Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:58 PM BST

PDB ID	:	6PD4
Title	:	Crystal Structure of Hendra Virus Attachment G Glycoprotein
Authors	:	Xu, K.; Nikolov, D.B.
Deposited on	:	2019-06-18
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:

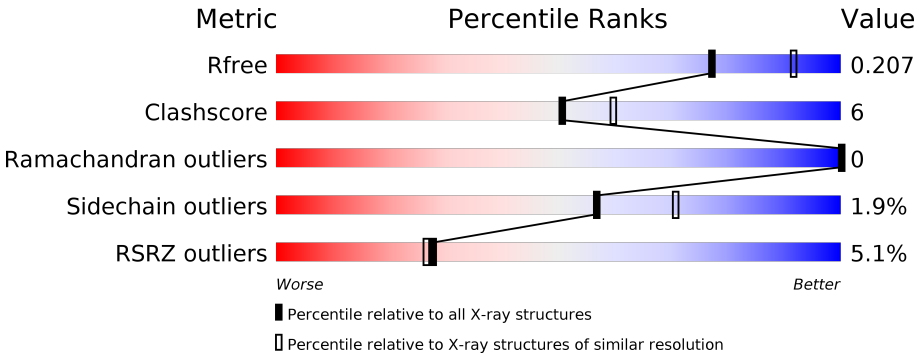
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	441	3% 88% 10%
1	B	441	7% 86% 11%
2	C	2	100%
2	D	2	50% 50%
2	F	2	100%
2	G	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	4	50% 50%
4	H	6	33% 67%

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
2	NAG	F	2	X	-	-	-
2	NAG	G	2	X	-	-	-
3	FUC	E	4	X	-	-	-
4	BMA	H	3	X	-	-	-
4	FUC	H	6	X	-	-	-
6	SO4	A	714	-	-	X	-
6	SO4	B	715	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7734 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3430	2182	580	649	19			
1	B	429	Total	C	N	O	S	0	0	0
			3378	2150	567	642	19			

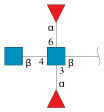
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	GLY	-	expression tag	UNP F4YH71
A	606	ARG	-	expression tag	UNP F4YH71
A	607	GLY	-	expression tag	UNP F4YH71
A	608	LEU	-	expression tag	UNP F4YH71
A	609	VAL	-	expression tag	UNP F4YH71
A	610	PRO	-	expression tag	UNP F4YH71
A	611	ARG	-	expression tag	UNP F4YH71
B	605	GLY	-	expression tag	UNP F4YH71
B	606	ARG	-	expression tag	UNP F4YH71
B	607	GLY	-	expression tag	UNP F4YH71
B	608	LEU	-	expression tag	UNP F4YH71
B	609	VAL	-	expression tag	UNP F4YH71
B	610	PRO	-	expression tag	UNP F4YH71
B	611	ARG	-	expression tag	UNP F4YH71

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

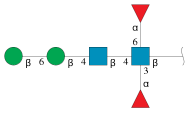
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0
2	F	2	Total C N O 28 16 2 10	0	0	0
2	G	2	Total C N O 28 16 2 10	0	0	0

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



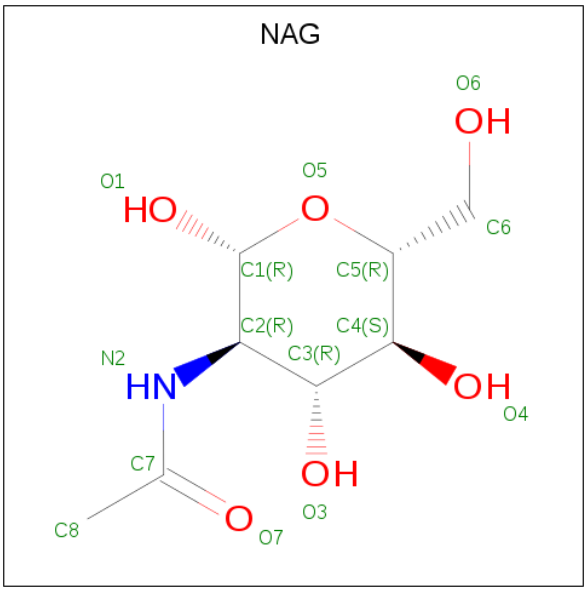
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	4	Total C N O 48 28 2 18	0	0	0

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



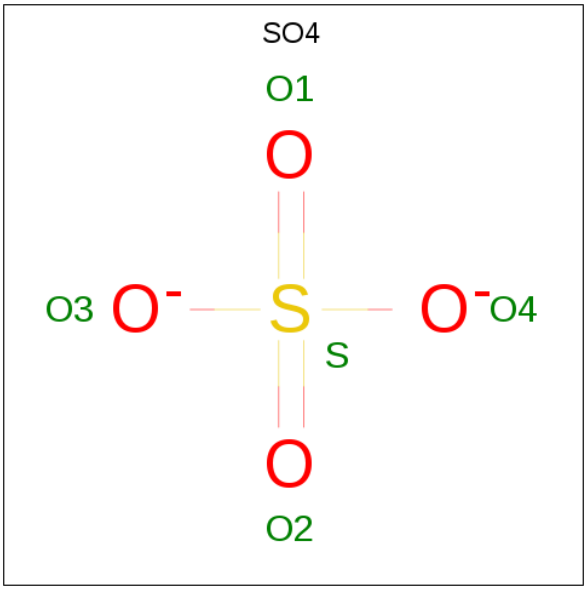
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	6	Total C N O 70 40 2 28	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

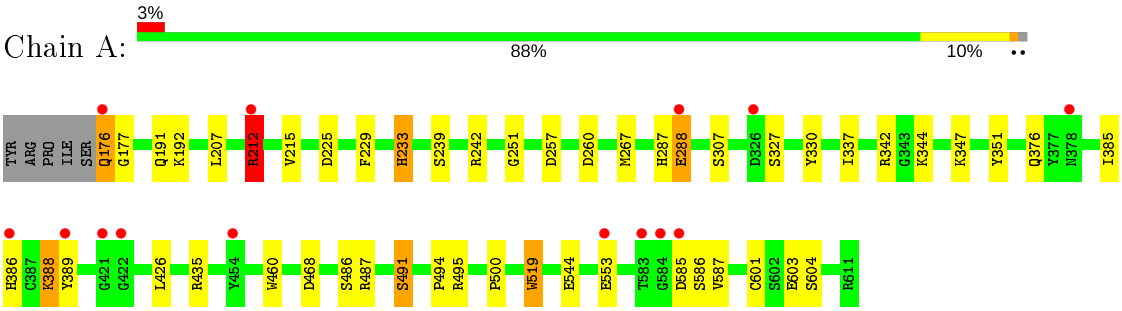
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	330	Total O 330 330	0	0
7	B	273	Total O 273 273	0	0

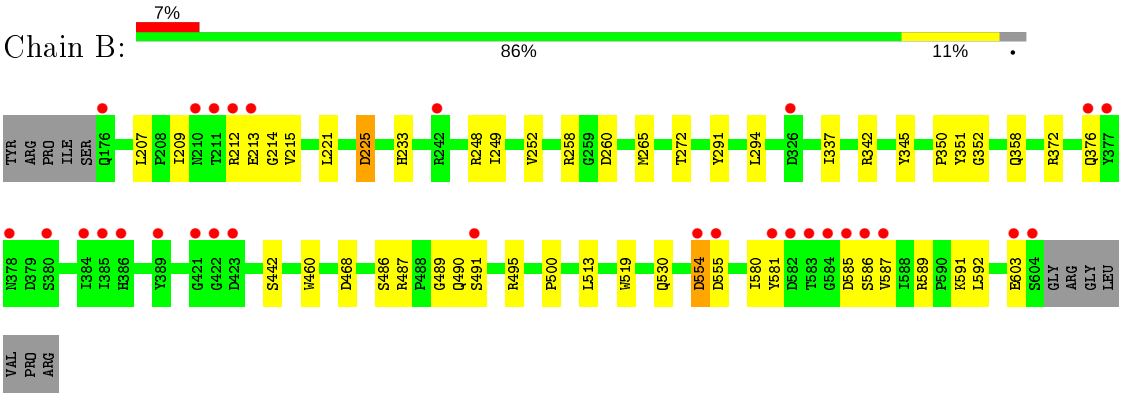
3 Residue-property plots (i)

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.

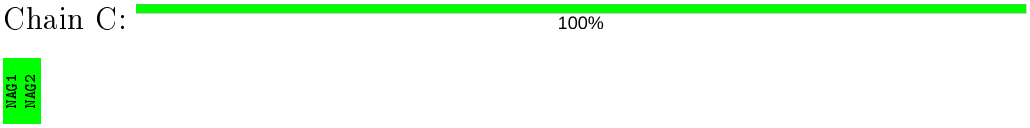
• Molecule 1: Attachment glycoprotein



• Molecule 1: Attachment glycoprotein



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



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

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

Chain F:

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

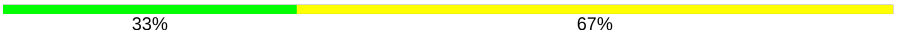
Chain G:

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

Chain E:

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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.15Å 73.24Å 109.13Å 90.00° 91.85° 90.00°	Depositor
Resolution (Å)	36.92 – 2.20 36.92 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.6 (36.92-2.20) 96.6 (36.92-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.167 , 0.207 0.167 , 0.207	Depositor DCC
R_{free} test set	2619 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7734	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, SO4, NAG

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	0.51	4/3512 (0.1%)	0.74	11/4782 (0.2%)
1	B	0.46	1/3459 (0.0%)	0.71	5/4711 (0.1%)
All	All	0.48	5/6971 (0.1%)	0.73	16/9493 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	SER	CB-OG	-6.95	1.33	1.42
1	A	225	ASP	CB-CG	-5.98	1.39	1.51
1	A	288	GLU	CD-OE2	5.51	1.31	1.25
1	A	225	ASP	CG-OD2	5.06	1.36	1.25
1	B	603	GLU	CB-CG	5.03	1.61	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	376	GLN	CA-CB-CG	8.25	131.56	113.40
1	A	212	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	212	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	288	GLU	CA-CB-CG	7.04	128.89	113.40
1	B	554	ASP	CB-CG-OD1	-6.99	112.00	118.30
1	A	176	GLN	N-CA-C	-6.95	92.23	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	603	GLU	CA-CB-CG	6.76	128.28	113.40
1	A	225	ASP	CB-CG-OD1	6.71	124.33	118.30
1	B	554	ASP	CB-CA-C	5.80	122.00	110.40
1	A	225	ASP	OD1-CG-OD2	-5.65	112.57	123.30
1	A	212	ARG	CB-CA-C	-5.48	99.44	110.40
1	A	225	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	176	GLN	CA-CB-CG	-5.10	102.17	113.40
1	B	221	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	176	GLN	C-N-CA	5.08	132.96	122.30
1	A	288	GLU	N-CA-CB	-5.05	101.52	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	490	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3375	37	0
1	B	3378	0	3316	34	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	F	28	0	25	3	0
2	G	28	0	25	0	0
3	E	48	0	43	0	0
4	H	70	0	61	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	35	0	0	4	0
6	B	30	0	0	2	0
7	A	330	0	0	9	3
7	B	273	0	0	14	1
All	All	7734	0	6921	80	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (80) 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:176:GLN:CG	1:A:177:GLY:H	1.19	1.29
1:A:388:LYS:HD2	1:A:389:TYR:CE1	1.90	1.06
1:A:176:GLN:HG2	1:A:177:GLY:N	1.44	1.04
1:A:176:GLN:CG	1:A:177:GLY:N	1.93	1.01
1:A:388:LYS:HD2	1:A:389:TYR:CZ	2.01	0.94
1:A:376:GLN:HG2	7:A:816:HOH:O	1.64	0.94
1:A:176:GLN:HG3	1:A:177:GLY:N	1.79	0.93
6:A:713:SO4:O1	7:A:801:HOH:O	1.85	0.93
1:A:176:GLN:HG3	1:A:177:GLY:H	1.26	0.90
1:A:176:GLN:HG2	1:A:177:GLY:H	0.71	0.87
6:B:715:SO4:O3	7:B:801:HOH:O	1.96	0.83
6:B:715:SO4:O1	7:B:802:HOH:O	1.99	0.80
1:A:388:LYS:CD	1:A:389:TYR:CE1	2.67	0.77
6:A:714:SO4:O4	7:A:802:HOH:O	2.03	0.75
6:A:714:SO4:O1	7:A:803:HOH:O	2.06	0.73
1:B:491:SER:OG	7:B:803:HOH:O	2.06	0.72
1:B:225:ASP:HB2	7:B:808:HOH:O	1.89	0.72
7:B:805:HOH:O	2:F:2:NAG:O7	2.10	0.68
1:A:191:GLN:HG2	1:A:601:CYS:SG	2.36	0.65
1:B:212:ARG:HD2	1:B:214:GLY:H	1.63	0.64
1:B:580:ILE:HG21	1:B:591:LYS:HE2	1.81	0.63
1:A:342:ARG:NH1	7:A:804:HOH:O	2.08	0.62
1:A:287:HIS:CE1	1:A:288:GLU:OE1	2.54	0.61
1:B:212:ARG:HE	1:B:215:VAL:HG23	1.65	0.61
1:A:176:GLN:NE2	1:A:257:ASP:HB2	2.15	0.61
1:A:251:GLY:HA3	1:A:267:MET:CE	2.31	0.60
1:B:258:ARG:HB2	7:B:804:HOH:O	2.02	0.60
1:A:251:GLY:HA3	1:A:267:MET:HE1	1.84	0.60
1:A:553:GLU:H	1:A:553:GLU:CD	2.05	0.59
1:A:435:ARG:NH1	7:A:807:HOH:O	2.19	0.58
1:B:248:ARG:HD3	7:B:821:HOH:O	2.03	0.58
1:B:587:VAL:HG23	1:B:589:ARG:HG2	1.87	0.57
1:B:207:LEU:HD11	1:B:592:LEU:HD11	1.87	0.57
1:B:554:ASP:OD2	1:B:555:ASP:N	2.39	0.56
1:B:585:ASP:O	1:B:587:VAL:N	2.39	0.55
1:A:468:ASP:OD1	1:A:519:TRP:HZ2	1.91	0.54
7:B:809:HOH:O	2:F:1:NAG:H2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:HA	1:B:587:VAL:CG1	2.39	0.53
6:A:712:SO4:O1	7:A:808:HOH:O	2.19	0.51
1:B:486:SER:HB3	1:B:495:ARG:HG3	1.91	0.51
1:B:352:GLY:HA3	1:B:442:SER:O	2.12	0.50
1:B:252:VAL:HG11	1:B:291:TYR:HB2	1.94	0.49
1:A:192:LYS:HE2	1:A:544:GLU:OE2	2.12	0.49
1:A:486:SER:HB3	1:A:495:ARG:HG3	1.94	0.48
1:B:248:ARG:NH2	7:B:825:HOH:O	2.47	0.48
1:B:294:LEU:HG	1:B:350:PRO:HG3	1.96	0.48
1:A:603:GLU:HG2	1:A:604:SER:N	2.28	0.48
1:B:337:ILE:O	7:B:807:HOH:O	2.20	0.47
1:B:460:TRP:CD2	1:B:500:PRO:HA	2.49	0.47
1:B:468:ASP:CG	1:B:519:TRP:HZ2	2.17	0.47
1:A:491:SER:O	1:A:494:PRO:HD3	2.14	0.47
1:B:213:GLU:HA	1:B:587:VAL:HG12	1.96	0.47
1:A:344:LYS:NZ	7:A:810:HOH:O	2.23	0.47
1:A:307:SER:O	1:A:347:LYS:NZ	2.40	0.46
1:B:265:MET:SD	1:B:592:LEU:HD13	2.55	0.46
1:B:460:TRP:CG	1:B:500:PRO:HA	2.51	0.46
1:A:207:LEU:HD21	1:A:229:PHE:HE1	1.80	0.46
1:A:327:SER:HB2	1:A:330:TYR:HB3	1.98	0.45
1:A:287:HIS:HE1	1:A:288:GLU:OE1	1.97	0.45
1:A:242:ARG:NH1	7:A:821:HOH:O	2.49	0.45
1:B:258:ARG:CB	7:B:804:HOH:O	2.64	0.44
1:B:342:ARG:HG3	1:B:345:TYR:O	2.17	0.44
7:B:809:HOH:O	2:F:1:NAG:O7	2.21	0.44
1:B:209:ILE:HG21	1:B:589:ARG:CZ	2.48	0.44
1:A:585:ASP:O	1:A:587:VAL:N	2.51	0.43
1:B:489:GLY:O	1:B:530:GLN:HA	2.18	0.43
1:A:385:ILE:HG22	1:A:386:HIS:CD2	2.54	0.43
1:A:460:TRP:CD2	1:A:500:PRO:HA	2.54	0.43
1:A:460:TRP:CG	1:A:500:PRO:HA	2.53	0.43
1:B:291:TYR:OH	7:B:808:HOH:O	2.20	0.42
1:B:468:ASP:OD1	1:B:519:TRP:HZ2	2.03	0.42
1:B:249:ILE:HG22	1:B:272:THR:HG22	2.01	0.42
1:A:251:GLY:HA3	1:A:267:MET:HE2	2.00	0.42
1:A:337:ILE:HD13	1:A:426:LEU:HD11	2.01	0.41
1:A:212:ARG:O	1:A:215:VAL:HG22	2.20	0.41
1:B:358:GLN:NE2	7:B:813:HOH:O	2.33	0.41
1:B:260:ASP:OD1	1:B:260:ASP:N	2.51	0.41
1:A:233:HIS:C	1:A:233:HIS:CD2	2.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:HD13	1:B:519:TRP:CE3	2.56	0.40
1:B:213:GLU:HG2	1:B:586:SER:H	1.85	0.40

All (4) 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)
7:A:1000:HOH:O	7:A:1089:HOH:O[2_544]	1.98	0.22
7:A:905:HOH:O	7:A:965:HOH:O[2_554]	2.03	0.17
7:B:968:HOH:O	7:B:1053:HOH:O[2_455]	2.14	0.06
7:A:1110:HOH:O	7:A:1120:HOH:O[2_554]	2.17	0.03

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	434/441 (98%)	420 (97%)	14 (3%)	0	100	100
1	B	427/441 (97%)	409 (96%)	18 (4%)	0	100	100
All	All	861/882 (98%)	829 (96%)	32 (4%)	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	389/394 (99%)	380 (98%)	9 (2%)	50 63
1	B	384/394 (98%)	378 (98%)	6 (2%)	62 76
All	All	773/788 (98%)	758 (98%)	15 (2%)	57 71

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

Mol	Chain	Res	Type
1	A	212	ARG
1	A	233	HIS
1	A	239	SER
1	A	260	ASP
1	A	351	TYR
1	A	388	LYS
1	A	487	ARG
1	A	519	TRP
1	A	586	SER
1	B	225	ASP
1	B	233	HIS
1	B	351	TYR
1	B	372	ARG
1	B	487	ARG
1	B	581	TYR

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

Mol	Chain	Res	Type
1	A	176	GLN
1	B	450	GLN
1	B	490	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)

18 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	0.34	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.39	0
2	NAG	D	1	1,2	14,14,15	0.28	0	17,19,21	0.65	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.68	1 (7%)	17,19,21	1.59	2 (11%)
3	FUC	E	2	3	10,10,11	0.98	0	14,14,16	0.92	0
3	NAG	E	3	3	14,14,15	0.30	0	17,19,21	0.36	0
3	FUC	E	4	3	10,10,11	0.86	0	14,14,16	1.11	1 (7%)
2	NAG	F	1	1,2	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
2	NAG	F	2	2	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
2	NAG	G	2	2	14,14,15	0.32	0	17,19,21	0.34	0
4	NAG	H	1	1,4	14,14,15	0.49	0	17,19,21	1.38	2 (11%)
4	NAG	H	2	4	14,14,15	0.21	0	17,19,21	0.55	0
4	BMA	H	3	4	11,11,12	1.07	1 (9%)	15,15,17	1.07	1 (6%)
4	BMA	H	4	4	11,11,12	0.76	0	15,15,17	1.39	2 (13%)
4	FUC	H	5	4	10,10,11	0.84	0	14,14,16	1.02	0
4	FUC	H	6	4	10,10,11	0.77	0	14,14,16	1.14	1 (7%)

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	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.31	1.40	1.43
4	H	3	BMA	C1-C2	2.21	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	C1-O5-C5	5.40	119.51	112.19
4	H	1	NAG	C1-O5-C5	4.79	118.68	112.19
2	D	2	NAG	C1-O5-C5	3.17	116.49	112.19
4	H	4	BMA	C1-O5-C5	3.15	116.46	112.19
2	F	2	NAG	C1-O5-C5	2.65	115.79	112.19
4	H	6	FUC	O2-C2-C1	2.61	114.49	109.15
2	F	1	NAG	C1-O5-C5	2.47	115.53	112.19
3	E	1	NAG	O5-C5-C6	-2.28	103.62	107.20
3	E	4	FUC	C1-O5-C5	2.28	117.95	112.78
4	H	4	BMA	O2-C2-C1	2.22	113.69	109.15
2	G	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	H	3	BMA	O5-C5-C6	2.13	110.54	107.20
4	H	1	NAG	O5-C5-C6	-2.11	103.90	107.20

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	4	FUC	C1
4	H	6	FUC	C1
2	G	2	NAG	C1
4	H	3	BMA	C1
2	F	2	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
4	H	4	BMA	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
4	H	4	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

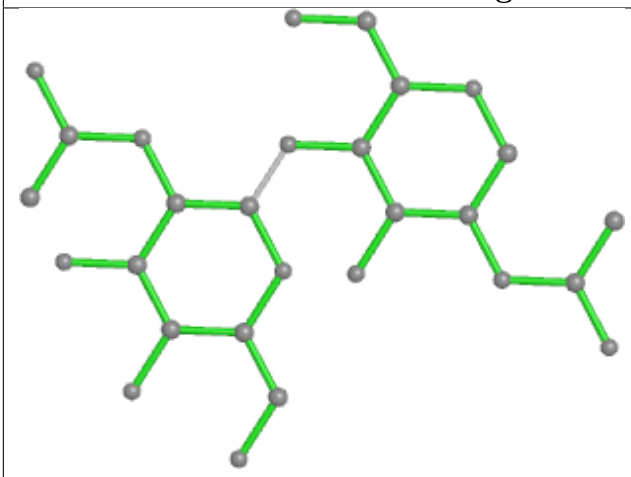
Mol	Chain	Res	Type	Atoms
4	H	3	BMA	C1-C2-C3-C4-C5-O5
4	H	4	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

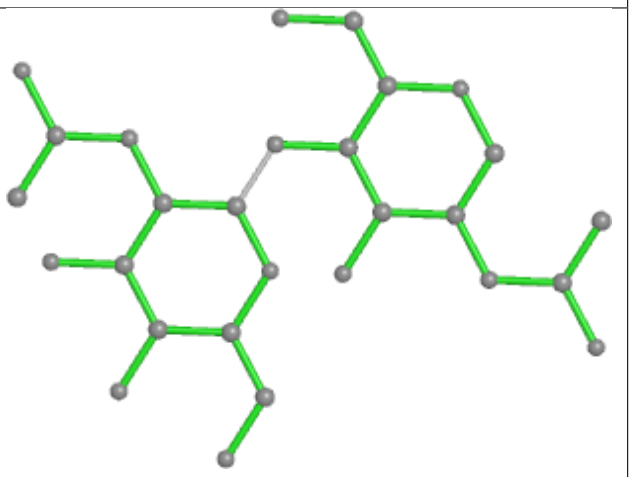
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	F	2	NAG	1	0

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

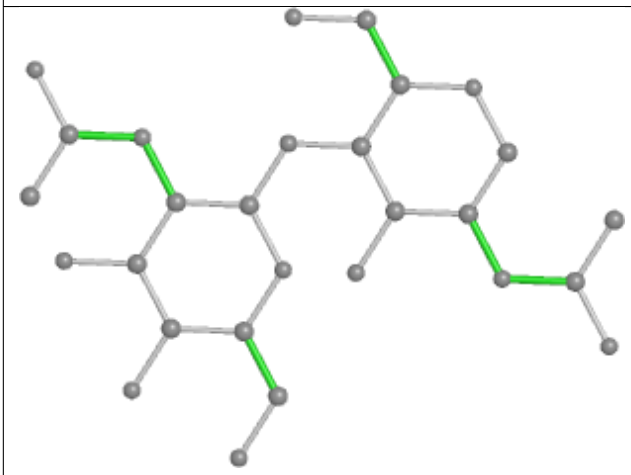
Oligosaccharide Chain C



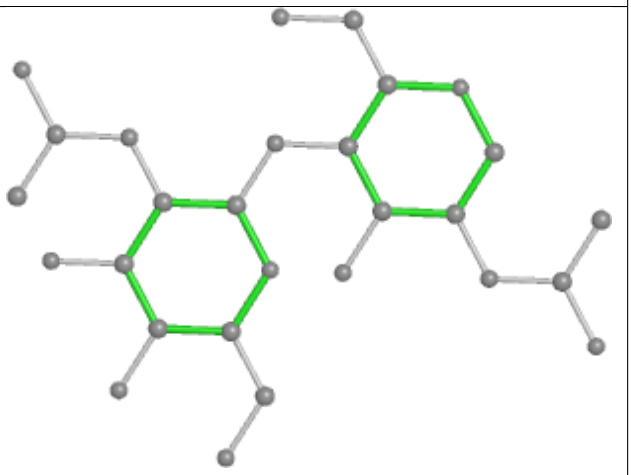
Bond lengths



Bond angles

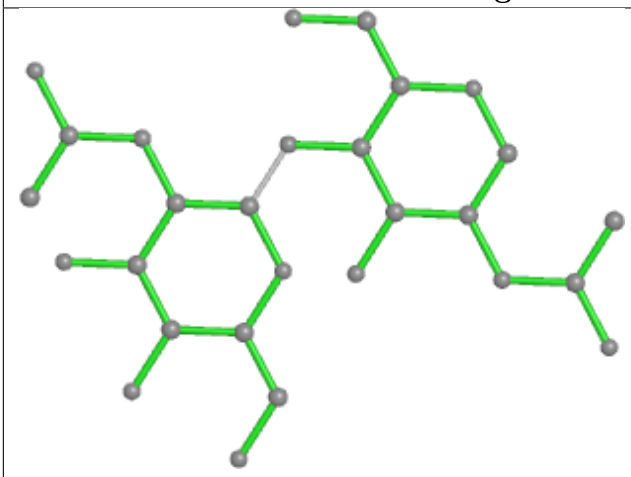


Torsions

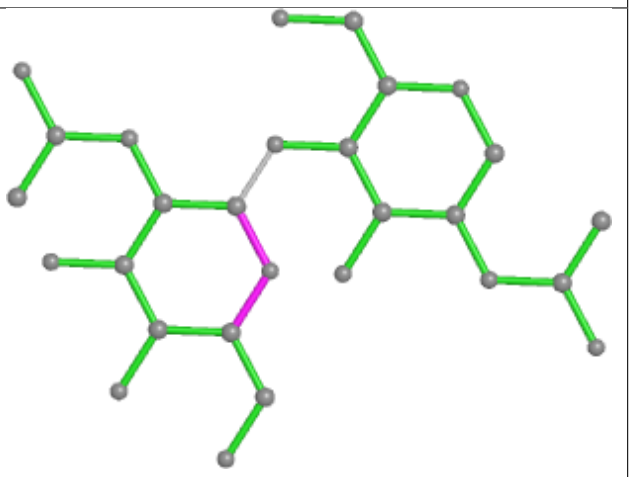


Rings

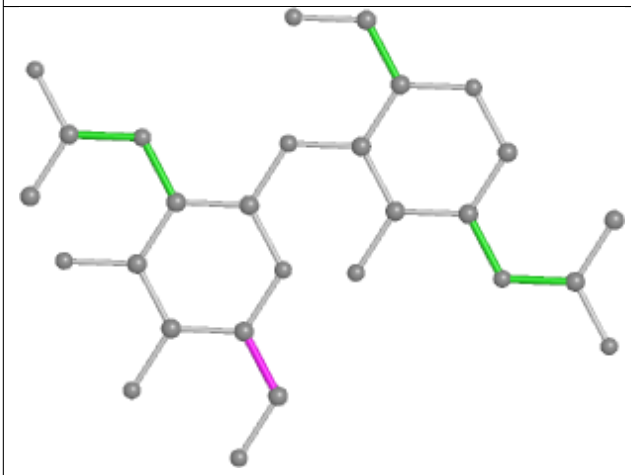
Oligosaccharide Chain D



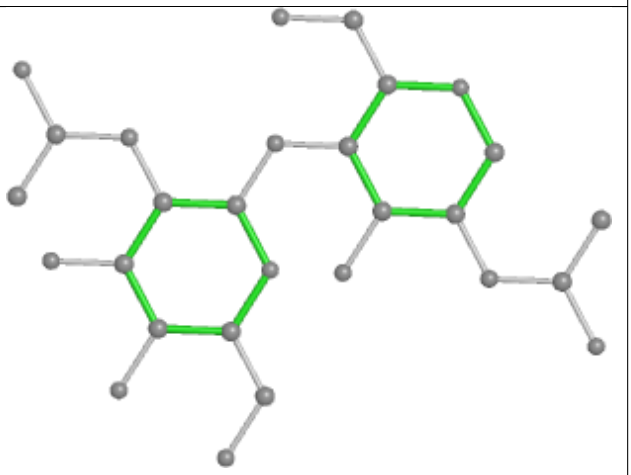
Bond lengths



Bond angles

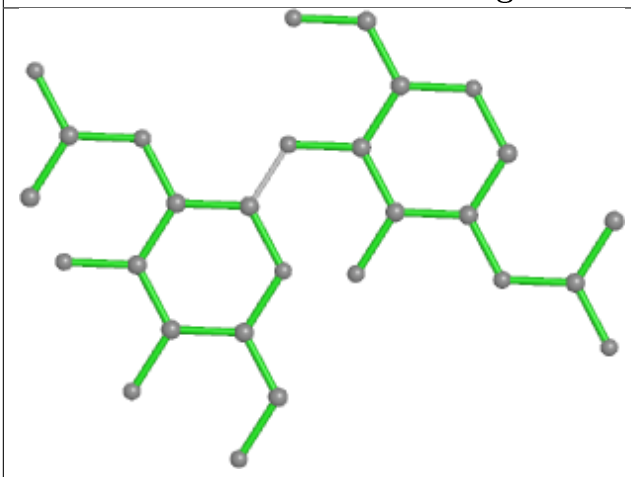


Torsions

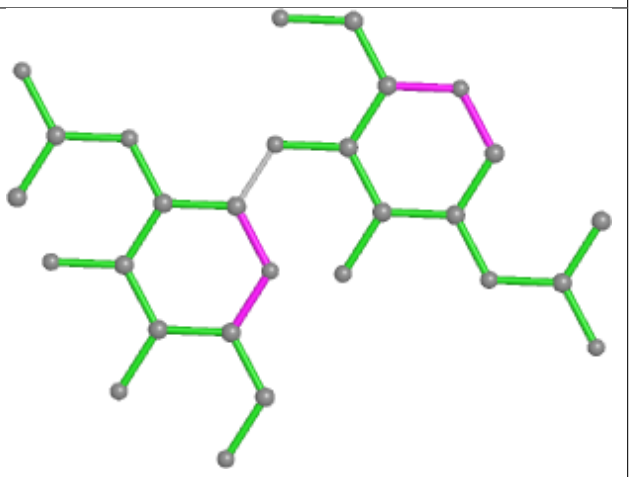


Rings

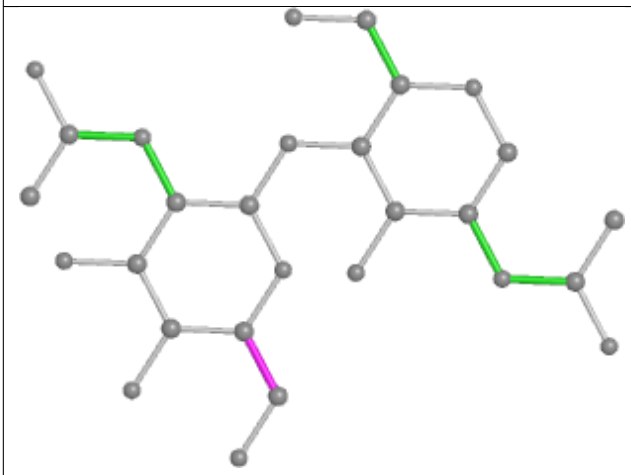
Oligosaccharide Chain F



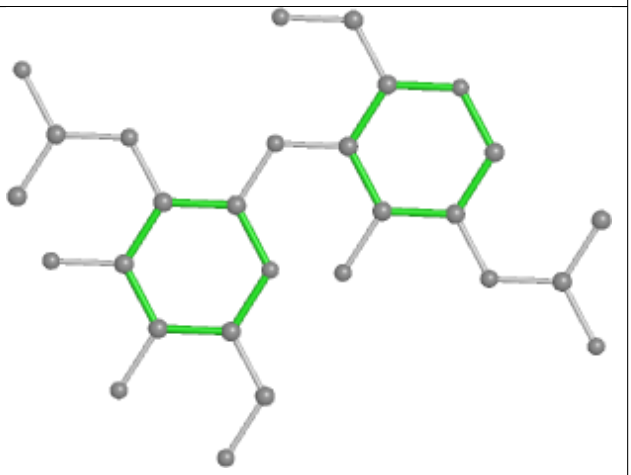
Bond lengths



Bond angles

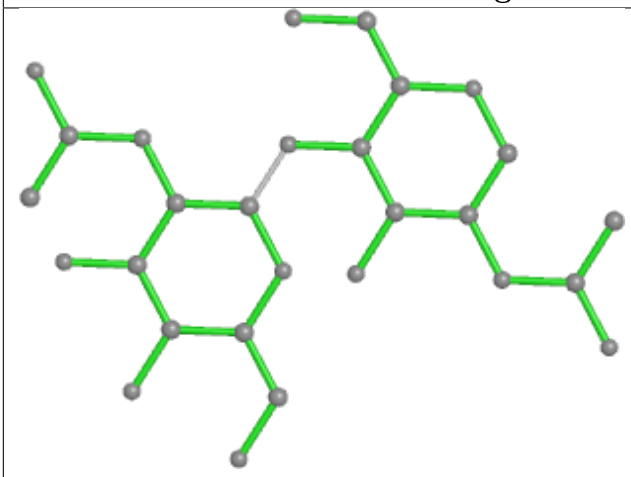


Torsions

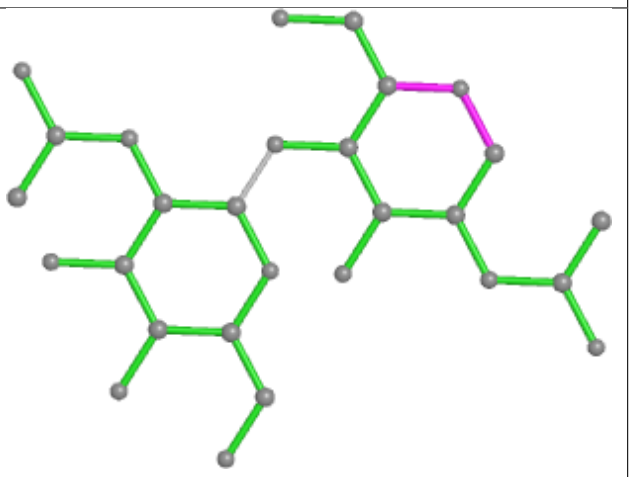


Rings

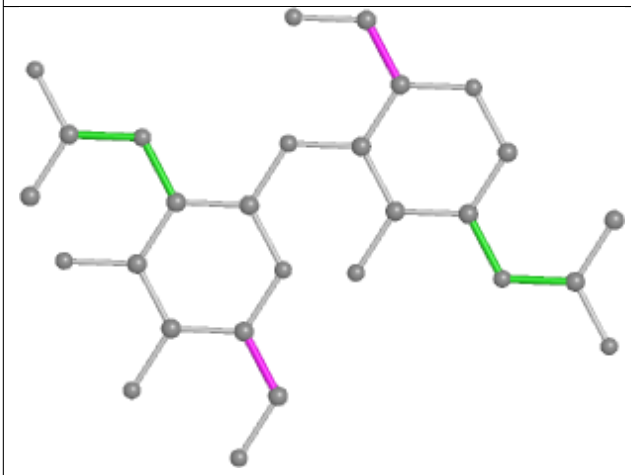
Oligosaccharide Chain G



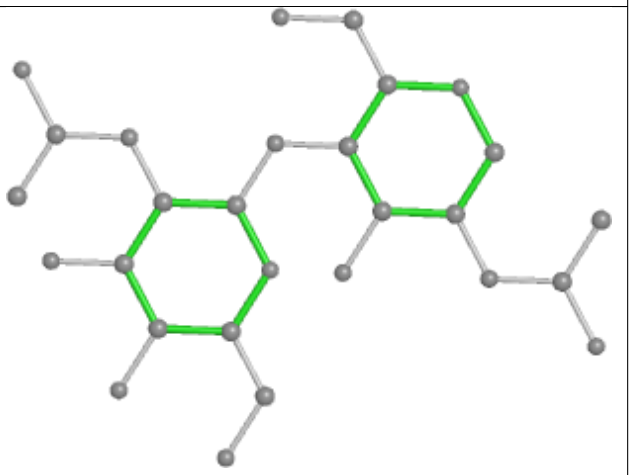
Bond lengths



Bond angles

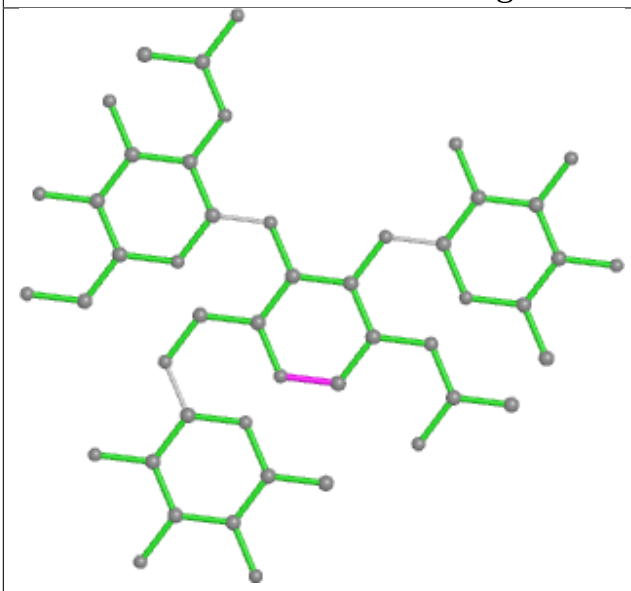


Torsions

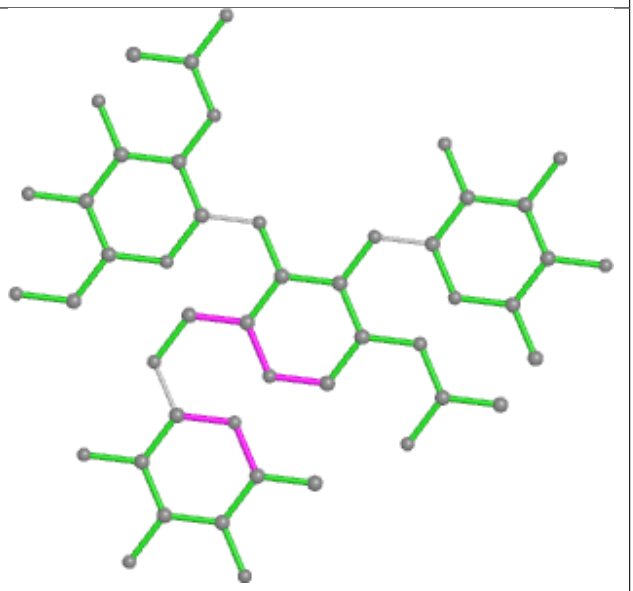


Rings

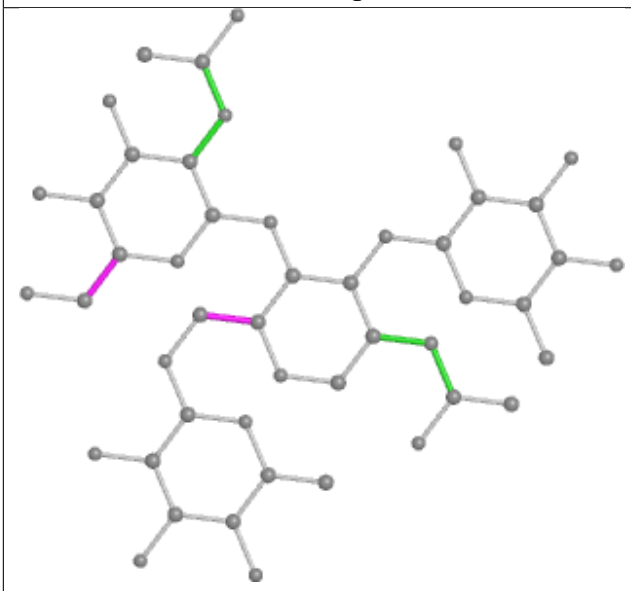
Oligosaccharide Chain E



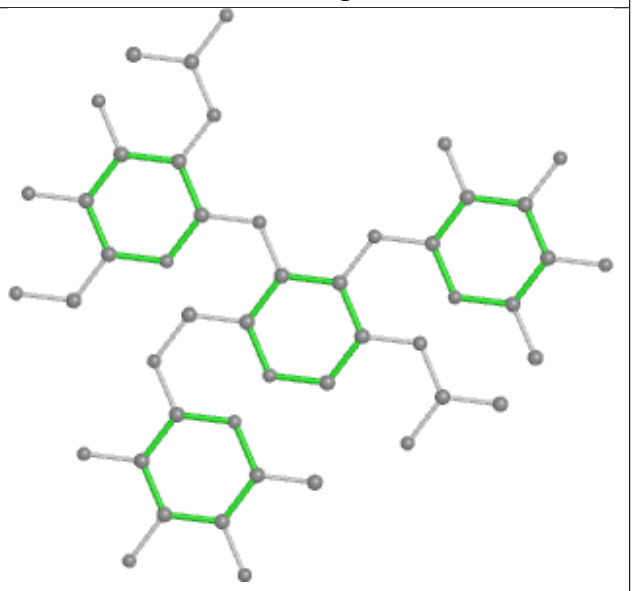
Bond lengths



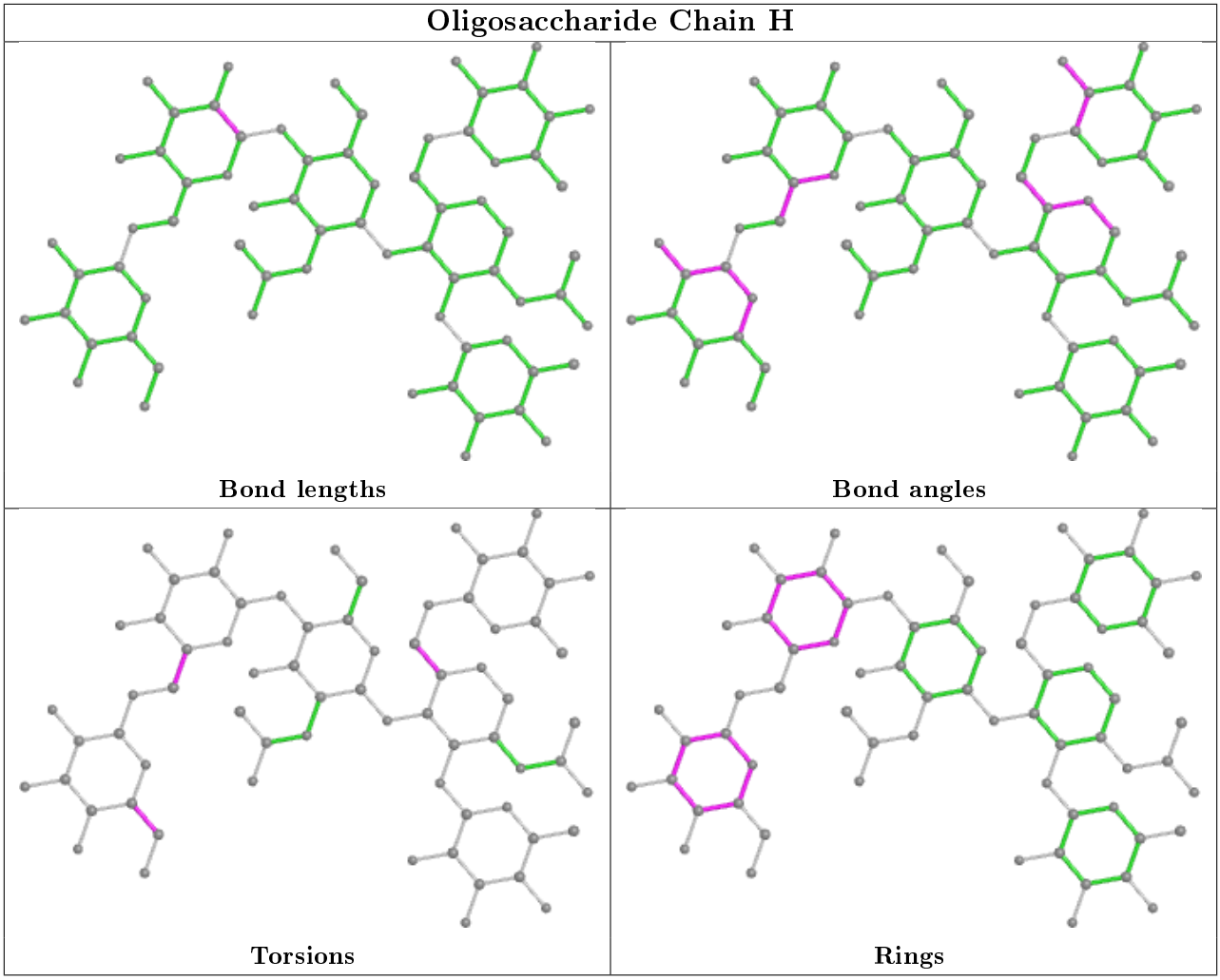
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
6	SO4	A	715	-	4,4,4	0.19	0	6,6,6	0.08	0
6	SO4	B	713	-	4,4,4	0.19	0	6,6,6	0.10	0
6	SO4	B	714	-	4,4,4	0.14	0	6,6,6	0.40	0
6	SO4	A	711	-	4,4,4	0.11	0	6,6,6	0.24	0
6	SO4	A	716	-	4,4,4	0.12	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	B	716	-	4,4,4	0.19	0	6,6,6	0.30	0
6	SO4	A	712	-	4,4,4	0.20	0	6,6,6	0.27	0
6	SO4	B	712	-	4,4,4	0.20	0	6,6,6	0.20	0
6	SO4	A	713	-	4,4,4	0.22	0	6,6,6	0.23	0
6	SO4	B	715	-	4,4,4	0.15	0	6,6,6	0.50	0
6	SO4	A	714	-	4,4,4	0.13	0	6,6,6	0.20	0
5	NAG	A	705	1	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
5	NAG	B	705	1	14,14,15	0.32	0	17,19,21	0.44	0
6	SO4	A	710	-	4,4,4	0.13	0	6,6,6	0.36	0
6	SO4	B	717	-	4,4,4	0.14	0	6,6,6	0.51	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
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	B	705	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	705	NAG	C1-O5-C5	2.42	115.47	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	NAG	O5-C5-C6-O6
5	B	705	NAG	C4-C5-C6-O6
5	A	705	NAG	C4-C5-C6-O6
5	B	705	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	712	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	713	SO4	1	0
6	B	715	SO4	2	0
6	A	714	SO4	2	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	436/441 (98%)	-0.23	14 (3%)	47	45	16, 26, 50, 80	0
1	B	429/441 (97%)	-0.05	30 (6%)	16	15	18, 29, 64, 104	0
All	All	865/882 (98%)	-0.14	44 (5%)	28	26	16, 27, 56, 104	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	GLY	7.5
1	B	585	ASP	6.7
1	B	581	TYR	6.2
1	A	176	GLN	6.0
1	B	604	SER	6.0
1	B	583	THR	5.6
1	B	389	TYR	5.4
1	A	583	THR	4.4
1	B	603	GLU	4.3
1	A	585	ASP	4.1
1	B	213	GLU	3.9
1	A	421	GLY	3.9
1	A	584	GLY	3.6
1	A	389	TYR	3.5
1	B	210	ASN	3.4
1	B	554	ASP	3.4
1	B	582	ASP	3.3
1	B	421	GLY	3.3
1	B	376	GLN	3.3
1	A	326	ASP	3.2
1	A	288	GLU	3.1
1	B	211	THR	3.0
1	B	380	SER	2.9
1	B	386	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	553	GLU	2.8
1	A	212	ARG	2.8
1	B	176	GLN	2.8
1	B	385	ILE	2.6
1	A	422	GLY	2.5
1	A	454	TYR	2.5
1	B	326	ASP	2.4
1	B	384	ILE	2.4
1	B	555	ASP	2.4
1	B	586	SER	2.3
1	B	378	ASN	2.2
1	B	242	ARG	2.2
1	B	212	ARG	2.1
1	B	422	GLY	2.1
1	B	423	ASP	2.1
1	A	386	HIS	2.1
1	B	377	TYR	2.1
1	B	587	VAL	2.1
1	A	378	ASN	2.0
1	B	491	SER	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
2	NAG	C	2	14/15	0.64	0.40	50,79,85,89	0
2	NAG	F	2	14/15	0.74	0.36	58,69,80,82	0
4	BMA	H	3	11/12	0.75	0.36	71,75,81,87	0
4	BMA	H	4	11/12	0.79	0.29	62,71,80,82	0
2	NAG	D	2	14/15	0.87	0.40	61,72,83,90	0
2	NAG	G	2	14/15	0.87	0.31	53,67,77,81	0
4	NAG	H	2	14/15	0.88	0.24	42,52,62,75	0
3	NAG	E	3	14/15	0.88	0.26	48,56,65,71	0

Continued on next page...

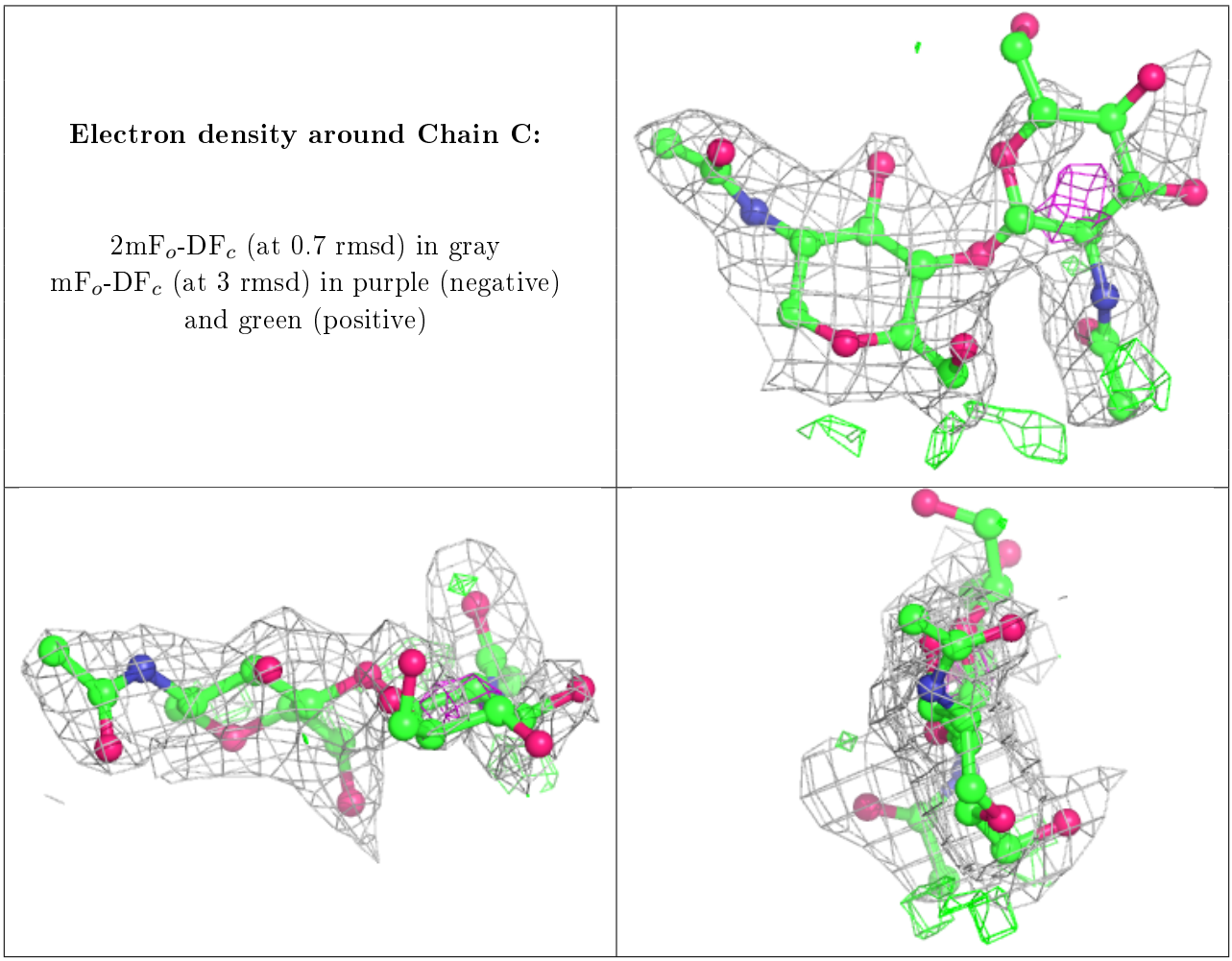
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	1	14/15	0.88	0.14	41,48,60,62	0
3	FUC	E	2	10/11	0.90	0.27	51,55,58,58	0
4	FUC	H	5	10/11	0.91	0.18	43,49,51,51	0
4	FUC	H	6	10/11	0.91	0.18	40,45,52,55	0
2	NAG	D	1	14/15	0.92	0.13	30,39,56,62	0
4	NAG	H	1	14/15	0.92	0.16	37,43,50,51	0
2	NAG	G	1	14/15	0.92	0.12	29,38,48,56	0
2	NAG	C	1	14/15	0.92	0.18	39,46,56,61	0
3	NAG	E	1	14/15	0.93	0.16	37,42,51,56	0
3	FUC	E	4	10/11	0.94	0.20	35,50,58,65	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.

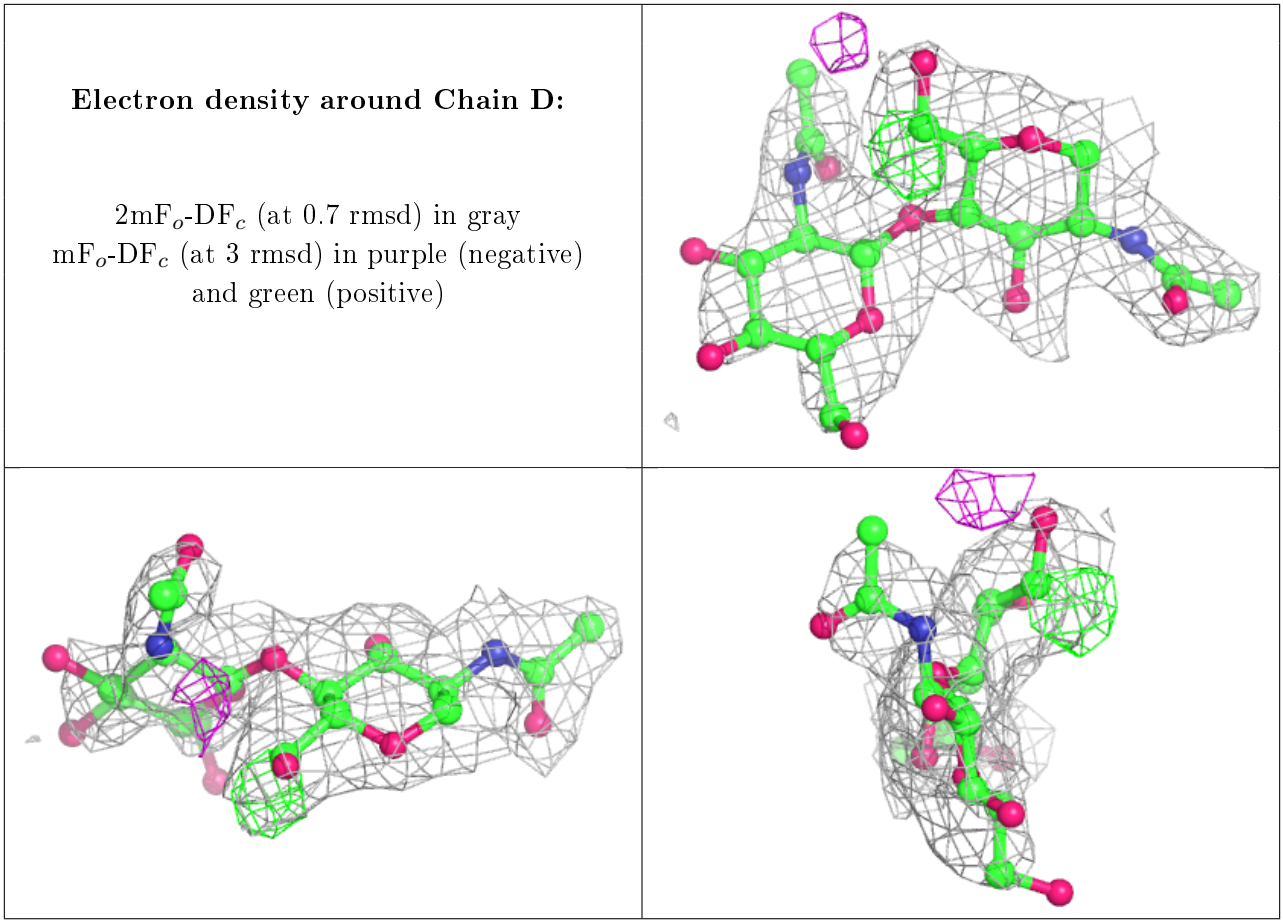
Electron density around Chain C:

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



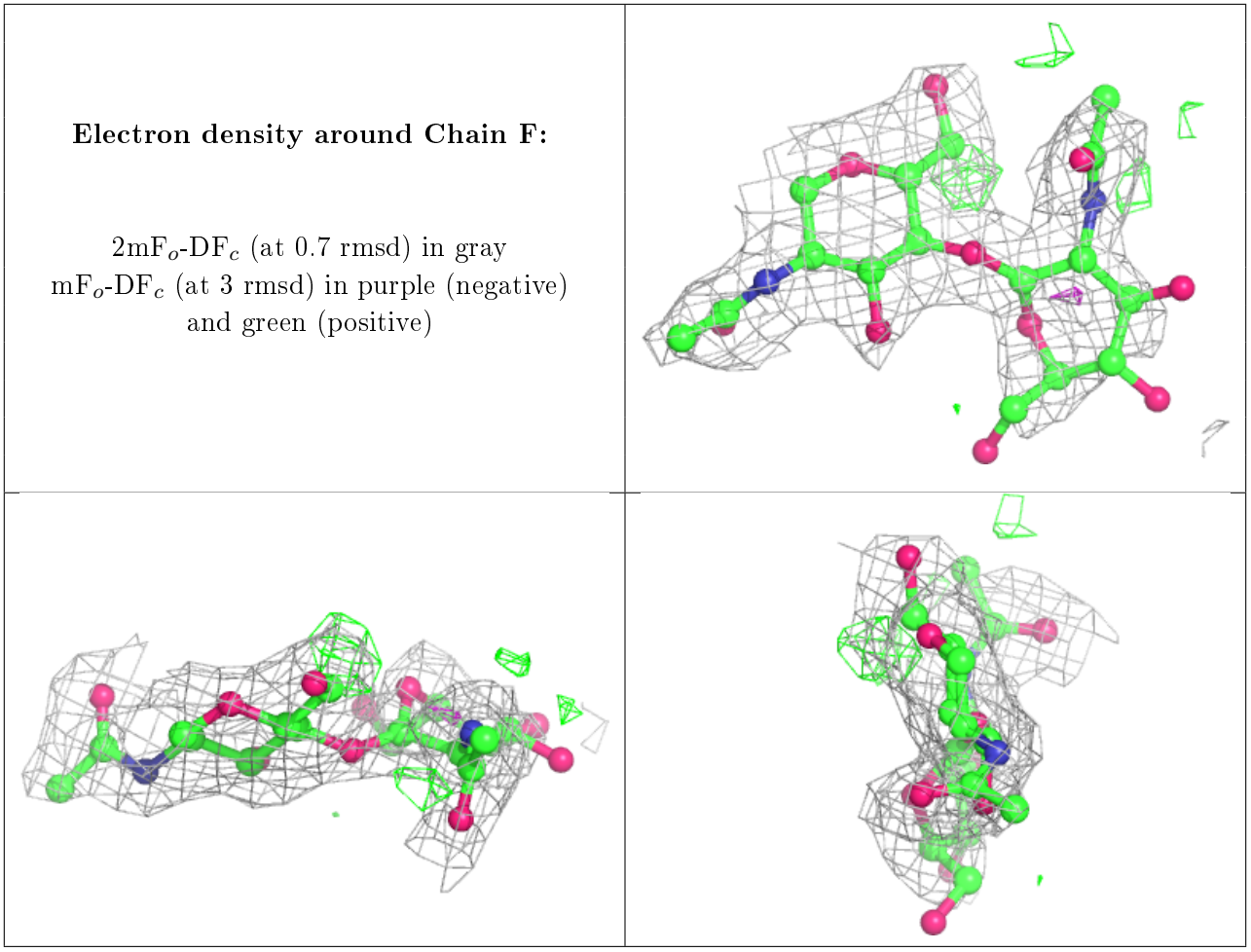
Electron density around Chain D:

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



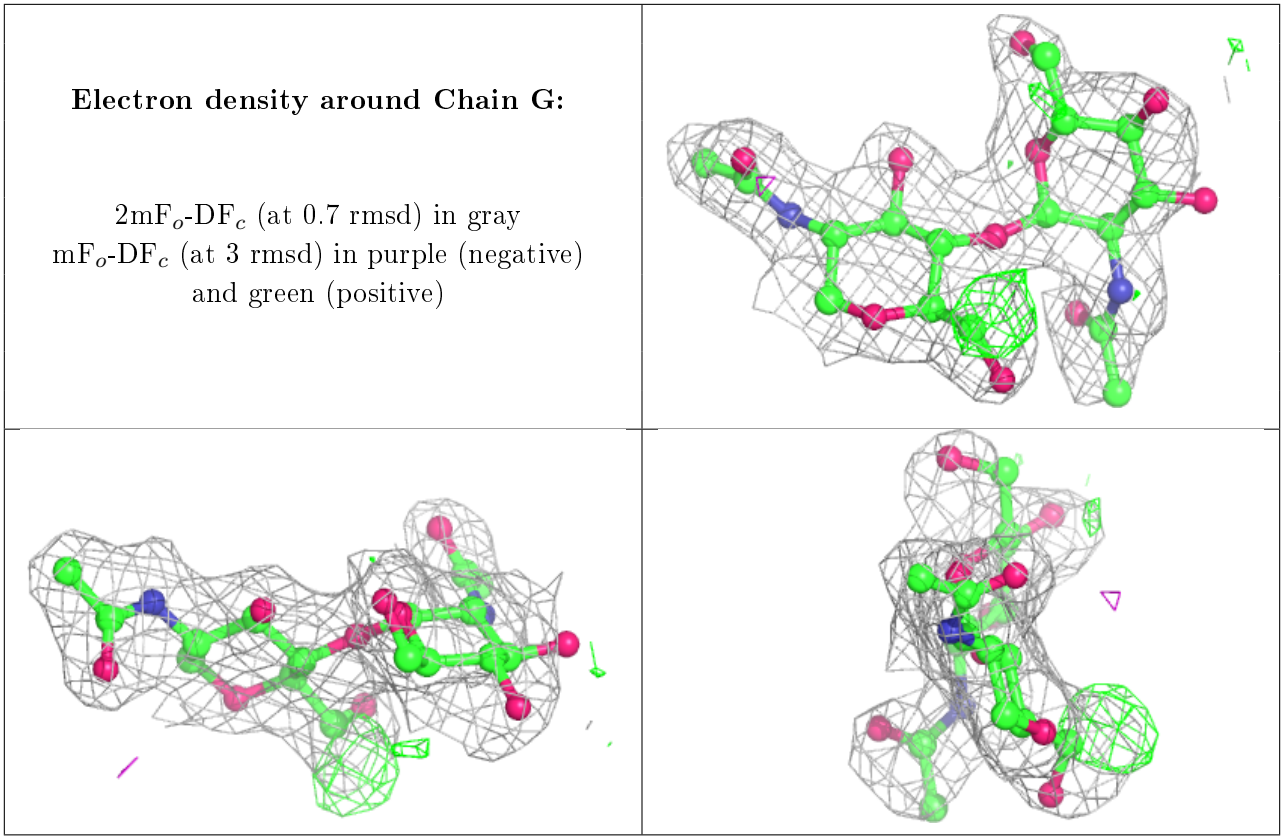
Electron density around Chain F:

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



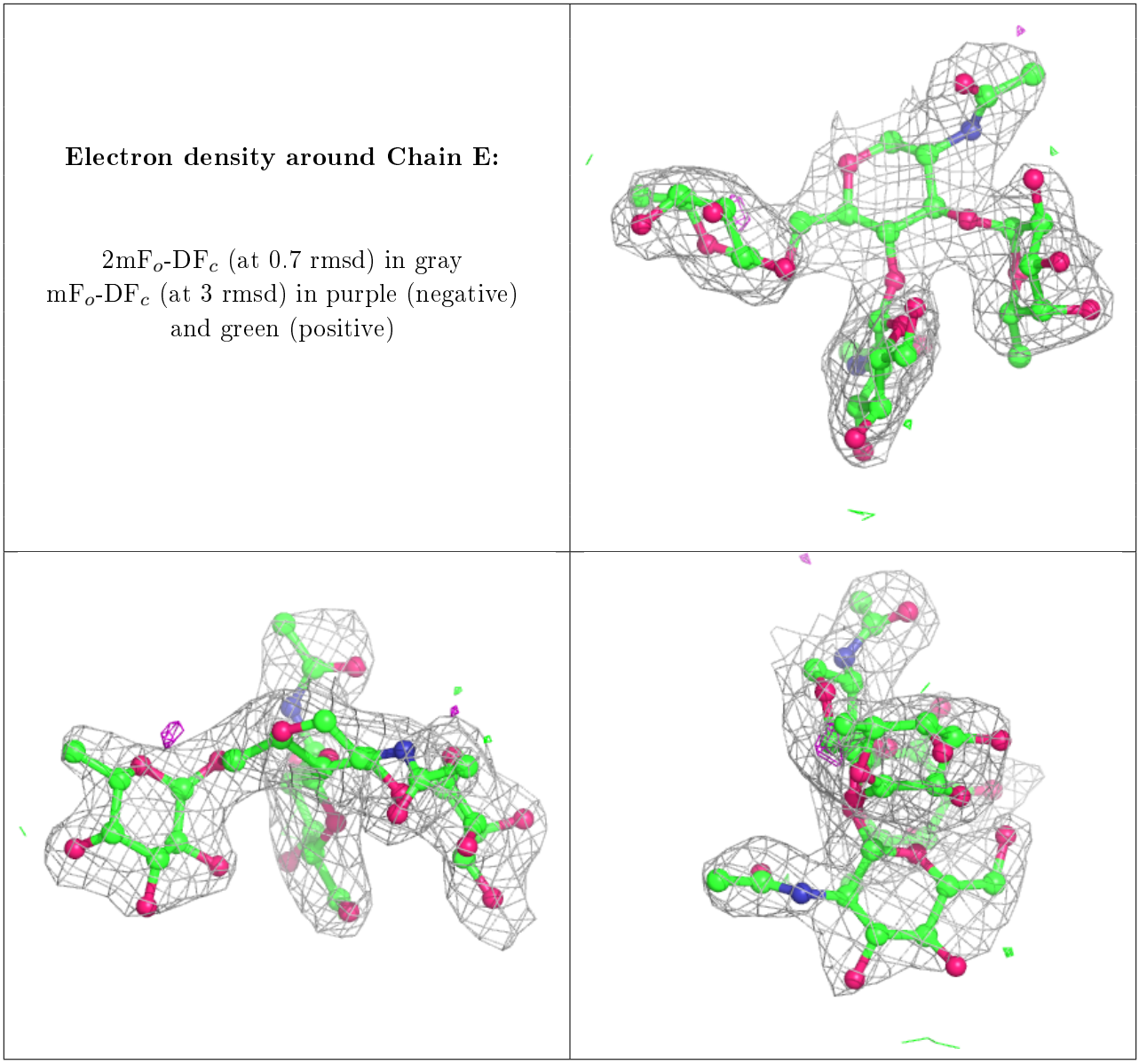
Electron density around Chain G:

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



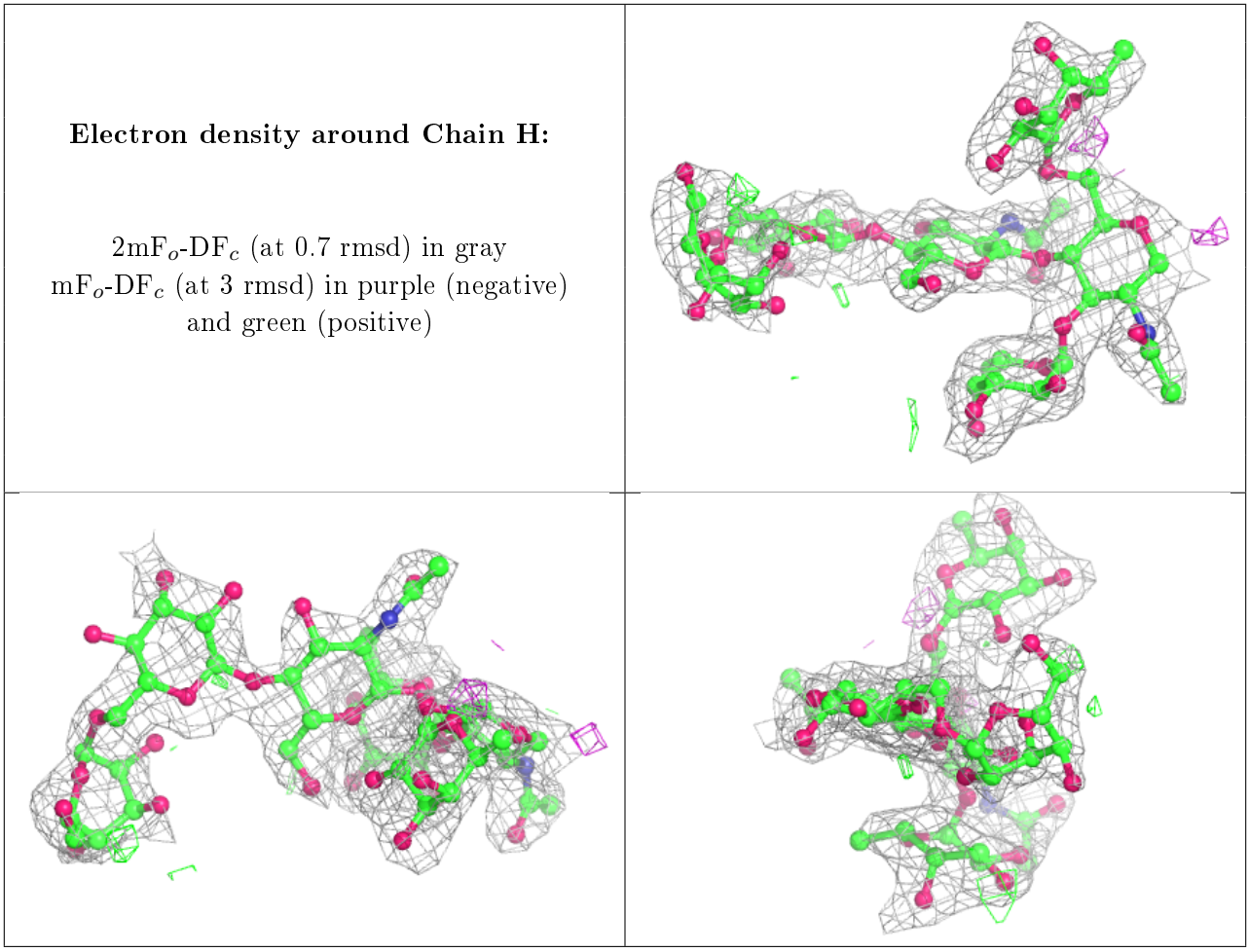
Electron density around Chain E:

$2mF_o$-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 H:

$2mF_o$-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
6	SO4	A	714	5/5	0.84	0.29	44,48,71,79	0
5	NAG	B	705	14/15	0.84	0.25	37,55,69,72	0
5	NAG	A	705	14/15	0.87	0.21	30,54,63,74	0
6	SO4	B	715	5/5	0.94	0.14	46,55,68,70	0
6	SO4	A	711	5/5	0.94	0.24	52,54,66,68	0
6	SO4	A	710	5/5	0.95	0.21	39,40,53,55	0
6	SO4	B	717	5/5	0.95	0.17	44,46,57,60	0
6	SO4	B	716	5/5	0.96	0.17	43,47,59,64	0
6	SO4	A	715	5/5	0.97	0.20	44,45,53,56	0
6	SO4	B	713	5/5	0.97	0.22	52,58,66,72	0
6	SO4	A	712	5/5	0.98	0.12	35,36,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	713	5/5	0.98	0.07	34,34,40,42	0
6	SO4	A	716	5/5	0.98	0.12	39,45,47,48	0
6	SO4	B	714	5/5	0.98	0.12	47,47,55,59	0
6	SO4	B	712	5/5	0.99	0.16	39,43,52,54	0

6.5 Other polymers

There are no such residues in this entry.