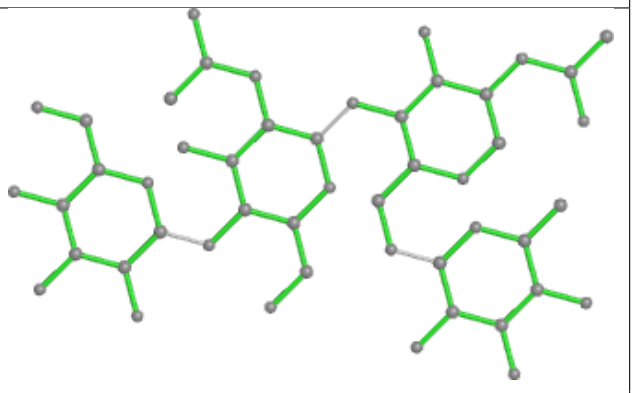


Rings

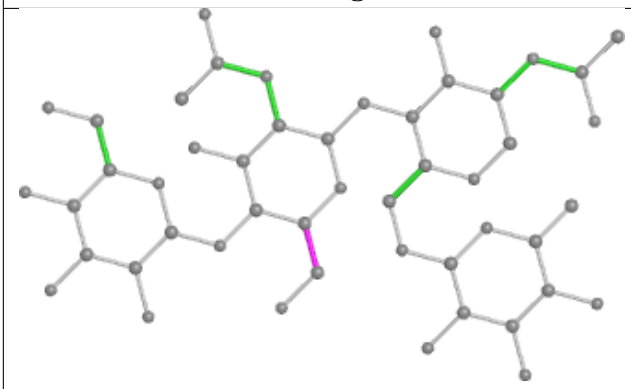
Oligosaccharide Chain M



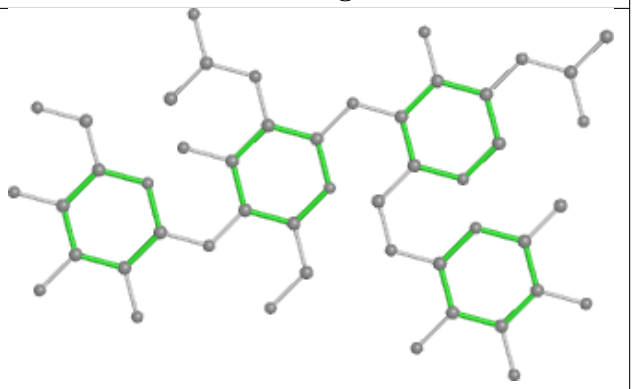
Bond lengths



Bond angles

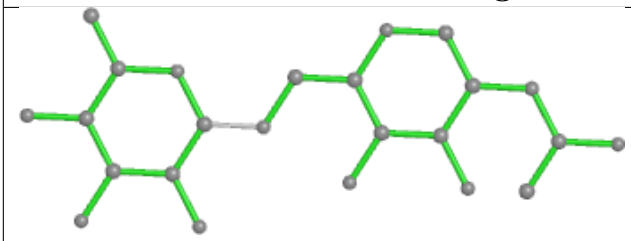


Torsions

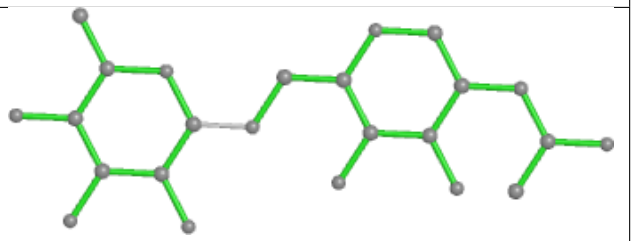


Rings

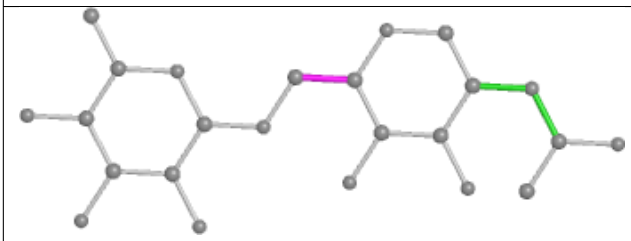
Oligosaccharide Chain H



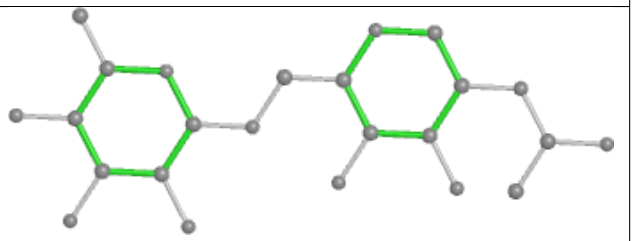
Bond lengths



Bond angles

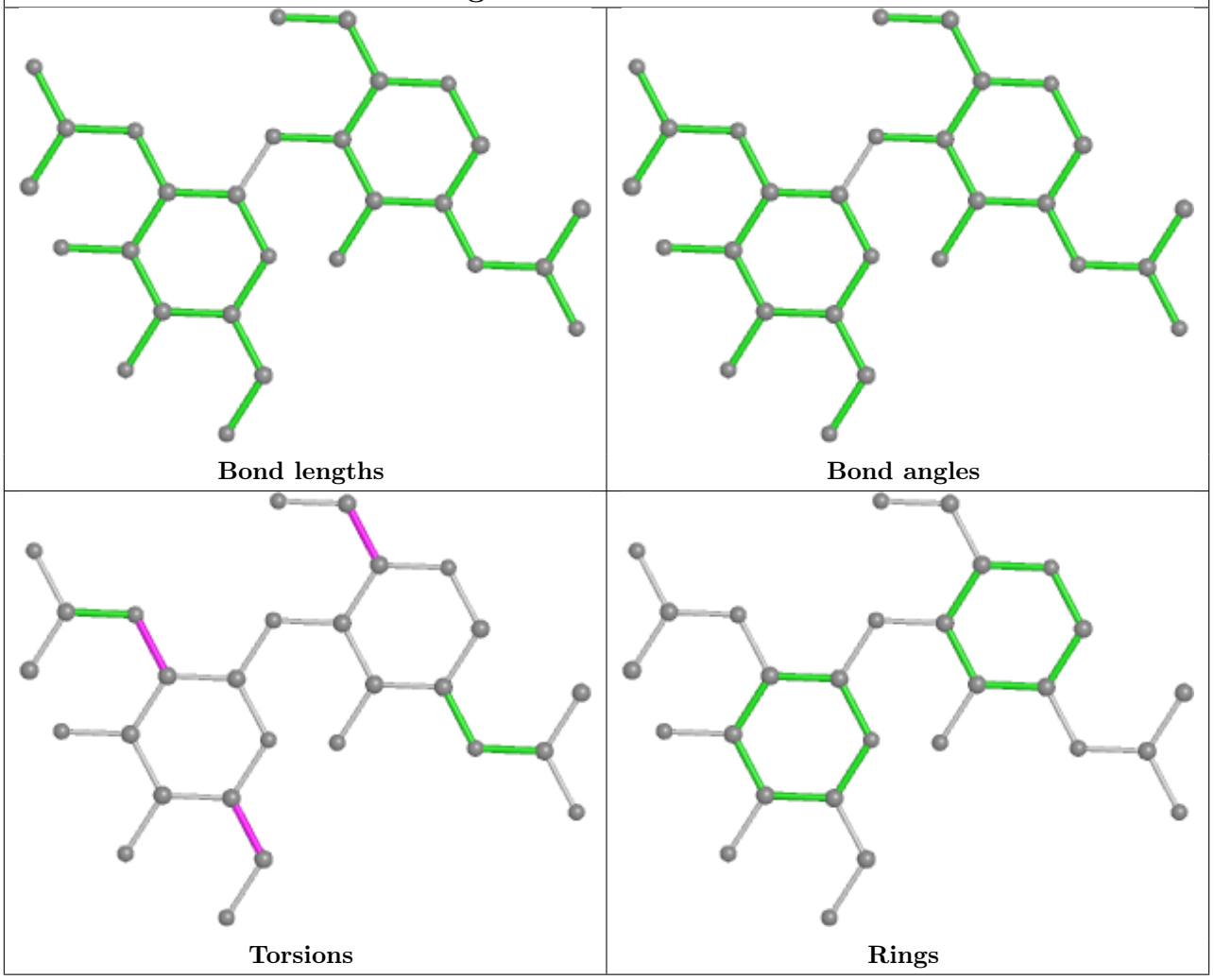


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
9	PEG	C	411	-	6,6,6	0.49	0	5,5,5	0.24	0
10	BU3	C	412	-	4,5,5	0.75	0	6,6,6	0.43	0
8	FLC	C	410	-	12,12,12	1.06	0	17,17,17	1.37	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BU3	C	413	-	4,5,5	0.72	0	6,6,6	0.38	0
8	FLC	C	409	-	12,12,12	1.06	0	17,17,17	1.41	1 (5%)
11	NAG	D	505	2	14,14,15	0.49	0	17,19,21	0.37	0
9	PEG	D	511	-	6,6,6	0.49	0	5,5,5	0.31	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
9	PEG	C	411	-	-	1/4/4/4	-
10	BU3	C	412	-	-	4/4/4/4	-
8	FLC	C	410	-	-	0/16/16/16	-
10	BU3	C	413	-	-	4/4/4/4	-
8	FLC	C	409	-	-	2/16/16/16	-
11	NAG	D	505	2	-	4/6/23/26	0/1/1/1
9	PEG	D	511	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	409	FLC	OB2-CBC-CB	3.99	119.98	113.05
8	C	410	FLC	OB2-CBC-CB	3.90	119.82	113.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	412	BU3	O5-C2-C3-O6
10	C	412	BU3	C1-C2-C3-O6
10	C	412	BU3	O5-C2-C3-C4
10	C	412	BU3	C1-C2-C3-C4
10	C	413	BU3	C1-C2-C3-O6
10	C	413	BU3	O5-C2-C3-C4
10	C	413	BU3	C1-C2-C3-C4
11	D	505	NAG	O5-C5-C6-O6
11	D	505	NAG	C8-C7-N2-C2
11	D	505	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	D	505	NAG	C4-C5-C6-O6
9	C	411	PEG	C1-C2-O2-C3
10	C	413	BU3	O5-C2-C3-O6
9	D	511	PEG	C4-C3-O2-C2
9	D	511	PEG	O1-C1-C2-O2
8	C	409	FLC	CB-CG-CGC-OG2
8	C	409	FLC	CB-CG-CGC-OG1

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	413	BU3	2	0
8	C	409	FLC	3	0
11	D	505	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	220/231 (95%)	-0.28	6 (2%) 54 38	28, 44, 103, 141	0
1	C	219/231 (94%)	-0.33	11 (5%) 28 18	28, 43, 111, 140	0
2	B	295/302 (97%)	-0.36	2 (0%) 87 76	26, 48, 97, 113	0
2	D	295/302 (97%)	-0.17	10 (3%) 45 29	27, 49, 139, 170	0
All	All	1029/1066 (96%)	-0.28	29 (2%) 53 36	26, 46, 113, 170	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	ASN	6.3
2	D	364	ASN	5.4
1	C	245	GLN	4.9
2	D	342	THR	4.9
1	A	245	GLN	4.7
1	A	284	GLU	4.6
1	A	103	TYR	4.5
1	A	242	THR	4.3
1	C	283	ALA	4.1
2	D	396	ILE	3.9
1	C	262	PHE	3.3
1	C	284	GLU	3.2
1	C	269	ALA	3.1
2	D	421	HIS	3.1
1	A	283	ALA	2.8
2	D	393	GLU	2.6
2	D	372	GLU	2.5
1	C	244	ALA	2.5
1	A	322	ASP	2.4
2	D	412	ASP	2.3
1	C	274	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	241	ALA	2.2
2	D	365	ASP	2.2
1	C	268	ASP	2.2
2	B	191	GLU	2.1
2	D	339	ALA	2.1
2	D	370	PRO	2.1
1	C	243	SER	2.0
2	B	372	GLU	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	NAG	O	2	14/15	0.57	0.61	116,159,174,175	0
5	BMA	G	3	11/12	0.61	0.40	113,127,133,141	0
3	NAG	J	2	14/15	0.71	0.58	104,139,154,159	0
3	NAG	K	2	14/15	0.72	0.59	86,127,141,144	0
3	NAG	E	2	14/15	0.75	0.59	107,139,157,165	0
3	FUC	N	3	10/11	0.76	0.79	142,155,165,168	0
3	FUC	J	3	10/11	0.76	0.59	90,121,134,135	0
7	NAG	O	1	14/15	0.76	0.47	111,160,166,170	0
3	NAG	J	1	14/15	0.76	0.37	97,122,139,146	0
4	MAN	L	4	11/12	0.79	0.40	108,128,141,161	0
6	NAG	H	1	14/15	0.79	0.38	97,122,134,135	0
6	FUC	H	2	10/11	0.83	0.55	95,121,128,131	0
3	FUC	E	3	10/11	0.83	0.36	93,119,128,133	0
3	NAG	N	1	14/15	0.83	0.31	70,115,143,155	0
3	NAG	N	2	14/15	0.85	0.59	94,142,151,153	0
4	MAN	F	4	11/12	0.86	0.39	81,105,112,113	0
4	BMA	L	3	11/12	0.87	0.21	72,101,117,119	0
3	NAG	I	2	14/15	0.88	0.45	91,118,131,133	0
5	BMA	M	3	11/12	0.89	0.44	89,108,113,116	0
5	NAG	G	2	14/15	0.90	0.25	63,79,102,118	0

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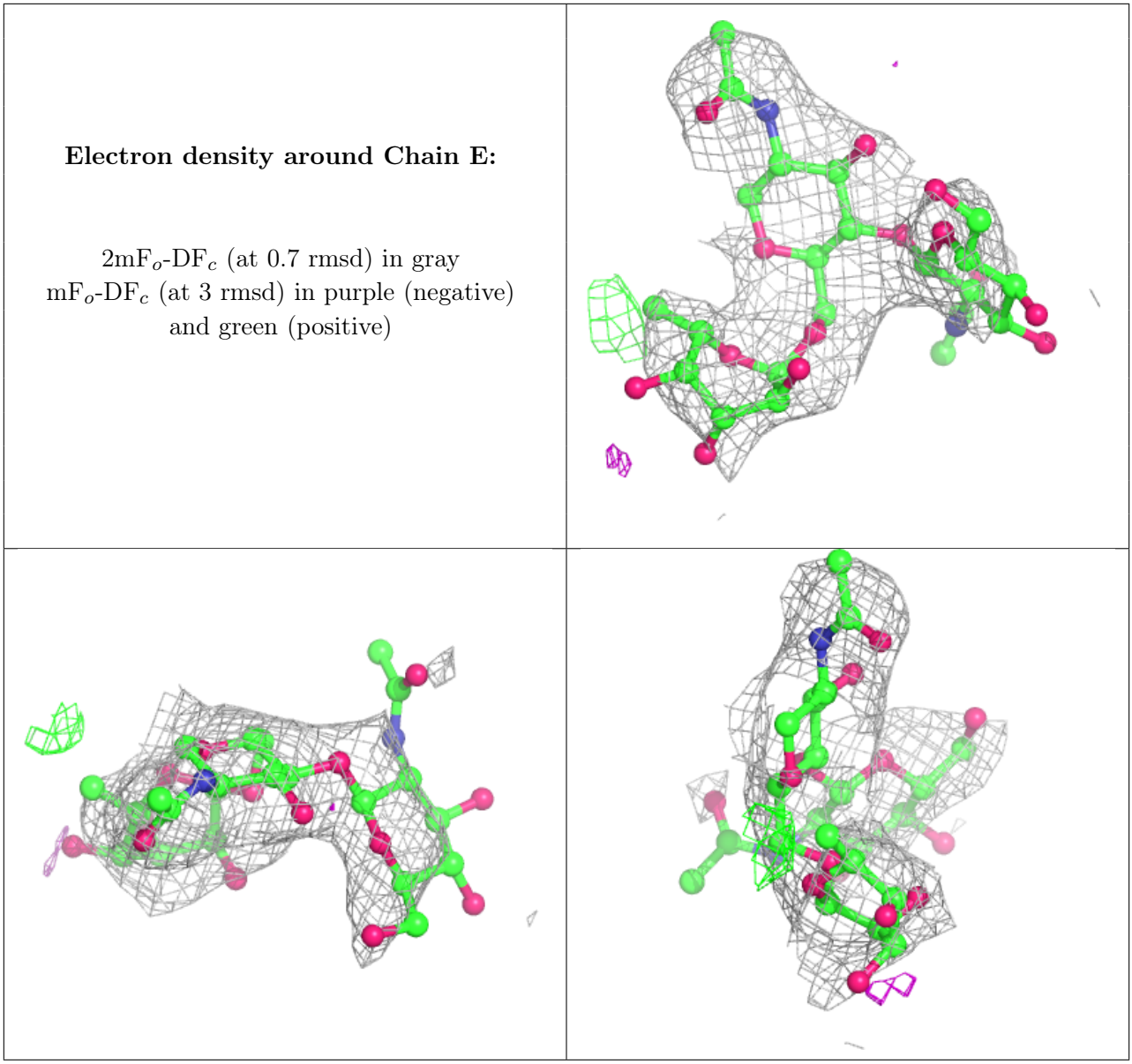
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	K	3	10/11	0.91	0.38	77,104,109,114	0
4	BMA	F	3	11/12	0.91	0.29	72,86,104,108	0
3	NAG	K	1	14/15	0.92	0.24	64,82,108,119	0
5	NAG	M	2	14/15	0.93	0.26	53,67,82,99	0
3	FUC	I	3	10/11	0.94	0.35	83,105,111,115	0
5	FUC	G	4	10/11	0.94	0.28	67,74,80,81	0
3	NAG	I	1	14/15	0.94	0.23	59,74,108,111	0
3	NAG	E	1	14/15	0.94	0.16	61,92,114,123	0
5	FUC	M	4	10/11	0.95	0.22	48,65,74,84	0
5	NAG	G	1	14/15	0.96	0.15	41,46,66,73	0
4	FUC	F	5	10/11	0.96	0.13	35,41,61,65	0
4	NAG	F	1	14/15	0.96	0.15	21,34,54,63	0
4	NAG	F	2	14/15	0.96	0.20	23,45,72,79	0
5	NAG	M	1	14/15	0.96	0.14	24,38,53,54	0
4	FUC	L	5	10/11	0.96	0.17	40,48,60,65	0
4	NAG	L	2	14/15	0.97	0.22	29,41,57,66	0
4	NAG	L	1	14/15	0.97	0.15	28,37,50,58	0

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

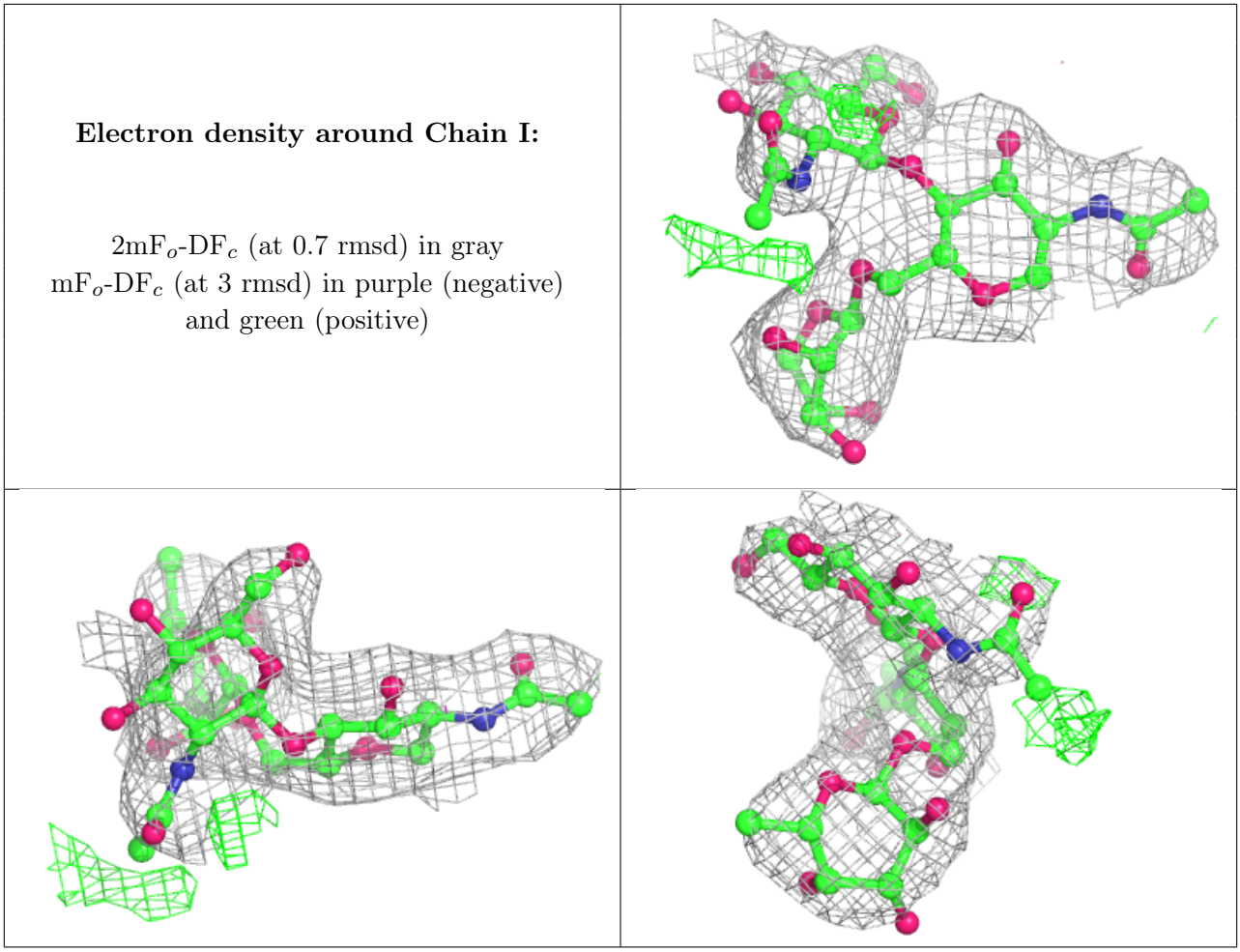
Electron density around Chain E:

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



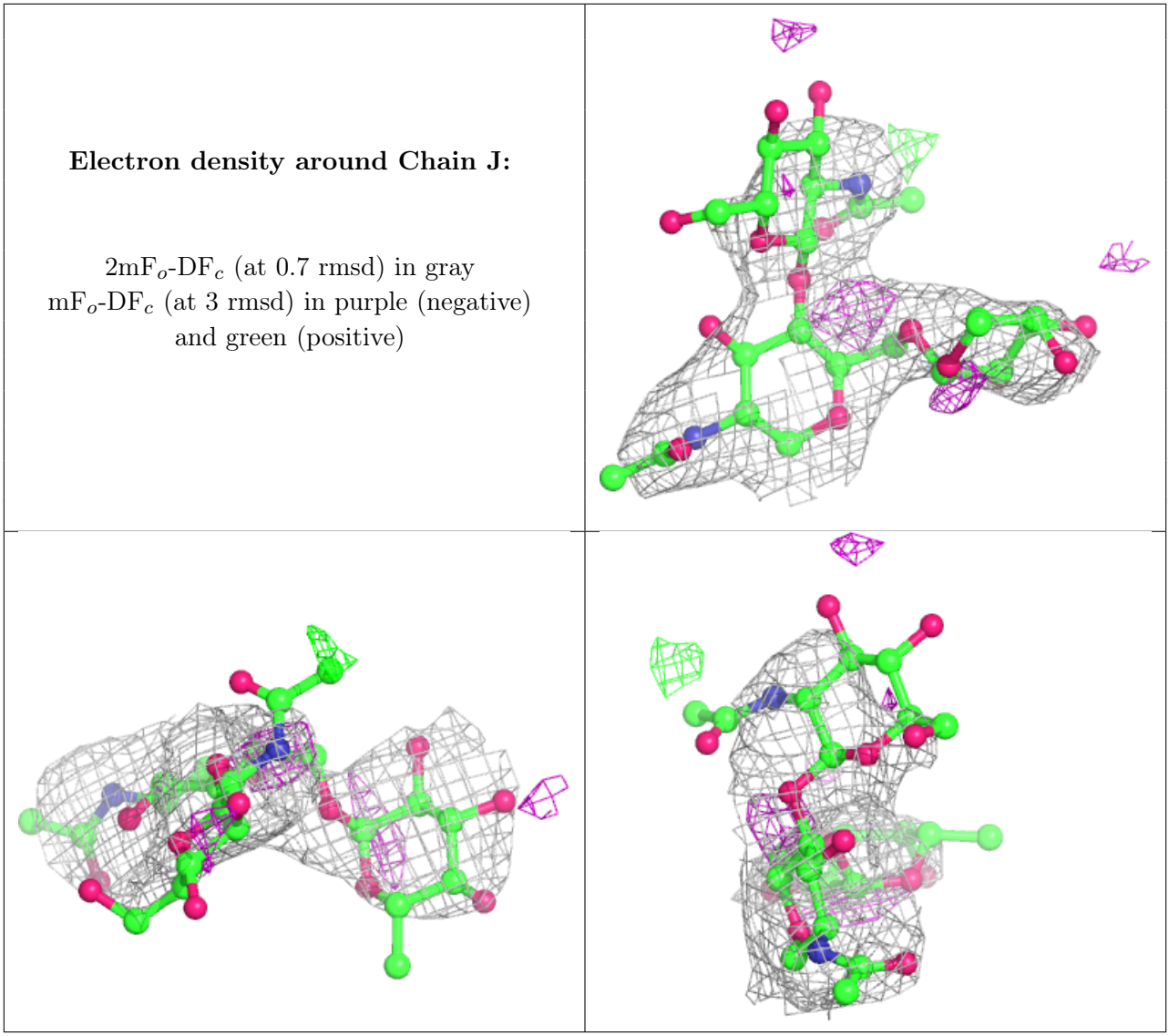
Electron density around Chain I:

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



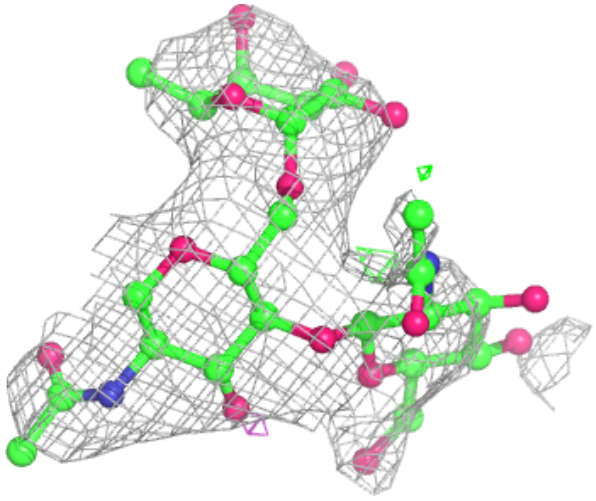
Electron density around Chain J:

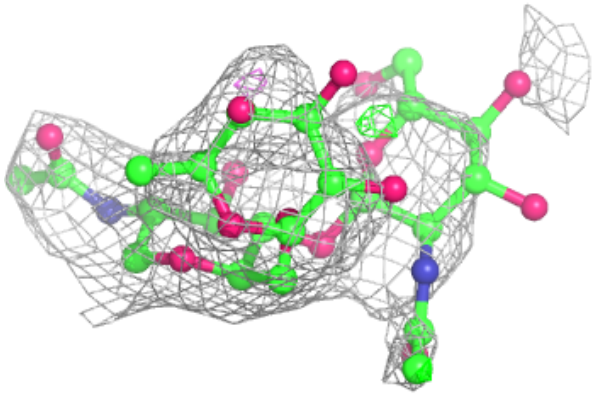
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

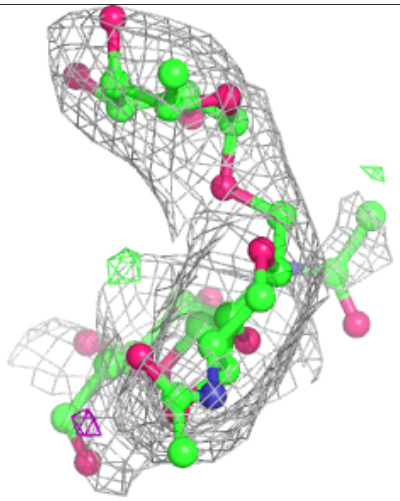


Electron density around Chain K:

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

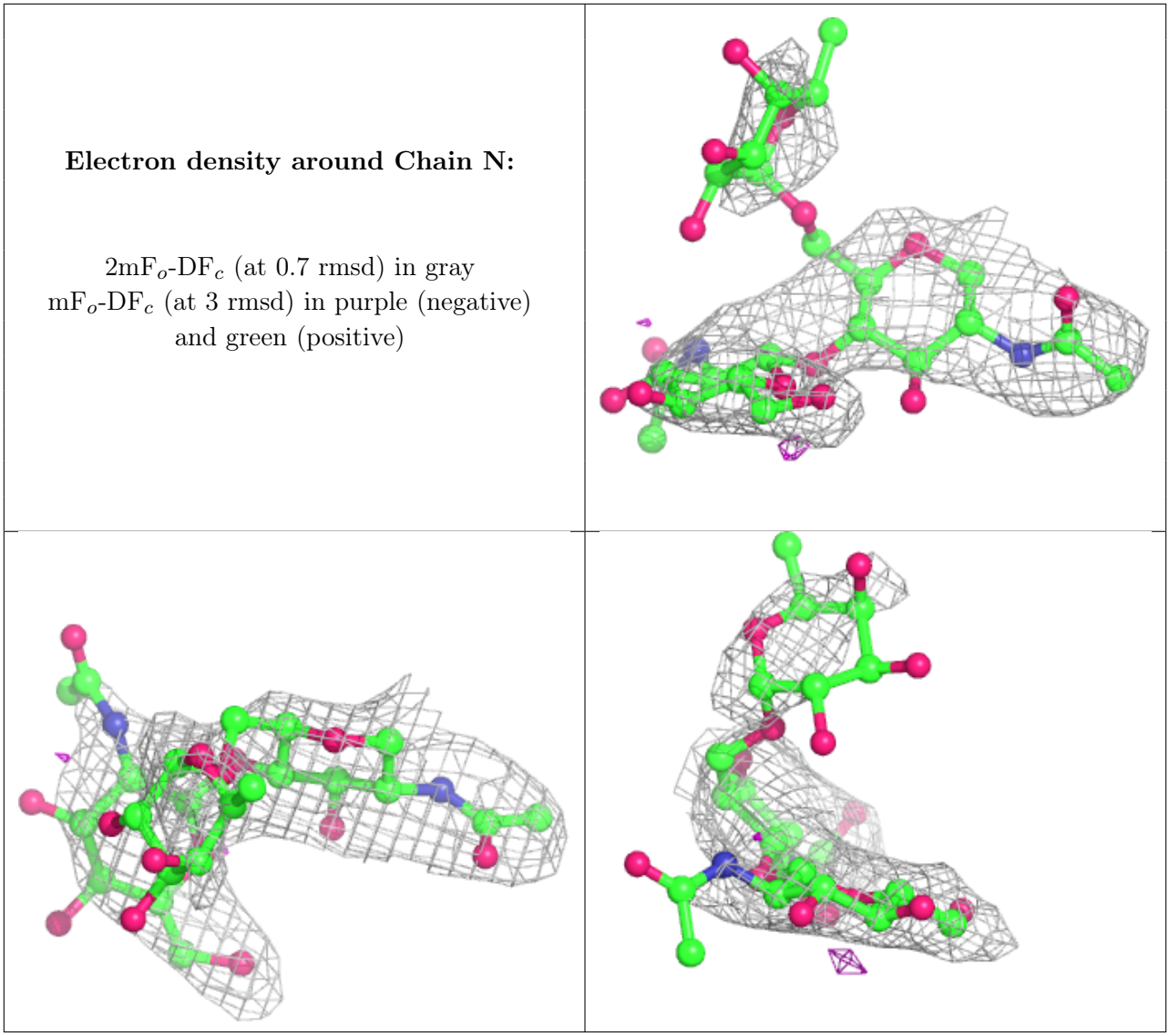






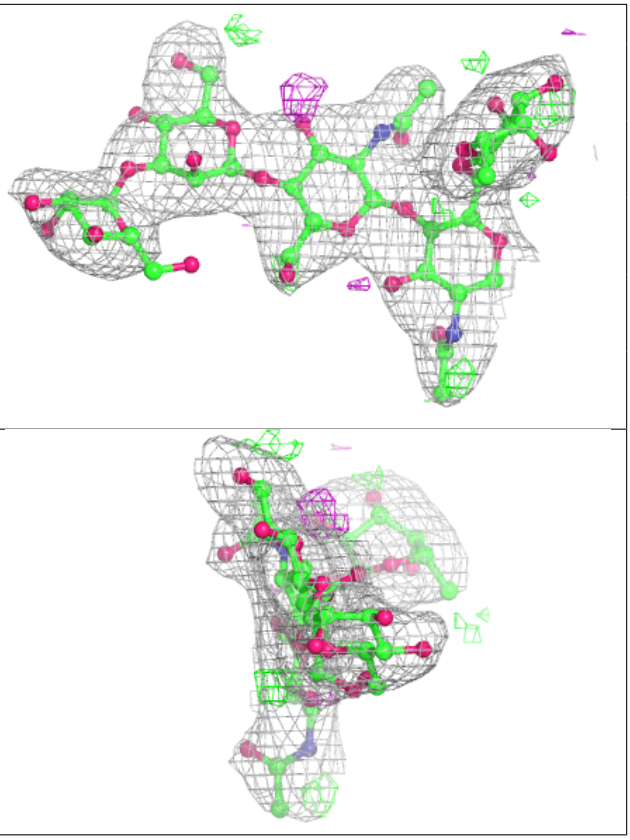
Electron density around Chain N:

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



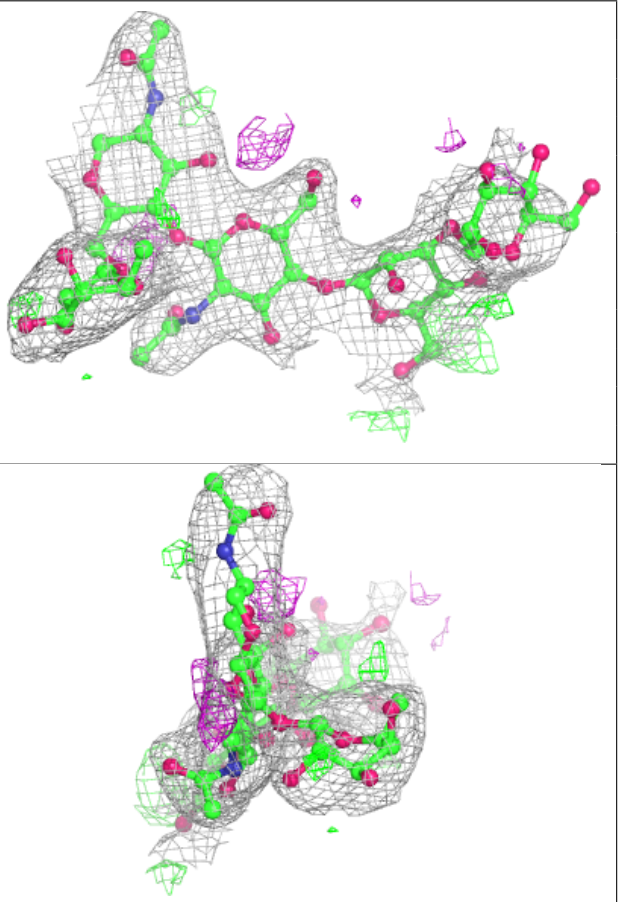
Electron density around Chain F:

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



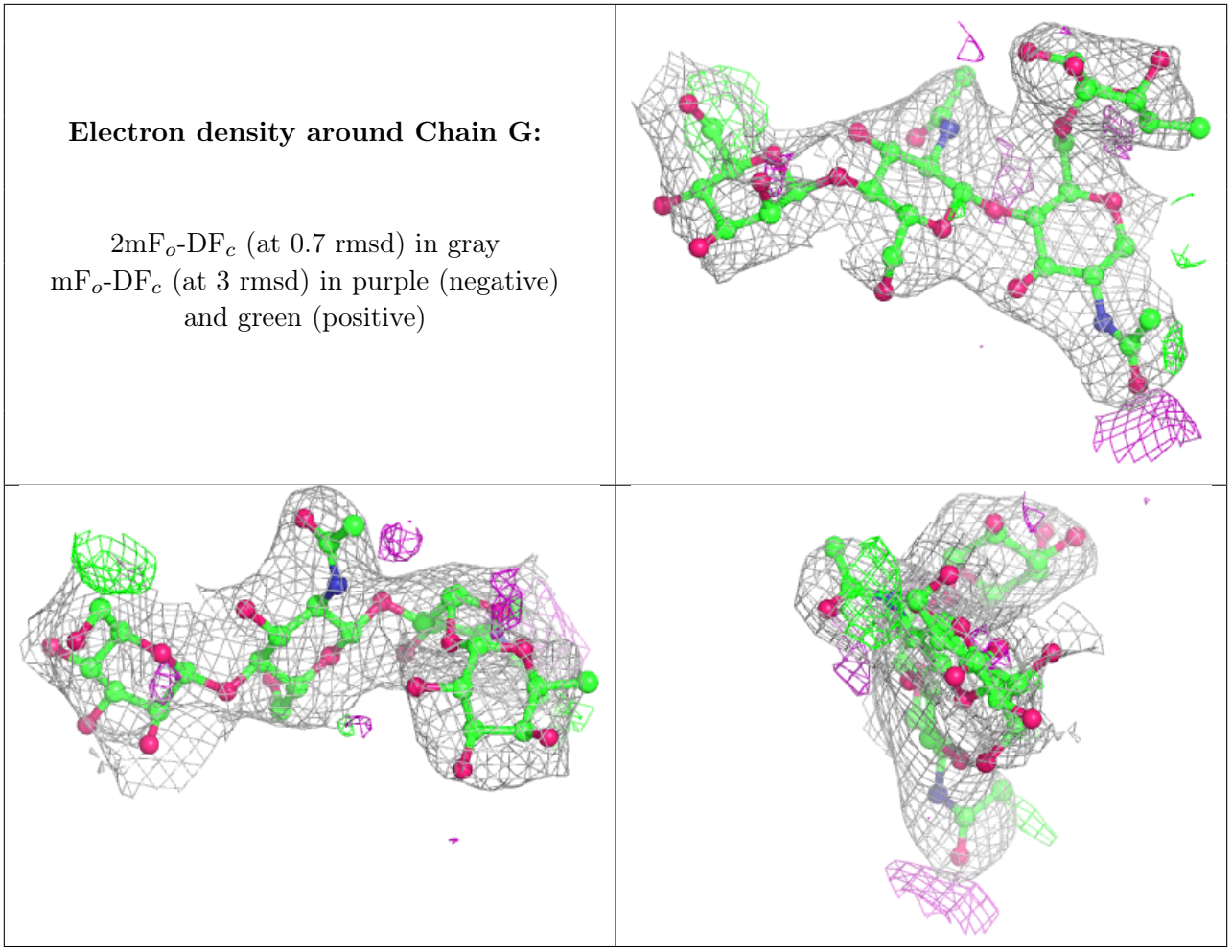
Electron density around Chain L:

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



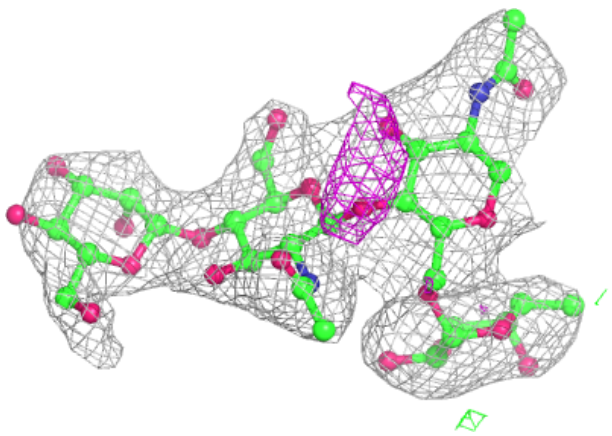
Electron density around Chain G:

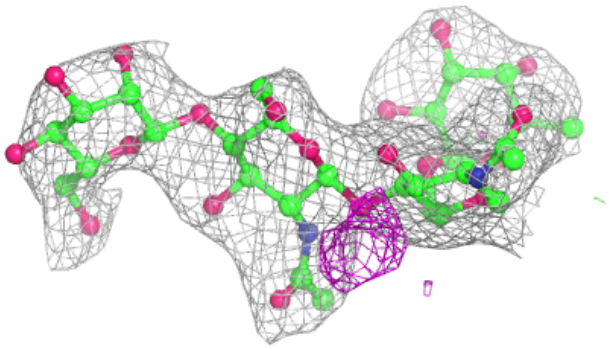
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

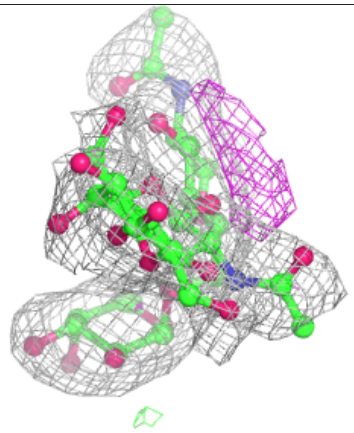


Electron density around Chain M:

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

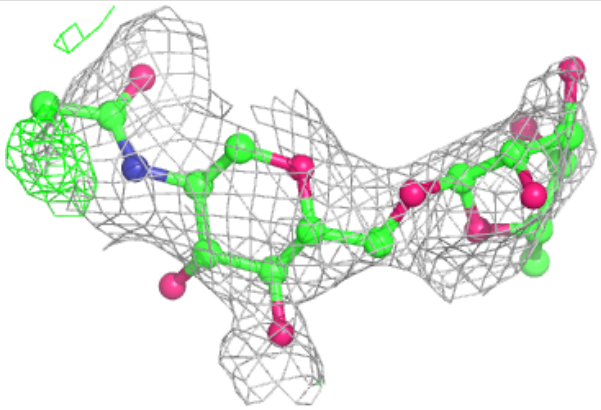


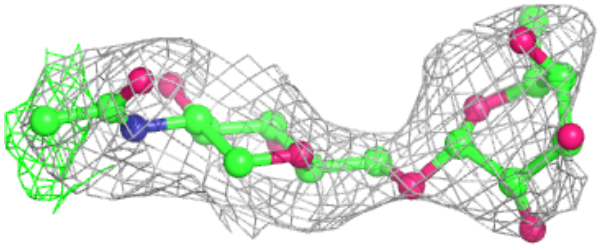


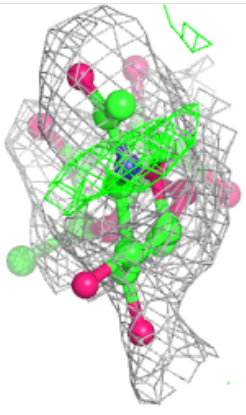


Electron density around Chain H:

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

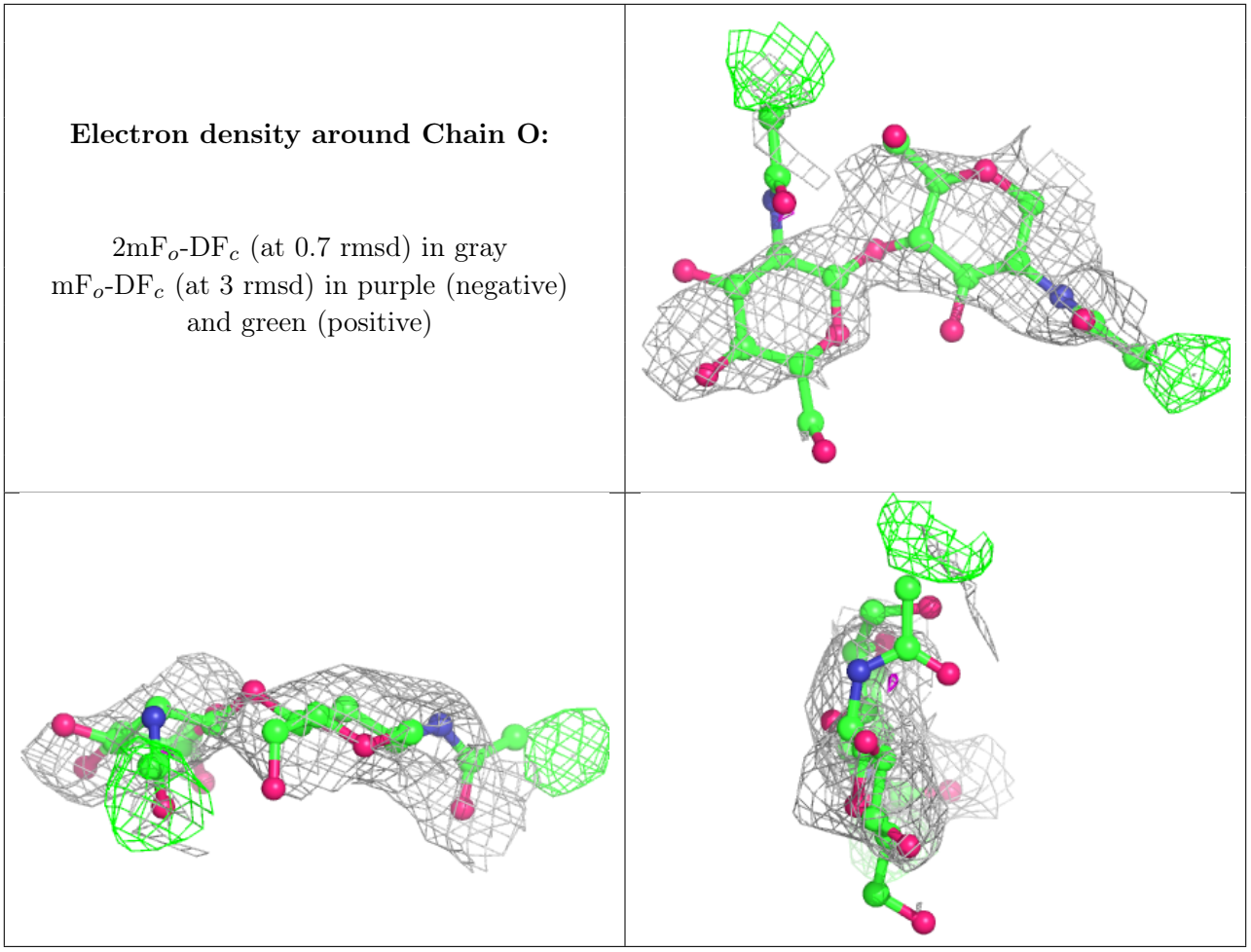






Electron density around Chain O:

$2mF_o$-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
11	NAG	D	505	14/15	0.77	0.46	86,131,146,151	0
9	PEG	C	411	7/7	0.87	0.31	58,69,73,88	0
10	BU3	C	413	6/6	0.88	0.29	56,89,109,129	0
10	BU3	C	412	6/6	0.91	0.31	48,79,104,104	0
8	FLC	C	409	13/13	0.91	0.27	59,74,87,94	0
9	PEG	D	511	7/7	0.91	0.23	51,67,84,88	0
8	FLC	C	410	13/13	0.93	0.22	50,64,82,97	0

6.5 Other polymers (i)

There are no such residues in this entry.