



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:18 AM BST

PDB ID : 3M5H
Title : Crystal structure of a H7 influenza virus hemagglutinin complexed with 3SLN
Authors : Yang, H.; Chen, L.M.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on : 2010-03-12
Resolution : 2.70 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

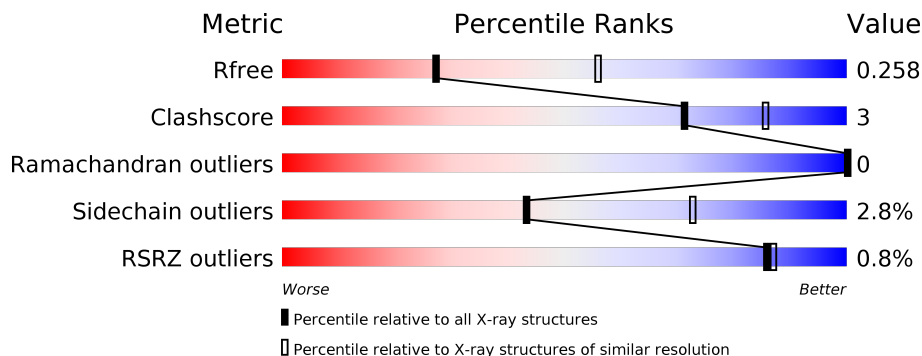
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	
1	C	317	
1	E	317	
2	B	182	
2	D	182	
2	F	182	

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Mol	Chain	Length	Quality of chain
3	G	3	 100%
3	K	3	 67%
4	H	2	 100%
4	J	2	 100%
5	I	2	 50%

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
4	NAG	H	2	-	-	-	X
4	NAG	J	2	-	-	-	X
6	NAG	E	331	X	-	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 11875 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2392	1488	433	458	13	0	0	0
1	C	309	2388	1486	432	457	13	0	0	0
1	E	309	2383	1482	431	457	13	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP B7NY59
A	8	ASP	-	expression tag	UNP B7NY59
A	9	PRO	-	expression tag	UNP B7NY59
A	216	ASN	SER	SEE REMARK 999	UNP B7NY59
A	257	THR	ALA	SEE REMARK 999	UNP B7NY59
A	309	VAL	ILE	SEE REMARK 999	UNP B7NY59
C	7	ALA	-	expression tag	UNP B7NY59
C	8	ASP	-	expression tag	UNP B7NY59
C	9	PRO	-	expression tag	UNP B7NY59
C	216	ASN	SER	SEE REMARK 999	UNP B7NY59
C	257	THR	ALA	SEE REMARK 999	UNP B7NY59
C	309	VAL	ILE	SEE REMARK 999	UNP B7NY59
E	7	ALA	-	expression tag	UNP B7NY59
E	8	ASP	-	expression tag	UNP B7NY59
E	9	PRO	-	expression tag	UNP B7NY59
E	216	ASN	SER	SEE REMARK 999	UNP B7NY59
E	257	THR	ALA	SEE REMARK 999	UNP B7NY59
E	309	VAL	ILE	SEE REMARK 999	UNP B7NY59

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1419	876	248	288	7			
2	D	172	Total	C	N	O	S	0	0	0
			1393	861	244	281	7			
2	F	171	Total	C	N	O	S	0	0	0
			1384	856	242	279	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
B	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
B	179	VAL	-	expression tag	UNP B7NYS1
B	180	PRO	-	expression tag	UNP B7NYS1
B	181	ARG	-	expression tag	UNP B7NYS1
B	182	GLY	-	expression tag	UNP B7NYS1
D	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
D	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
D	179	VAL	-	expression tag	UNP B7NYS1
D	180	PRO	-	expression tag	UNP B7NYS1
D	181	ARG	-	expression tag	UNP B7NYS1
D	182	GLY	-	expression tag	UNP B7NYS1
F	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
F	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
F	179	VAL	-	expression tag	UNP B7NYS1
F	180	PRO	-	expression tag	UNP B7NYS1
F	181	ARG	-	expression tag	UNP B7NYS1
F	182	GLY	-	expression tag	UNP B7NYS1

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	K	3	Total	C	N	O	0	0	0
			46	25	2	19			

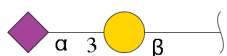
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



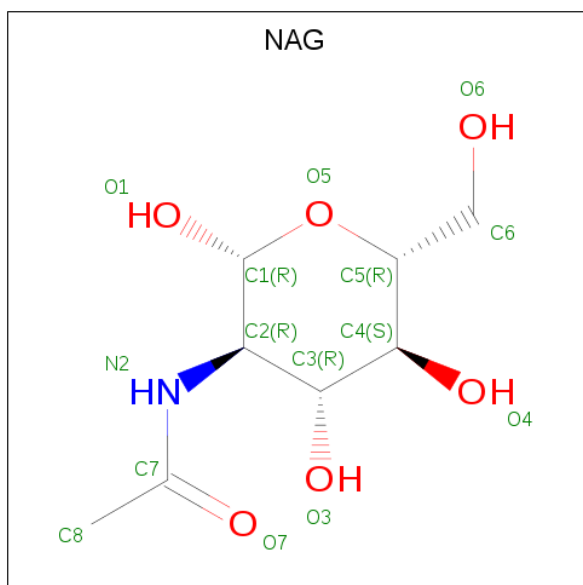
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



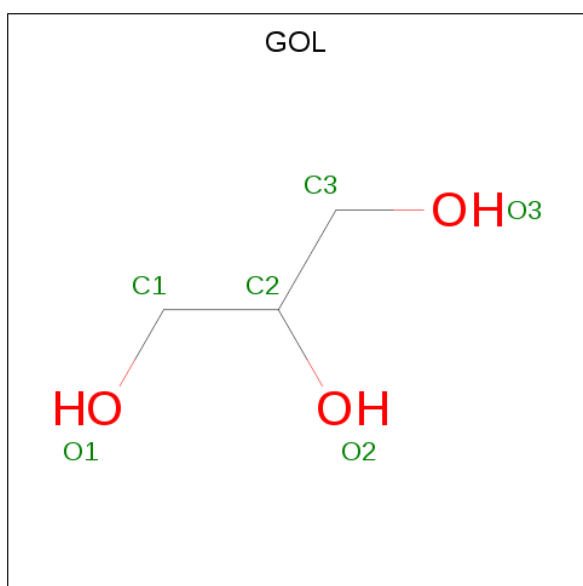
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	2	31	17	1	13	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	44	Total	O	0	0
			44	44		

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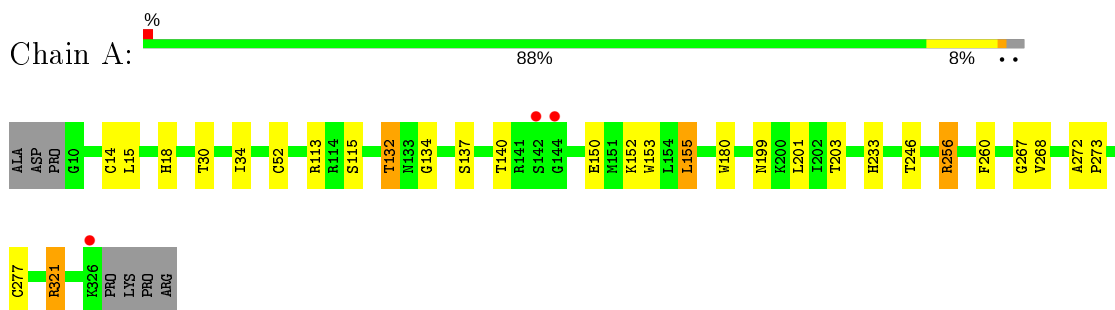
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	46	Total 46	O 46	0	0
8	D	29	Total 29	O 29	0	0
8	E	56	Total 56	O 56	0	0
8	F	33	Total 33	O 33	0	0

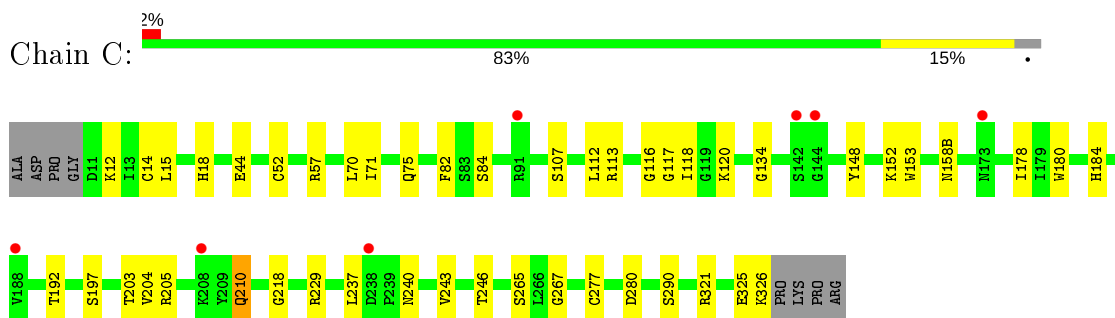
3 Residue-property plots [i](#)

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.

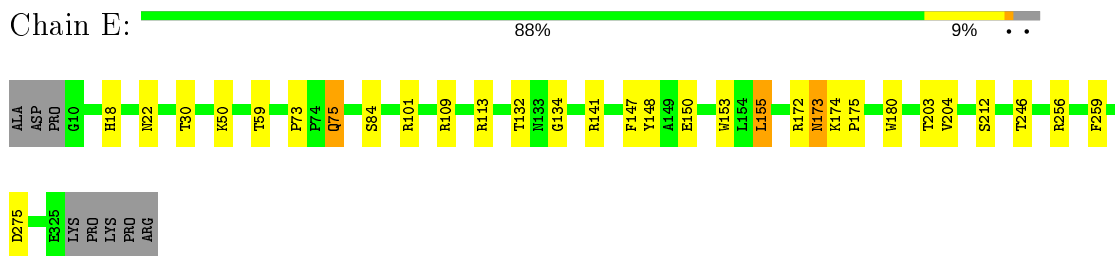
- Molecule 1: Hemagglutinin



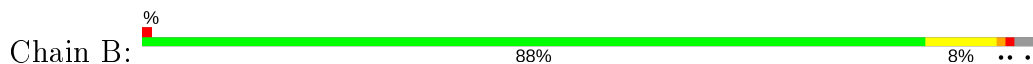
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

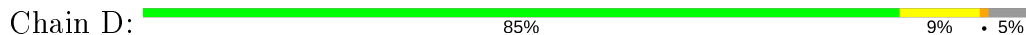


- Molecule 2: Hemagglutinin

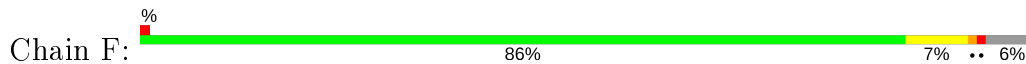




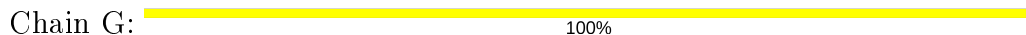
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



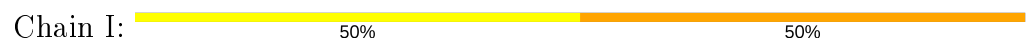
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



GAL1
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.80Å 116.70Å 249.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 26.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.70) 98.5 (26.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.214 , 0.264 0.211 , 0.258	Depositor DCC
R_{free} test set	2769 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SIA, GAL, 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	0.34	0/2440	0.51	1/3297 (0.0%)
1	C	0.35	0/2436	0.49	0/3292
1	E	0.35	0/2431	0.53	1/3286 (0.0%)
2	B	0.34	0/1443	0.48	1/1945 (0.1%)
2	D	0.34	0/1417	0.50	0/1910
2	F	0.34	0/1408	0.52	1/1898 (0.1%)
All	All	0.35	0/11575	0.51	4/15628 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	155	LEU	CA-CB-CG	5.30	127.49	115.30
2	F	110	LEU	CA-CB-CG	5.12	127.07	115.30
1	E	155	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2392	0	2353	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2388	0	2350	24	0
1	E	2383	0	2340	15	0
2	B	1419	0	1324	10	0
2	D	1393	0	1301	14	0
2	F	1384	0	1293	11	0
3	G	46	0	40	0	0
3	K	46	0	40	1	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
5	I	31	0	26	1	0
6	A	14	0	13	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	B	12	0	16	0	0
7	D	6	0	8	1	0
7	F	6	0	8	1	0
8	A	49	0	0	0	0
8	B	44	0	0	0	0
8	C	46	0	0	0	0
8	D	29	0	0	0	0
8	E	56	0	0	0	0
8	F	33	0	0	0	0
All	All	11875	0	11201	79	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 3.

All (79) 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:C:205:ARG:HG3	1:C:210:GLN:HG3	1.48	0.93
2:F:121:ARG:HG2	2:F:121:ARG:HH11	1.34	0.89
1:E:141:ARG:NH2	1:E:147:PHE:O	2.20	0.74
1:C:237:LEU:HD22	1:C:243:VAL:HG23	1.74	0.70
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.74	0.68
2:B:97:GLU:HG2	7:F:184:GOL:H32	1.75	0.67
2:F:121:ARG:HG2	2:F:121:ARG:NH1	2.03	0.67
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.80	0.63
1:A:132:THR:HG23	1:A:152:LYS:HD2	1.85	0.59
1:E:174:LYS:HB2	1:E:175:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LYS:HD3	2:D:134:GLY:HA2	1.84	0.58
1:A:15:LEU:HD22	2:B:119:TYR:HA	1.84	0.58
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.86	0.57
1:C:57:ARG:O	1:C:84:SER:HB2	2.06	0.56
1:E:50:LYS:HG2	1:E:275:ASP:HB2	1.88	0.56
2:F:68:ASN:HB3	2:F:71:ASN:O	2.07	0.55
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.07	0.54
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.89	0.54
1:C:203:THR:HB	1:C:246:THR:OG1	2.07	0.54
1:C:158(B):ASN:HA	1:C:192:THR:O	2.08	0.53
1:E:150:GLU:OE1	1:E:256:ARG:HD3	2.08	0.53
1:E:203:THR:OG1	1:E:246:THR:HB	2.10	0.52
2:F:121:ARG:CG	2:F:121:ARG:HH11	2.14	0.52
1:C:15:LEU:HD22	2:D:119:TYR:HA	1.92	0.51
2:B:77:ILE:HD11	2:D:80:VAL:HG21	1.92	0.51
1:C:178:ILE:HG13	1:C:243:VAL:HG21	1.93	0.50
1:E:109:ARG:O	1:E:113:ARG:HG3	2.11	0.50
1:A:30:THR:O	2:F:50:GLY:HA3	2.12	0.50
2:D:54:ARG:HH21	7:D:184:GOL:H32	1.77	0.49
1:A:201:LEU:HD22	1:C:218:GLY:HA3	1.94	0.49
2:D:88:MET:CE	2:D:88:MET:HA	2.43	0.49
1:C:107:SER:HB3	2:F:75:GLN:HB2	1.94	0.49
2:F:19:ASN:HB2	2:F:36:ALA:HB2	1.95	0.48
2:F:27:GLN:NE2	2:F:32:GLU:HG3	2.31	0.46
1:C:116:GLY:HA2	1:C:265:SER:HB3	1.97	0.46
2:B:47:GLN:HB3	2:B:110:LEU:HD11	1.98	0.46
2:D:47:GLN:HB3	2:D:110:LEU:HD11	1.98	0.46
1:A:52:CYS:HB3	1:A:277:CYS:O	2.16	0.46
1:C:44:GLU:HG2	1:C:290:SER:HB2	1.97	0.46
1:E:173:ASN:ND2	1:E:174:LYS:HE2	2.31	0.45
1:C:52:CYS:HB3	1:C:277:CYS:O	2.16	0.45
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.52	0.45
1:C:14:CYS:HA	2:D:137:CYS:HA	1.98	0.44
1:E:172:ARG:HG3	1:E:259:PHE:CZ	2.52	0.44
1:C:70:LEU:HD21	1:C:112:LEU:HD21	1.99	0.44
1:C:113:ARG:HB3	1:C:267:GLY:HA3	1.99	0.44
1:A:14:CYS:HA	2:B:137:CYS:HA	1.98	0.44
2:F:131:GLU:OE2	2:F:170:ARG:HD2	2.18	0.44
2:D:140:ILE:HG22	2:D:142:HIS:H	1.83	0.43
1:C:12:LYS:HA	2:D:140:ILE:HD12	2.01	0.43
1:A:113:ARG:HG2	1:A:267:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PHE:CE1	1:C:117:GLY:HA2	2.54	0.43
3:K:2:GAL:H3	3:K:3:SIA:H32	1.95	0.43
2:D:18:ILE:H	2:D:18:ILE:HG13	1.68	0.42
2:D:131:GLU:OE2	2:D:170:ARG:HD2	2.19	0.42
1:E:73:PRO:HB2	1:E:75:GLN:OE1	2.19	0.42
1:E:59:THR:OG1	1:E:84:SER:HB2	2.19	0.42
1:A:34:ILE:HG13	1:A:321:ARG:HH21	1.84	0.42
1:E:147:PHE:CG	1:E:148:TYR:N	2.87	0.42
2:B:66:ILE:HG13	2:B:66:ILE:H	1.61	0.42
1:E:203:THR:HG22	1:E:212:SER:HB3	2.01	0.42
1:C:118:ILE:HD12	1:C:120:LYS:HE3	2.01	0.42
2:B:3:PHE:HZ	2:D:2:LEU:HB3	1.85	0.42
2:B:141:PHE:CG	2:B:170:ARG:HG2	2.55	0.41
1:C:71:ILE:O	1:C:148:TYR:HB3	2.20	0.41
1:C:70:LEU:HD11	1:C:112:LEU:HD11	2.03	0.41
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.96	0.41
2:D:19:ASN:OD1	2:D:19:ASN:N	2.52	0.41
2:D:77:ILE:HD11	2:F:77:ILE:HG12	2.01	0.41
1:A:180:TRP:CE2	1:A:233:HIS:HB2	2.56	0.41
1:C:192:THR:HG22	1:C:197:SER:HA	2.03	0.41
5:I:1:GAL:H3	5:I:2:SIA:H32	1.98	0.41
1:A:137:SER:O	1:A:140:THR:HG23	2.22	0.40
1:A:203:THR:HB	1:A:246:THR:OG1	2.22	0.40
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.56	0.40
1:E:150:GLU:OE1	1:E:256:ARG:CD	2.70	0.40
1:A:115:SER:HB2	1:A:260:PHE:CD1	2.57	0.40
1:C:184:HIS:HB2	1:C:229:ARG:HG2	2.03	0.40
2:F:47:GLN:HB3	2:F:110:LEU:HD11	2.04	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	308/317 (97%)	294 (96%)	14 (4%)	0	100	100
1	C	307/317 (97%)	296 (96%)	11 (4%)	0	100	100
1	E	307/317 (97%)	295 (96%)	12 (4%)	0	100	100
2	B	174/182 (96%)	169 (97%)	5 (3%)	0	100	100
2	D	170/182 (93%)	165 (97%)	5 (3%)	0	100	100
2	F	169/182 (93%)	165 (98%)	4 (2%)	0	100	100
All	All	1435/1497 (96%)	1384 (96%)	51 (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	265/271 (98%)	258 (97%)	7 (3%)	46	75
1	C	265/271 (98%)	256 (97%)	9 (3%)	37	66
1	E	264/271 (97%)	256 (97%)	8 (3%)	41	70
2	B	150/155 (97%)	145 (97%)	5 (3%)	38	67
2	D	147/155 (95%)	144 (98%)	3 (2%)	55	81
2	F	146/155 (94%)	143 (98%)	3 (2%)	53	80
All	All	1237/1278 (97%)	1202 (97%)	35 (3%)	43	73

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	132	THR
1	A	155	LEU
1	A	199	ASN
1	A	256	ARG
1	A	268	VAL
1	A	321	ARG

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Mol	Chain	Res	Type
2	B	12	ASN
2	B	66	ILE
2	B	72	GLU
2	B	110	LEU
2	B	154	ASN
1	C	18	HIS
1	C	75	GLN
1	C	152	LYS
1	C	210	GLN
1	C	240	ASN
1	C	280	ASP
1	C	321	ARG
1	C	325	GLU
1	C	326	LYS
2	D	12	ASN
2	D	19	ASN
2	D	154	ASN
1	E	18	HIS
1	E	22	ASN
1	E	30	THR
1	E	75	GLN
1	E	101	ARG
1	E	132	THR
1	E	155	LEU
1	E	173	ASN
2	F	65	LEU
2	F	110	LEU
2	F	121	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

12 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	G	1	3	15,15,15	0.48	0	21,21,21	1.18	2 (9%)
3	GAL	G	2	3	11,11,12	0.60	0	15,15,17	1.04	1 (6%)
3	SIA	G	3	3	17,20,21	0.41	0	21,28,31	1.08	2 (9%)
4	NAG	H	1	2,4	14,14,15	0.54	0	17,19,21	1.27	2 (11%)
4	NAG	H	2	4	14,14,15	0.70	0	17,19,21	1.38	3 (17%)
5	GAL	I	1	5	11,11,12	0.65	0	15,15,17	0.80	0
5	SIA	I	2	5	17,20,21	0.58	0	21,28,31	1.15	1 (4%)
4	NAG	J	1	1,4	14,14,15	0.55	0	17,19,21	0.94	1 (5%)
4	NAG	J	2	4	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
3	NAG	K	1	3	15,15,15	0.44	0	21,21,21	0.85	1 (4%)
3	GAL	K	2	3	11,11,12	0.61	0	15,15,17	0.68	0
3	SIA	K	3	3	17,20,21	0.44	0	21,28,31	0.91	1 (4%)

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	G	1	3	-	2/6/26/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	SIA	G	3	3	-	4/14/34/38	0/1/1/1
4	NAG	H	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
5	GAL	I	1	5	-	1/2/19/22	0/1/1/1
5	SIA	I	2	5	-	4/14/34/38	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	3	-	2/6/26/26	0/1/1/1
3	GAL	K	2	3	-	2/2/19/22	0/1/1/1
3	SIA	K	3	3	-	2/14/34/38	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	SIA	C6-O6-C2	3.79	119.44	111.34
3	G	1	NAG	C4-C3-C2	3.51	115.48	110.34
4	H	1	NAG	C4-C3-C2	3.36	115.94	111.02
3	K	3	SIA	C6-O6-C2	3.22	118.22	111.34
4	H	2	NAG	C4-C3-C2	3.19	115.69	111.02
4	J	1	NAG	C4-C3-C2	2.79	115.11	111.02
4	H	2	NAG	C2-N2-C7	2.76	126.83	122.90
3	G	3	SIA	C6-O6-C2	2.69	117.09	111.34
3	G	3	SIA	C4-C3-C2	2.44	114.18	109.81
3	G	1	NAG	C3-C4-C5	2.39	114.50	110.24
4	H	2	NAG	O5-C5-C6	2.35	110.88	107.20
4	J	2	NAG	C1-O5-C5	2.28	115.28	112.19
4	H	1	NAG	O5-C1-C2	-2.28	107.68	111.29
3	G	2	GAL	C1-C2-C3	2.17	112.33	109.67
3	K	1	NAG	C4-C3-C2	2.11	113.44	110.34

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	SIA	C7-C8-C9-O9
5	I	2	SIA	O8-C8-C9-O9
3	K	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	G	3	SIA	C11-C10-N5-C5
3	G	3	SIA	O10-C10-N5-C5
5	I	2	SIA	C11-C10-N5-C5
5	I	2	SIA	O10-C10-N5-C5
3	K	3	SIA	C11-C10-N5-C5
3	K	3	SIA	O10-C10-N5-C5
3	G	1	NAG	C4-C5-C6-O6

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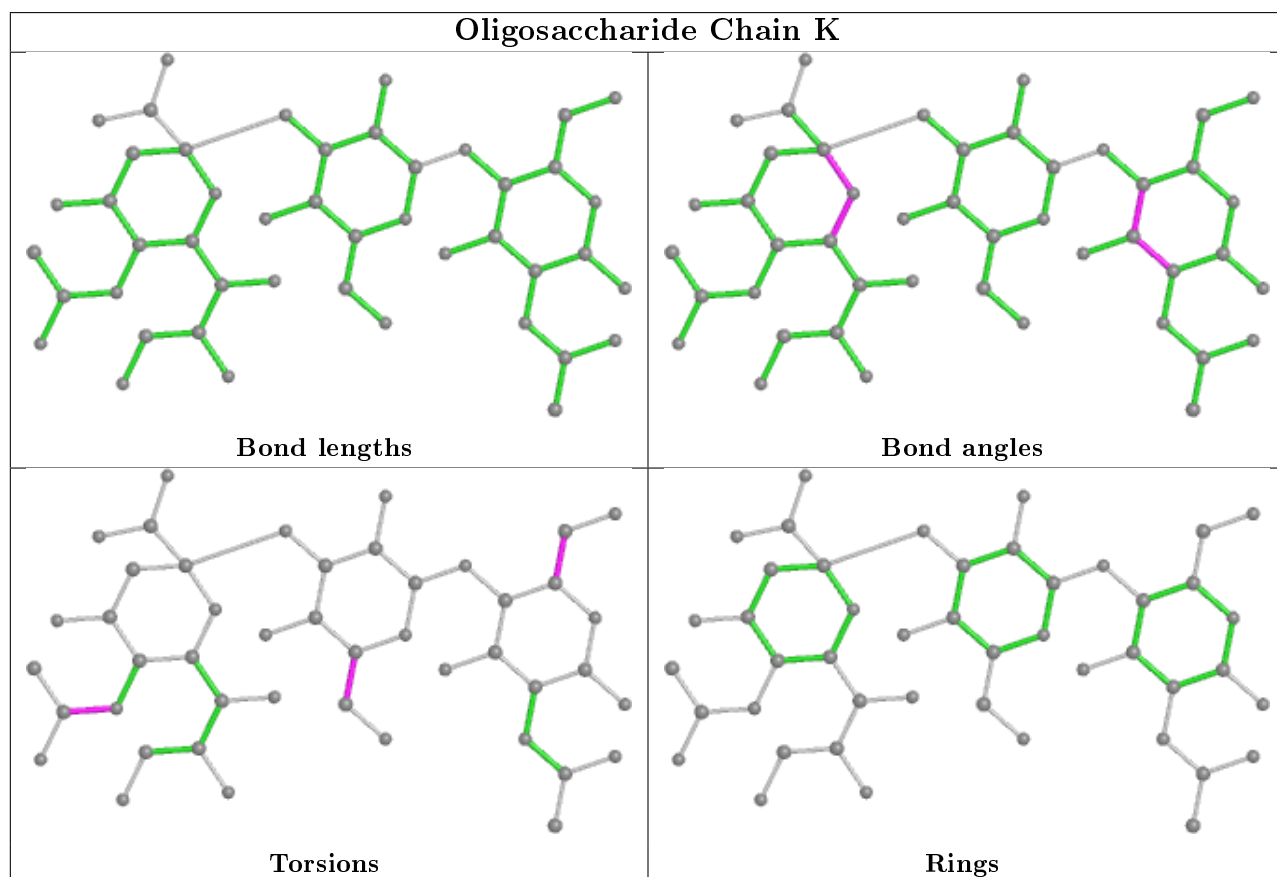
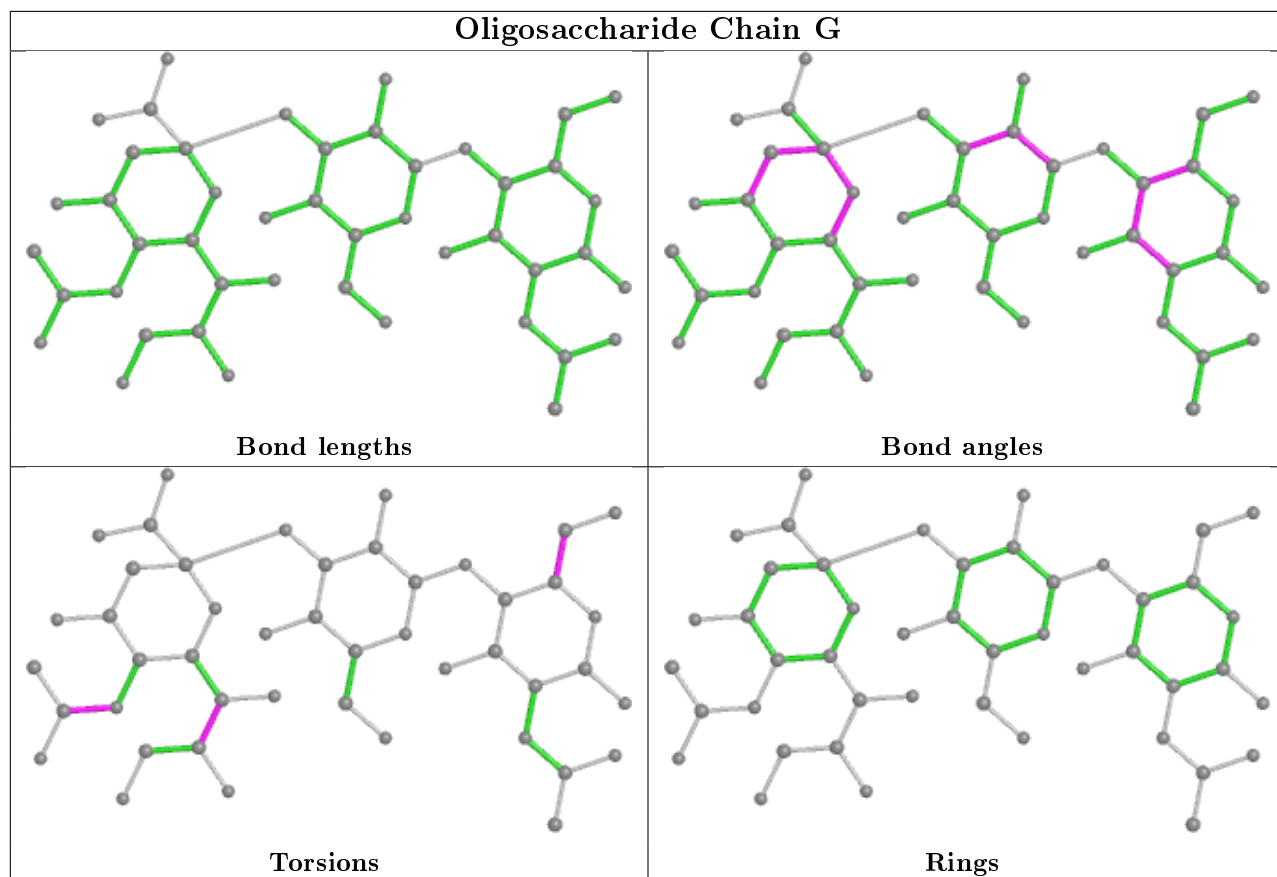
Mol	Chain	Res	Type	Atoms
3	K	2	GAL	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	K	2	GAL	C4-C5-C6-O6
3	G	3	SIA	C6-C7-C8-O8
4	H	2	NAG	C1-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6
5	I	1	GAL	C4-C5-C6-O6
3	G	3	SIA	C6-C7-C8-C9

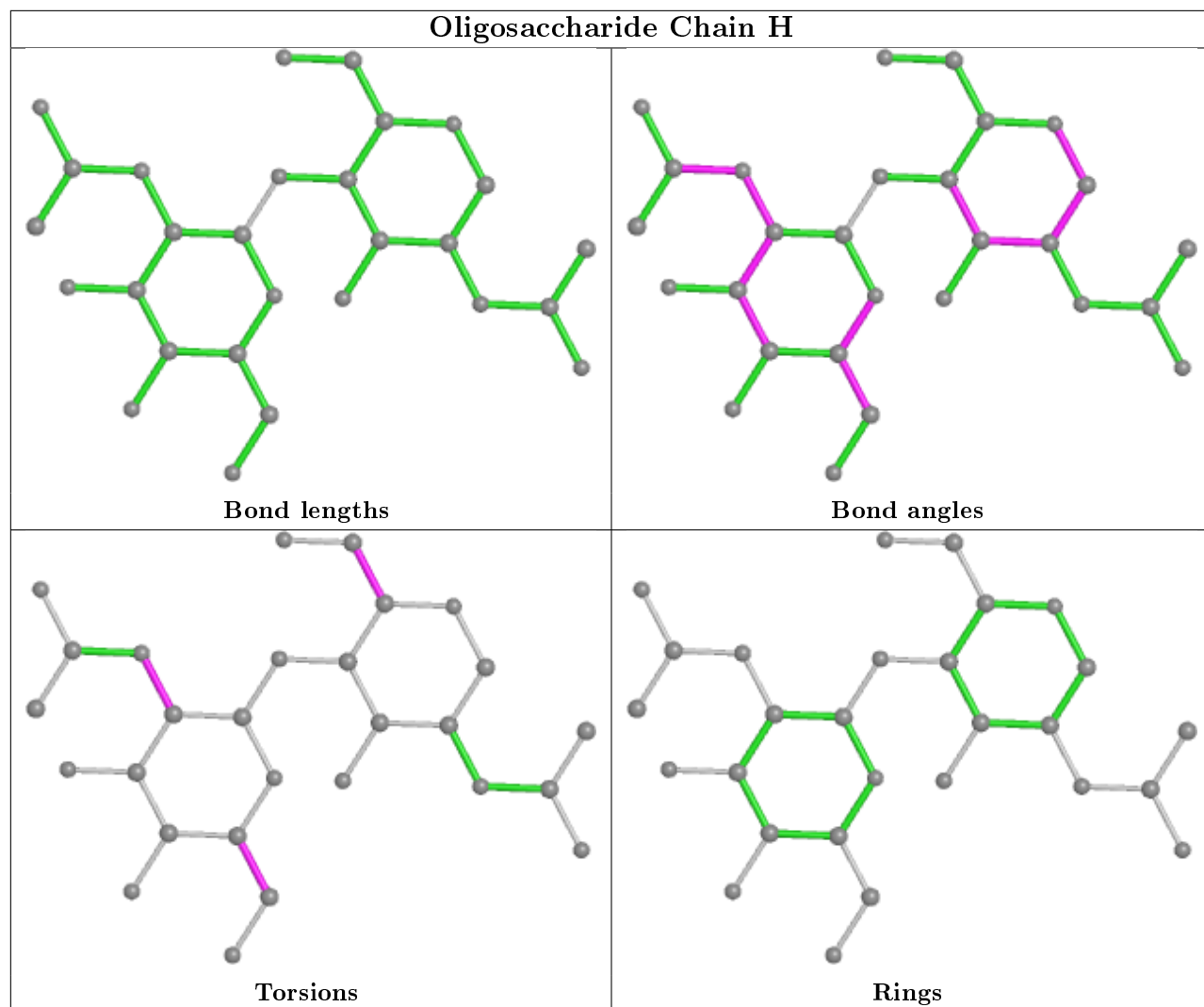
There are no ring outliers.

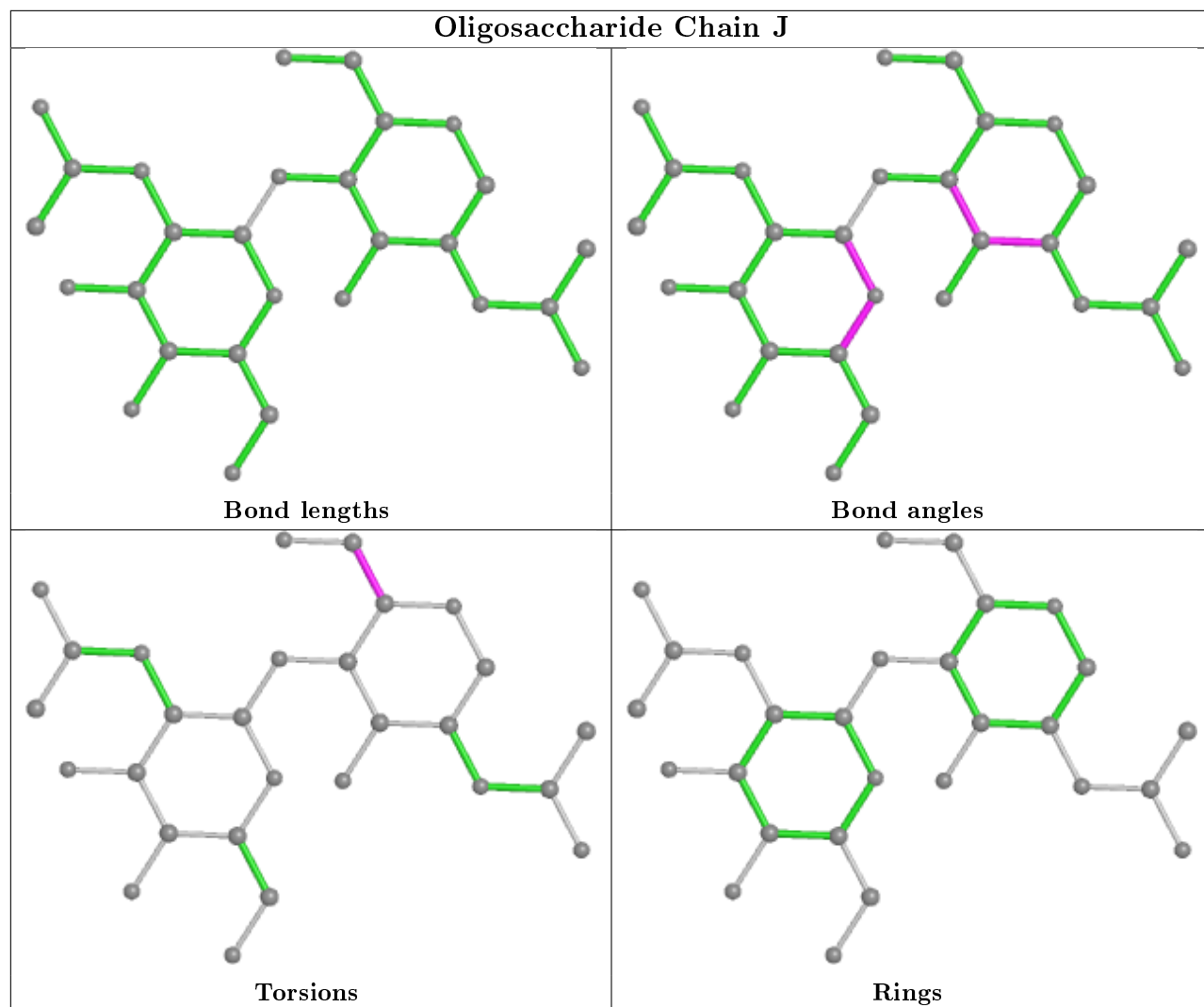
4 monomers are involved in 2 short contacts:

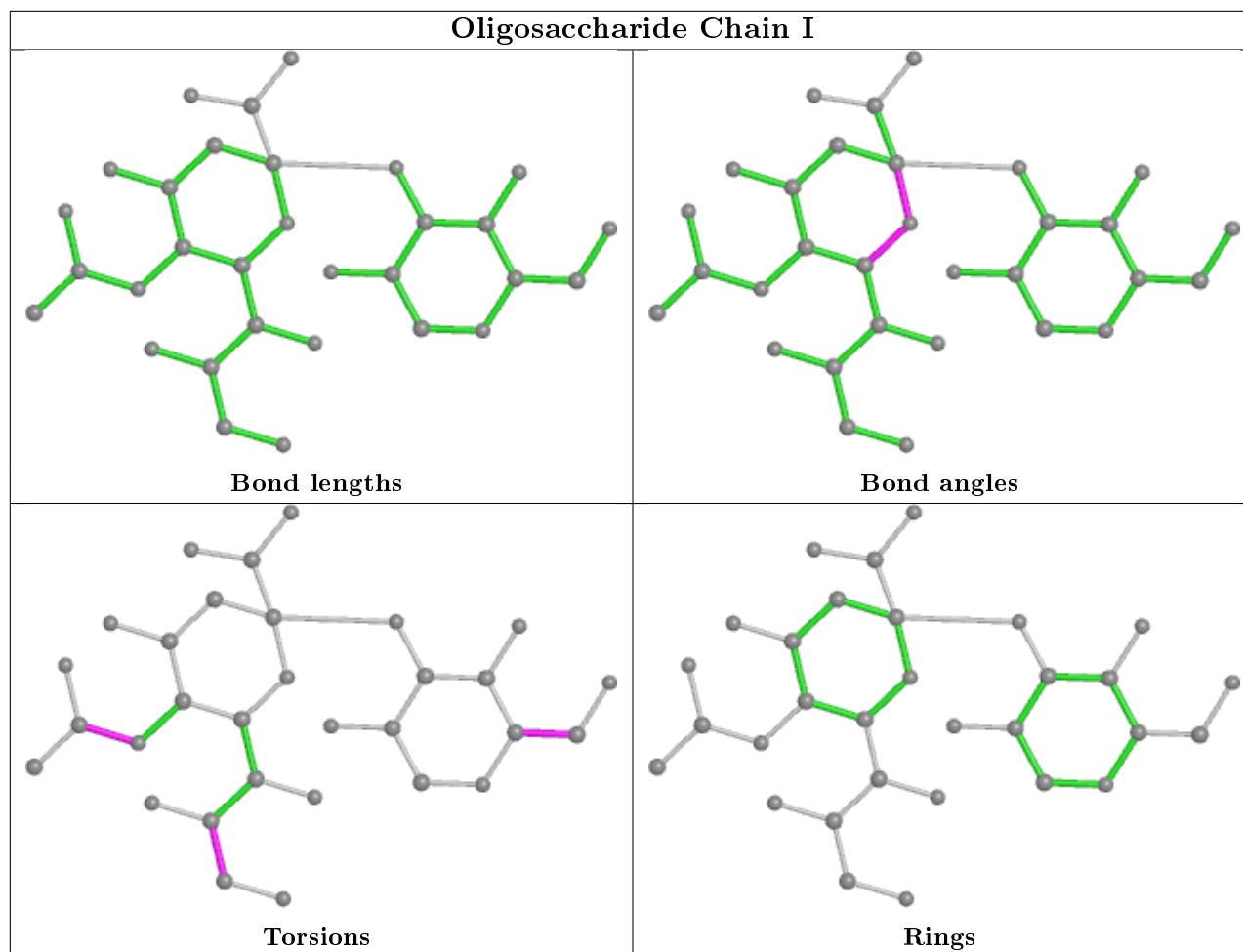
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2	GAL	1	0
5	I	1	GAL	1	0
5	I	2	SIA	1	0
3	K	3	SIA	1	0

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









5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
7	GOL	D	184	-	5,5,5	0.34	0	5,5,5	0.44	0
7	GOL	F	184	-	5,5,5	0.35	0	5,5,5	0.51	0
6	NAG	F	183	2	14,14,15	0.49	0	17,19,21	1.16	1 (5%)
6	NAG	A	331	1	14,14,15	0.61	0	17,19,21	1.45	3 (17%)
6	NAG	E	331	1	14,14,15	0.53	0	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	183	2	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
7	GOL	B	186	-	5,5,5	0.35	0	5,5,5	0.40	0
7	GOL	B	185	-	5,5,5	0.37	0	5,5,5	0.38	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
7	GOL	D	184	-	-	4/4/4/4	-
7	GOL	F	184	-	-	2/4/4/4	-
6	NAG	F	183	2	-	0/6/23/26	0/1/1/1
6	NAG	A	331	1	-	1/6/23/26	0/1/1/1
6	NAG	E	331	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	D	183	2	-	0/6/23/26	0/1/1/1
7	GOL	B	186	-	-	2/4/4/4	-
7	GOL	B	185	-	-	0/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	183	NAG	C1-O5-C5	3.72	117.23	112.19
6	A	331	NAG	C2-N2-C7	3.40	127.75	122.90
6	E	331	NAG	C2-N2-C7	2.95	127.10	122.90
6	E	331	NAG	O5-C5-C6	2.61	111.29	107.20
6	D	183	NAG	C1-O5-C5	2.10	115.04	112.19
6	A	331	NAG	C4-C3-C2	2.08	114.07	111.02
6	A	331	NAG	C3-C4-C5	2.07	113.92	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	331	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	184	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	D	184	GOL	C1-C2-C3-O3
7	F	184	GOL	C1-C2-C3-O3
7	B	186	GOL	C1-C2-C3-O3
7	B	186	GOL	O2-C2-C3-O3
7	F	184	GOL	O2-C2-C3-O3
7	D	184	GOL	O2-C2-C3-O3
7	D	184	GOL	O1-C1-C2-O2
6	E	331	NAG	C4-C5-C6-O6
6	A	331	NAG	C1-C2-N2-C7
6	E	331	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	184	GOL	1	0
7	F	184	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	310/317 (97%)	-0.39	3 (0%) 82 83	5, 18, 28, 41	0
1	C	309/317 (97%)	-0.05	7 (2%) 60 62	2, 19, 34, 40	0
1	E	309/317 (97%)	-0.45	0 100 100	2, 12, 20, 27	0
2	B	176/182 (96%)	-0.52	1 (0%) 89 91	8, 16, 30, 39	0
2	D	172/182 (94%)	-0.43	0 100 100	7, 14, 24, 31	0
2	F	171/182 (93%)	-0.49	1 (0%) 89 91	6, 15, 25, 30	0
All	All	1447/1497 (96%)	-0.36	12 (0%) 86 87	2, 16, 30, 41	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	SER	4.8
1	C	142	SER	4.3
1	A	326	LYS	4.1
1	C	208	LYS	3.4
1	C	144	GLY	3.3
1	C	173	ASN	3.2
1	A	144	GLY	2.8
1	C	238	ASP	2.5
2	B	176	GLY	2.2
1	C	91	ARG	2.2
1	C	188	VAL	2.1
2	F	18	ILE	2.1

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

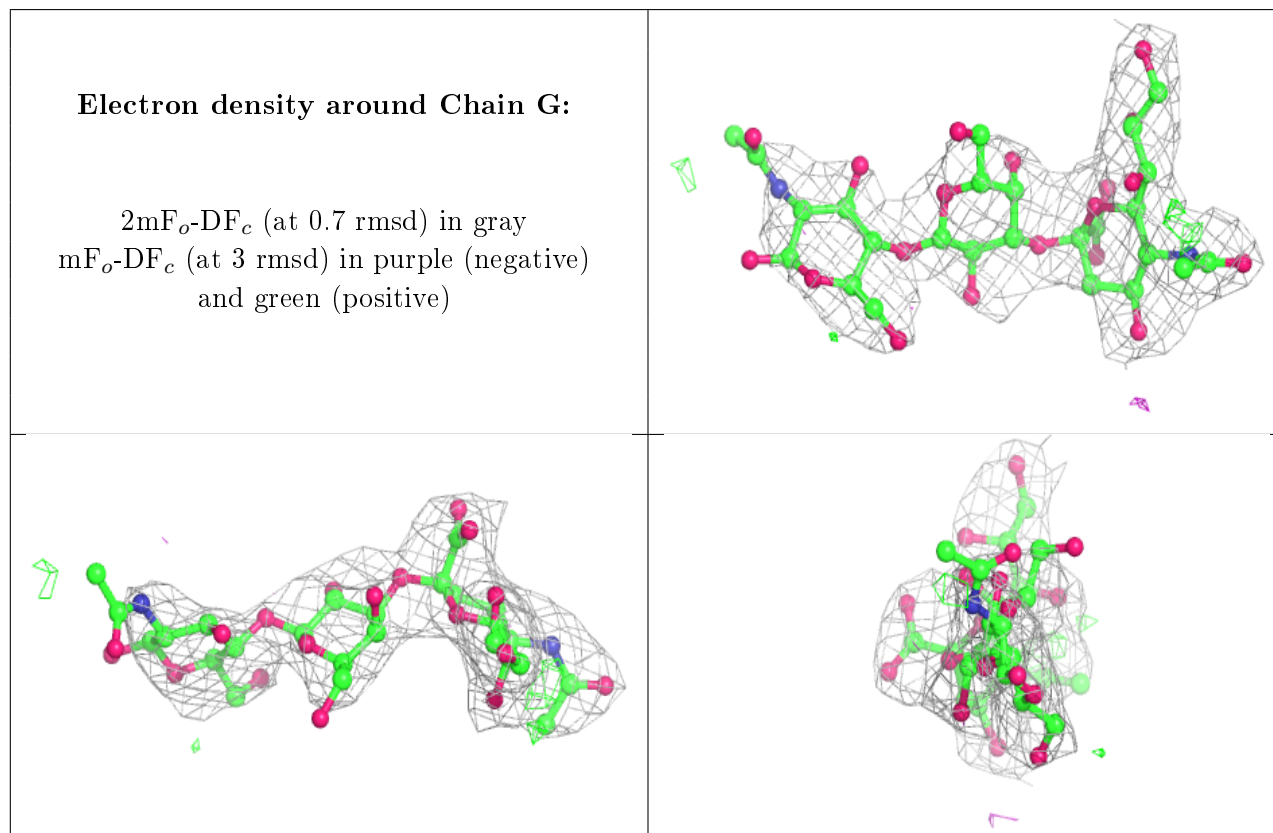
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

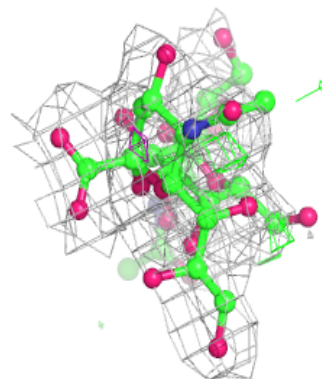
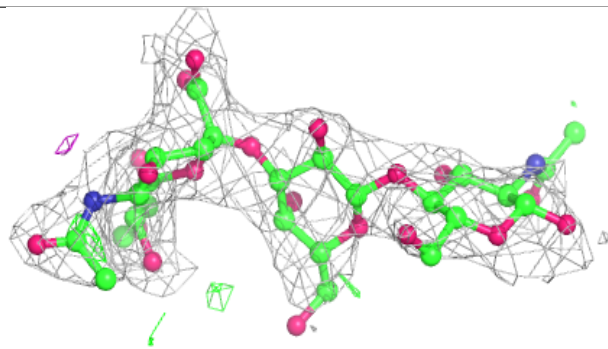
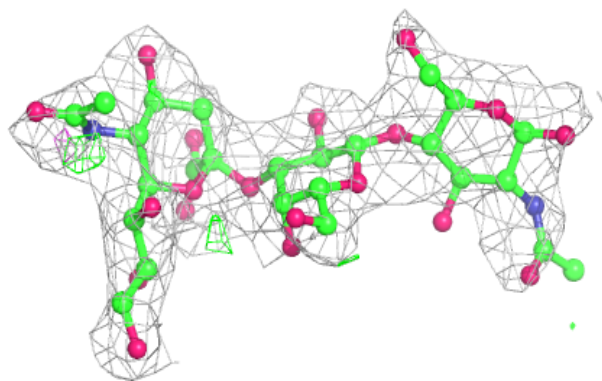
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	2	14/15	0.59	0.51	76,85,86,86	0
4	NAG	H	2	14/15	0.62	0.56	84,89,93,94	0
5	GAL	I	1	11/12	0.65	0.34	117,118,119,119	0
5	SIA	I	2	20/21	0.67	0.39	107,111,115,115	0
4	NAG	J	1	14/15	0.76	0.32	59,67,73,78	0
3	SIA	K	3	20/21	0.77	0.23	59,65,69,70	0
3	NAG	K	1	15/15	0.81	0.47	91,94,98,98	0
3	NAG	G	1	15/15	0.81	0.50	78,83,88,88	0
4	NAG	H	1	14/15	0.87	0.27	52,60,67,76	0
3	GAL	K	2	11/12	0.87	0.29	78,85,88,88	0
3	GAL	G	2	11/12	0.88	0.28	64,69,71,73	0
3	SIA	G	3	20/21	0.92	0.16	41,49,58,58	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.



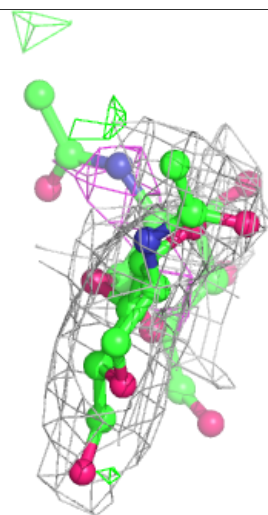
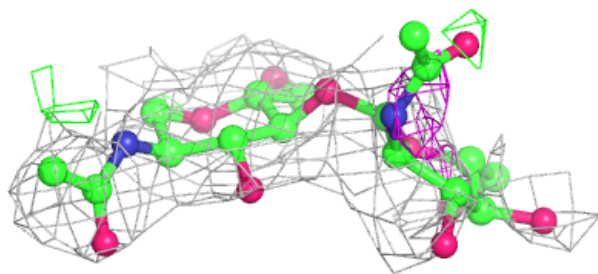
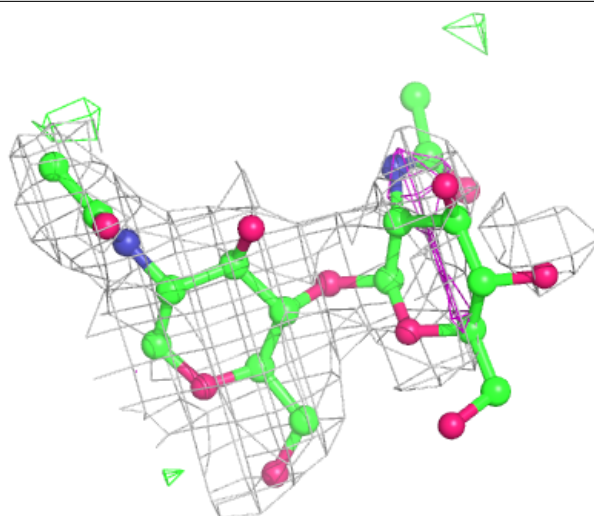
Electron density around Chain K:

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



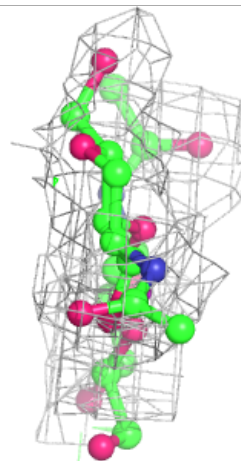
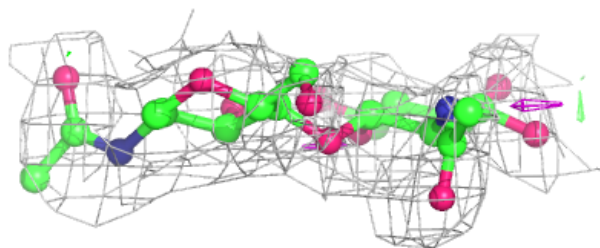
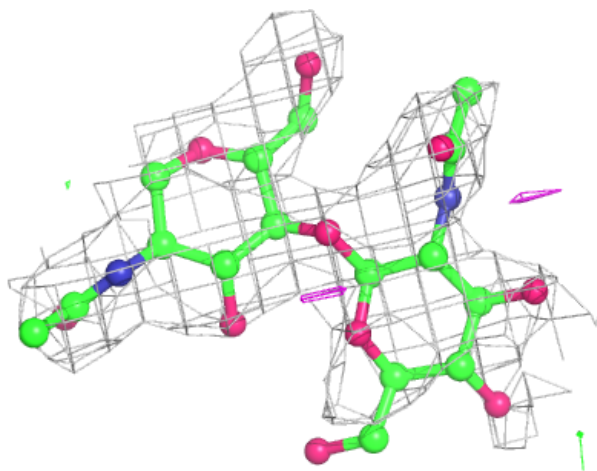
Electron density around Chain H:

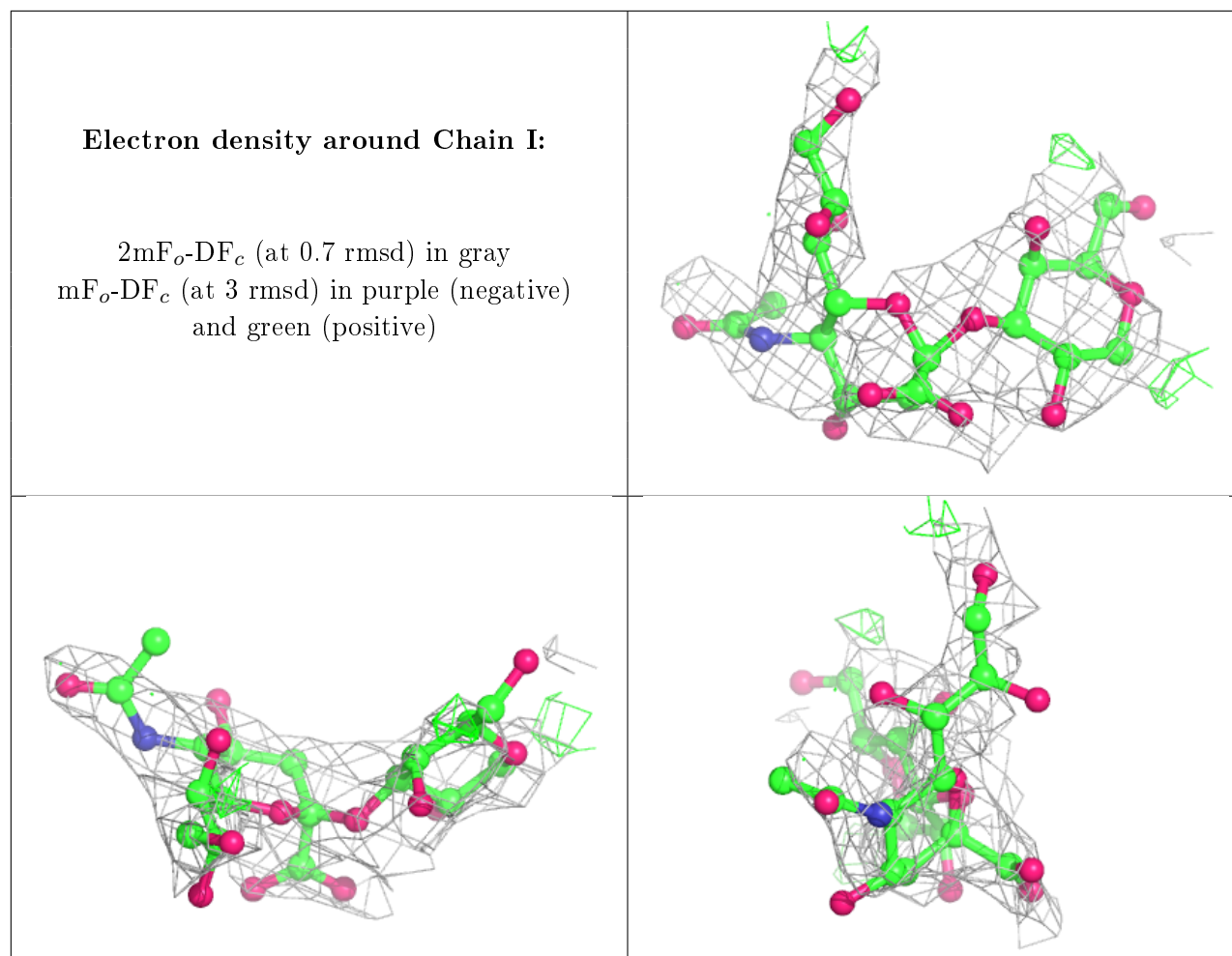
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	F	183	14/15	0.75	0.24	54,60,62,62	0
6	NAG	A	331	14/15	0.77	0.29	56,66,68,69	0
7	GOL	B	185	6/6	0.77	0.40	40,43,45,46	0
6	NAG	E	331	14/15	0.82	0.29	52,62,64,66	0
6	NAG	D	183	14/15	0.84	0.26	44,51,55,56	0
7	GOL	D	184	6/6	0.86	0.30	45,49,52,53	0
7	GOL	B	186	6/6	0.90	0.23	50,50,51,52	0
7	GOL	F	184	6/6	0.90	0.25	30,40,44,46	0

6.5 Other polymers

There are no such residues in this entry.