



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2022 – 04:12 PM EDT

PDB ID : 5VMG
Title : Influenza hemagglutinin H1 mutant DH1E in complex with 6'SLN
Authors : Ni, F.; Kondrashkina, E.; Wang, Q.
Deposited on : 2017-04-27
Resolution : 2.45 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 : 2.27
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) : 2.27

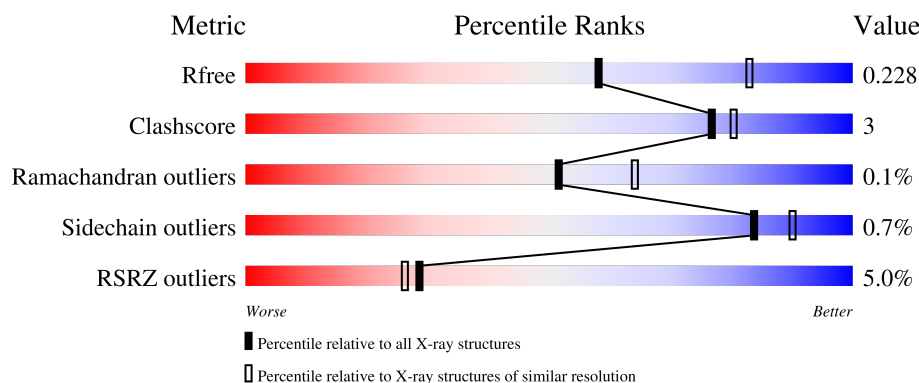
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 $\leq 5\%$. 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	326	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6% ..</div> </div> </div>
1	C	326	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6% .</div> </div> </div>
1	E	326	<div> <div></div> <div> <div></div> <div>92%</div> <div>6% ..</div> </div> </div>
2	B	191	<div> <div>16%</div> <div> <div></div> <div>83%</div> <div>14%</div> </div> </div>
2	D	191	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	191	
3	G	3	
4	H	2	
4	I	2	
5	J	2	
6	K	3	

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
7	NAG	A	1004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23445 atoms, of which 11090 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 HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	H	N	O	S	0	0	0
			4859	1561	2384	426	477	11			
1	C	321	Total	C	H	N	O	S	0	0	0
			4864	1562	2386	426	479	11			
1	E	321	Total	C	H	N	O	S	0	0	0
			4908	1572	2419	426	480	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLU	ASP	engineered mutation	UNP Q9WFX4
A	222	LEU	GLN	engineered mutation	UNP Q9WFX4
A	224	SER	GLY	engineered mutation	UNP Q9WFX4
C	186	GLU	ASP	engineered mutation	UNP Q9WFX4
C	222	LEU	GLN	engineered mutation	UNP Q9WFX4
C	224	SER	GLY	engineered mutation	UNP Q9WFX4
E	186	GLU	ASP	engineered mutation	UNP Q9WFX4
E	222	LEU	GLN	engineered mutation	UNP Q9WFX4
E	224	SER	GLY	engineered mutation	UNP Q9WFX4

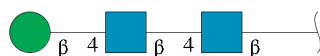
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	164	Total	C	H	N	O	S	0	0	0
			2551	825	1234	225	261	6			
2	D	164	Total	C	H	N	O	S	0	0	0
			2551	825	1234	225	261	6			
2	F	164	Total	C	H	N	O	S	0	0	0
			2552	825	1235	225	261	6			

There are 18 discrepancies between the modelled and reference sequences:

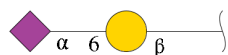
Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLY	-	expression tag	UNP Q9WFX3
B	187	ALA	-	expression tag	UNP Q9WFX3
B	188	LEU	-	expression tag	UNP Q9WFX3
B	189	VAL	-	expression tag	UNP Q9WFX3
B	190	PRO	-	expression tag	UNP Q9WFX3
B	191	ARG	-	expression tag	UNP Q9WFX3
D	186	GLY	-	expression tag	UNP Q9WFX3
D	187	ALA	-	expression tag	UNP Q9WFX3
D	188	LEU	-	expression tag	UNP Q9WFX3
D	189	VAL	-	expression tag	UNP Q9WFX3
D	190	PRO	-	expression tag	UNP Q9WFX3
D	191	ARG	-	expression tag	UNP Q9WFX3
F	186	GLY	-	expression tag	UNP Q9WFX3
F	187	ALA	-	expression tag	UNP Q9WFX3
F	188	LEU	-	expression tag	UNP Q9WFX3
F	189	VAL	-	expression tag	UNP Q9WFX3
F	190	PRO	-	expression tag	UNP Q9WFX3
F	191	ARG	-	expression tag	UNP Q9WFX3

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



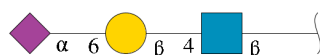
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	2	Total	C	H	N	O	0	0	0
			58	17	27	1	13			
4	I	2	Total	C	H	N	O	0	0	0
			58	17	27	1	13			

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



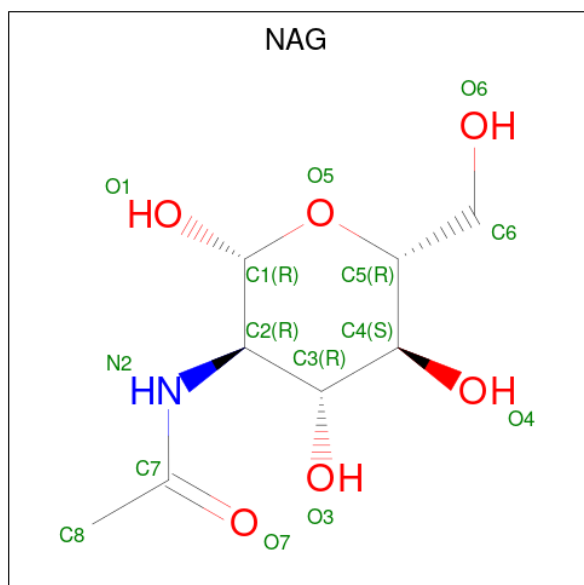
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	2	Total	C	H	N	O	0	0	0
			52	16	25	2	9			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	3	Total	C	H	N	O	0	0	0
			87	25	41	2	19			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

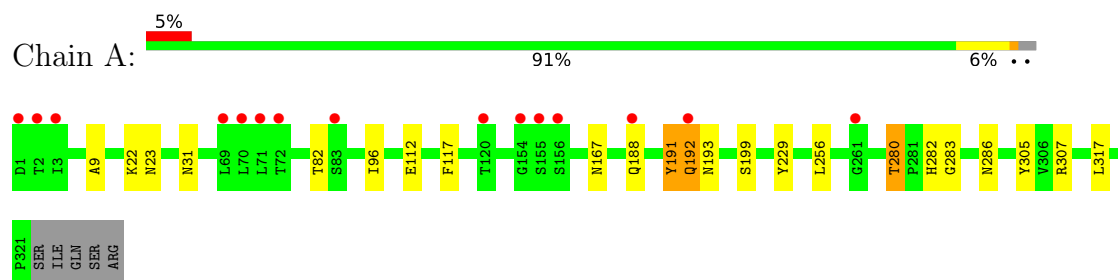
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	170	Total	O	0	0
			170	170		
8	B	57	Total	O	0	0
			57	57		
8	C	131	Total	O	0	0
			131	131		
8	D	75	Total	O	0	0
			75	75		
8	E	229	Total	O	0	0
			229	229		
8	F	84	Total	O	0	0
			84	84		

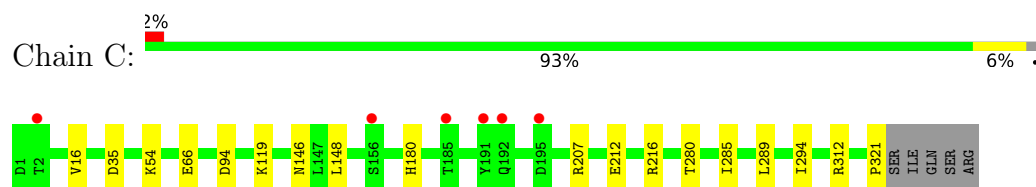
3 Residue-property plots [i](#)

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.

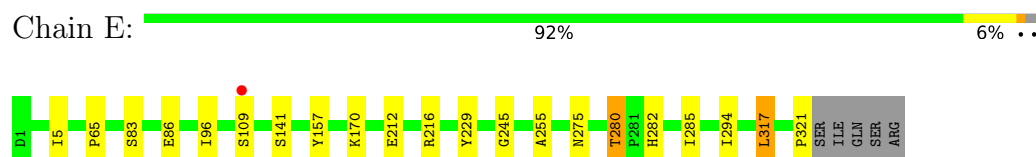
• Molecule 1: Hemagglutinin HA1



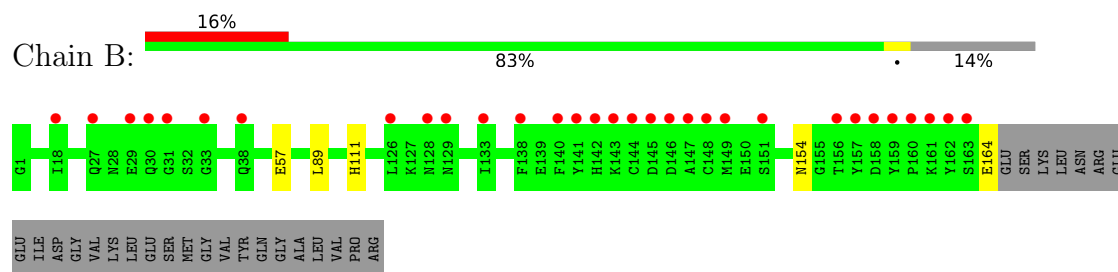
• Molecule 1: Hemagglutinin HA1



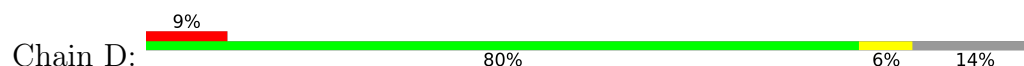
• Molecule 1: Hemagglutinin HA1

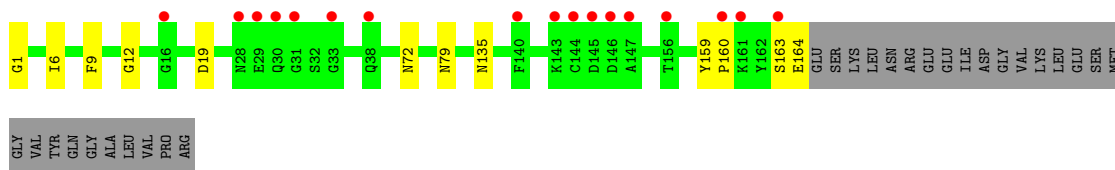


• Molecule 2: Hemagglutinin HA2

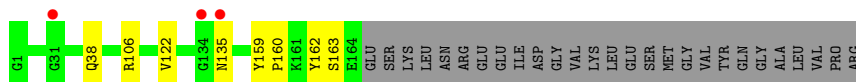
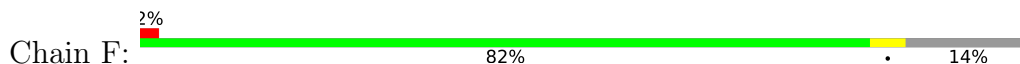


• Molecule 2: Hemagglutinin HA2





- Molecule 2: Hemagglutinin HA2



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



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose



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



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.38Å 81.37Å 120.96Å 90.00° 95.45° 90.00°	Depositor
Resolution (Å)	45.67 – 2.45 45.67 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.67-2.45) 100.0 (45.67-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.191 , 0.225 0.199 , 0.228	Depositor DCC
R_{free} test set	3449 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23445	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

5.1 Standard geometry

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

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	0.33	0/2539	0.57	0/3460
1	C	0.31	0/2542	0.52	0/3464
1	E	0.34	0/2553	0.56	1/3479 (0.0%)
2	B	0.31	0/1344	0.47	0/1811
2	D	0.33	0/1344	0.48	0/1811
2	F	0.32	0/1344	0.47	0/1811
All	All	0.32	0/11666	0.53	1/15836 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	317	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	TYR	Peptide

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	2475	2384	2384	19	0
1	C	2478	2386	2386	12	0
1	E	2489	2419	2419	14	0
2	B	1317	1234	1234	5	0
2	D	1317	1234	1234	9	0
2	F	1317	1235	1234	8	0
3	G	39	36	34	1	0
4	H	31	27	26	0	0
4	I	31	27	26	0	0
5	J	27	25	23	0	0
6	K	46	41	40	1	0
7	A	14	14	13	3	0
7	C	28	28	26	3	0
8	A	170	0	0	12	0
8	B	57	0	0	3	0
8	C	131	0	0	6	0
8	D	75	0	0	5	0
8	E	229	0	0	6	0
8	F	84	0	0	6	0
All	All	12355	11090	11079	69	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 (69) 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:207:ARG:NH2	8:C:1101:HOH:O	1.93	1.01
2:F:162:TYR:O	8:F:201:HOH:O	1.81	0.98
1:A:307:ARG:NH1	8:A:1104:HOH:O	2.01	0.90
1:E:141:SER:O	8:E:1101:HOH:O	1.90	0.89
2:B:57:GLU:OE1	8:B:201:HOH:O	1.91	0.87
1:A:82:THR:O	8:A:1101:HOH:O	1.92	0.86
2:D:79:ASN:OD1	8:D:201:HOH:O	1.93	0.86
2:F:135:ASN:N	8:F:202:HOH:O	2.00	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:PRO:O	8:C:1102:HOH:O	1.93	0.85
1:A:167:ASN:OD1	8:A:1102:HOH:O	1.96	0.82
1:C:146:ASN:OD1	8:C:1103:HOH:O	1.98	0.81
1:E:275:ASN:O	8:E:1102:HOH:O	2.02	0.78
1:A:23:ASN:ND2	8:A:1103:HOH:O	2.01	0.78
6:K:1:NAG:O3	6:K:2:GAL:O5	2.04	0.74
1:C:94:ASP:OD2	8:C:1104:HOH:O	2.06	0.73
1:A:286:ASN:HD21	7:A:1004:NAG:C6	1.99	0.73
2:F:135:ASN:CA	8:F:202:HOH:O	2.37	0.72
2:B:164:GLU:OE2	8:B:202:HOH:O	2.07	0.71
1:E:83:SER:OG	8:E:1103:HOH:O	2.09	0.70
7:C:1001:NAG:O7	7:C:1001:NAG:O3	2.10	0.69
2:D:72:ASN:OD1	8:D:203:HOH:O	2.12	0.68
1:C:54:LYS:NZ	1:C:66:GLU:OE1	2.27	0.68
8:A:1105:HOH:O	3:G:3:BMA:O4	2.13	0.65
1:A:286:ASN:ND2	7:A:1004:NAG:O6	2.28	0.65
2:D:6:ILE:O	8:D:205:HOH:O	2.14	0.65
2:F:135:ASN:CB	8:F:202:HOH:O	2.45	0.65
2:D:12:GLY:O	8:D:204:HOH:O	2.14	0.65
1:A:117:PHE:O	8:A:1106:HOH:O	2.16	0.63
7:A:1004:NAG:H2	8:A:1140:HOH:O	1.98	0.62
1:A:22:LYS:NZ	8:A:1110:HOH:O	2.24	0.60
7:C:1002:NAG:O3	8:C:1105:HOH:O	2.16	0.60
1:E:109:SER:O	8:E:1104:HOH:O	2.17	0.59
1:A:31:ASN:OD1	8:A:1107:HOH:O	2.16	0.59
1:C:212:GLU:O	1:C:216:ARG:NH2	2.36	0.58
1:A:112:GLU:OE1	8:A:1108:HOH:O	2.17	0.58
1:E:212:GLU:O	1:E:216:ARG:NH2	2.37	0.57
1:C:180:HIS:NE2	8:C:1109:HOH:O	2.29	0.56
2:F:135:ASN:HB3	8:F:202:HOH:O	2.02	0.56
2:B:154:ASN:OD1	8:B:203:HOH:O	2.18	0.55
1:C:119:LYS:HZ3	1:C:148:LEU:HD11	1.72	0.54
2:D:19:ASP:OD1	2:D:19:ASP:N	2.36	0.54
1:E:86:GLU:HB2	8:E:1119:HOH:O	2.08	0.54
1:A:96:ILE:HG13	1:A:229:TYR:CE1	2.43	0.53
1:A:191:TYR:O	1:A:193:ASN:N	2.40	0.52
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.94	0.49
1:E:285:ILE:HG21	1:E:294:ILE:HG13	1.95	0.49
1:C:289:LEU:HD11	7:C:1002:NAG:H82	1.93	0.48
1:E:96:ILE:HG13	1:E:229:TYR:CE1	2.49	0.48
1:A:9:ALA:O	8:A:1109:HOH:O	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:ARG:HD3	8:F:248:HOH:O	2.14	0.47
1:C:16:VAL:HG12	1:C:312:ARG:HG2	1.97	0.46
1:C:285:ILE:HG21	1:C:294:ILE:HG13	1.98	0.45
1:A:280:THR:HG22	1:A:282:HIS:H	1.81	0.45
1:A:305:TYR:CD2	2:B:89:LEU:HD13	2.51	0.45
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.99	0.45
1:A:280:THR:HB	1:A:283:GLY:O	2.18	0.44
1:A:188:GLN:HA	1:A:192:GLN:HA	2.00	0.43
1:E:280:THR:HG22	1:E:282:HIS:H	1.83	0.43
1:E:321:PRO:O	8:E:1107:HOH:O	2.22	0.43
1:A:23:ASN:ND2	8:A:1127:HOH:O	2.52	0.42
2:D:9:PHE:O	2:D:135:ASN:HA	2.19	0.42
1:E:157:TYR:CZ	1:E:245:GLY:HA2	2.55	0.42
1:E:170:LYS:HE3	1:E:255:ALA:HB1	2.02	0.42
1:E:5:ILE:HD11	2:F:122:VAL:HG21	2.02	0.41
1:E:280:THR:CG2	1:E:282:HIS:H	2.34	0.41
2:D:163:SER:C	2:D:164:GLU:HG3	2.41	0.41
1:A:317:LEU:HB3	2:B:111:HIS:CG	2.56	0.41
1:C:35:ASP:C	1:C:294:ILE:HD11	2.42	0.41
2:D:1:GLY:N	8:D:208:HOH:O	2.38	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	319/326 (98%)	312 (98%)	6 (2%)	1 (0%)	41	49
1	C	319/326 (98%)	315 (99%)	4 (1%)	0	100	100
1	E	319/326 (98%)	313 (98%)	6 (2%)	0	100	100
2	B	162/191 (85%)	160 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	162/191 (85%)	161 (99%)	1 (1%)	0	100	100
2	F	162/191 (85%)	161 (99%)	1 (1%)	0	100	100
All	All	1443/1551 (93%)	1422 (98%)	20 (1%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLN

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	272/282 (96%)	269 (99%)	3 (1%)	73	82
1	C	273/282 (97%)	272 (100%)	1 (0%)	91	94
1	E	277/282 (98%)	274 (99%)	3 (1%)	73	82
2	B	139/162 (86%)	139 (100%)	0	100	100
2	D	139/162 (86%)	139 (100%)	0	100	100
2	F	139/162 (86%)	137 (99%)	2 (1%)	67	77
All	All	1239/1332 (93%)	1230 (99%)	9 (1%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	256	LEU
1	A	280	THR
1	C	280	THR
1	E	65	PRO
1	E	280	THR
1	E	317	LEU
2	F	38	GLN
2	F	163	SER

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

Mol	Chain	Res	Type
2	F	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,3	14,14,15	0.51	0	17,19,21	0.74	0
3	NAG	G	2	3	14,14,15	0.83	1 (7%)	17,19,21	0.66	0
3	BMA	G	3	3	11,11,12	0.68	0	15,15,17	0.88	0
4	GAL	H	1	4	11,11,12	1.17	2 (18%)	15,15,17	1.32	2 (13%)
4	SIA	H	2	4	17,20,21	1.31	3 (17%)	21,28,31	1.11	2 (9%)
4	GAL	I	1	4	11,11,12	0.56	0	15,15,17	0.93	0
4	SIA	I	2	4	17,20,21	1.39	3 (17%)	21,28,31	1.35	3 (14%)
5	NAG	J	1	1,5	14,14,15	0.49	0	17,19,21	0.50	0
5	NAG	J	2	5	13,13,15	0.83	1 (7%)	16,17,21	0.87	1 (6%)
6	NAG	K	1	6	15,15,15	1.20	1 (6%)	21,21,21	1.32	3 (14%)
6	GAL	K	2	6	11,11,12	0.66	0	15,15,17	1.09	1 (6%)
6	SIA	K	3	6	17,20,21	1.14	3 (17%)	21,28,31	1.11	2 (9%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O5-C1	4.31	1.53	1.42
4	I	2	SIA	C4-C5	-3.32	1.50	1.53
3	G	2	NAG	O5-C1	-3.05	1.38	1.43
4	H	2	SIA	C4-C5	-3.00	1.50	1.53
5	J	2	NAG	C1-C2	2.87	1.54	1.51
4	H	1	GAL	C2-C3	2.78	1.56	1.52
4	I	2	SIA	C5-N5	-2.37	1.42	1.45
4	H	2	SIA	C10-N5	2.37	1.42	1.34
6	K	3	SIA	C10-N5	2.36	1.42	1.34
4	H	2	SIA	C5-N5	-2.34	1.42	1.45
6	K	3	SIA	C5-N5	-2.31	1.42	1.45
6	K	3	SIA	C4-C5	-2.28	1.51	1.53
4	I	2	SIA	C10-N5	2.26	1.42	1.34
4	H	1	GAL	O5-C1	-2.02	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C1-O5-C5	3.81	120.86	113.66
4	H	1	GAL	C1-C2-C3	3.69	114.20	109.67
4	I	2	SIA	O6-C2-C3	-3.34	104.02	109.87
4	I	2	SIA	C3-C4-C5	-2.77	108.11	111.46
4	H	2	SIA	C3-C4-C5	-2.74	108.15	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	SIA	O6-C2-C3	-2.70	105.14	109.87
6	K	1	NAG	C1-C2-N2	2.65	113.80	110.73
6	K	3	SIA	O6-C2-C3	-2.61	105.30	109.87
5	J	2	NAG	C4-C3-C2	-2.49	109.46	112.53
6	K	3	SIA	C3-C4-C5	-2.25	108.74	111.46
6	K	1	NAG	C4-C3-C2	-2.21	107.11	110.34
4	H	1	GAL	O3-C3-C4	-2.14	105.41	110.35
6	K	2	GAL	C1-O5-C5	2.10	115.03	112.19
4	I	2	SIA	C8-C7-C6	-2.02	109.20	113.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

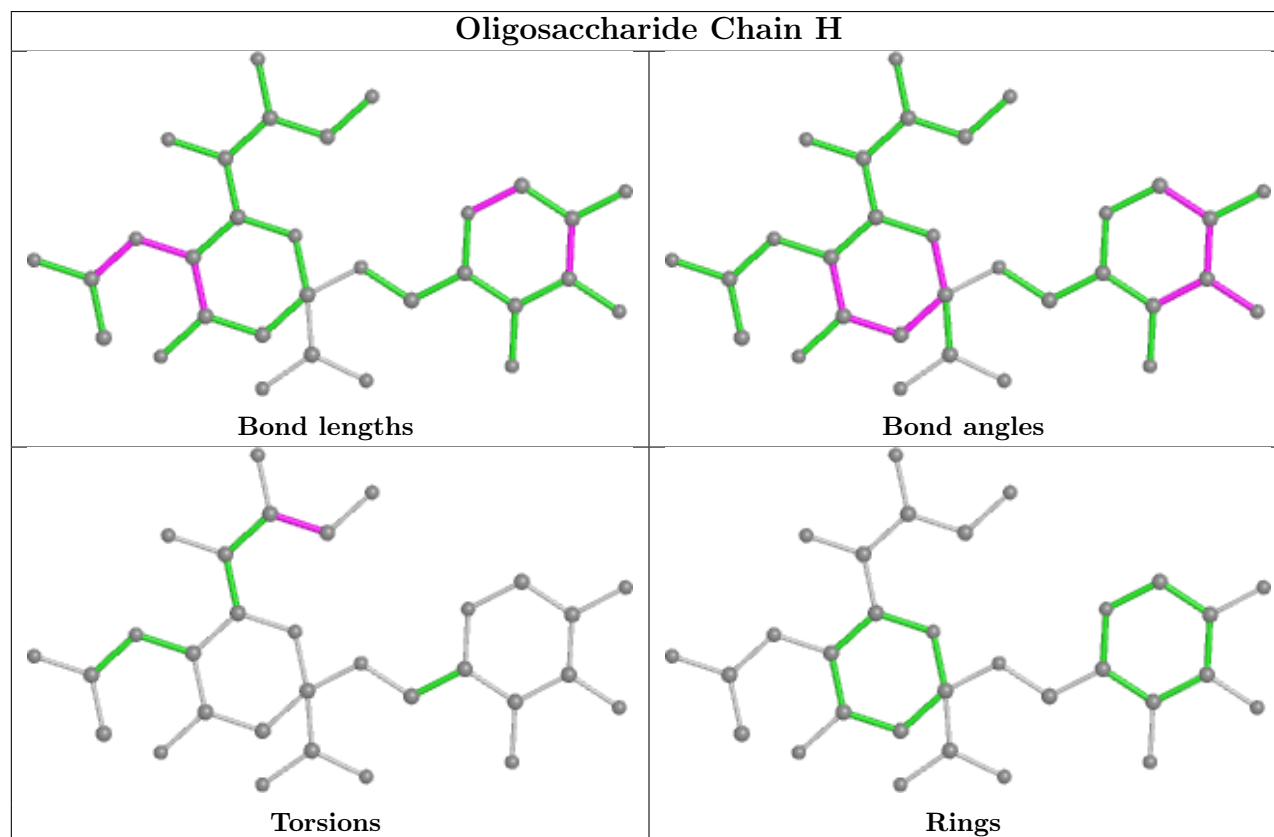
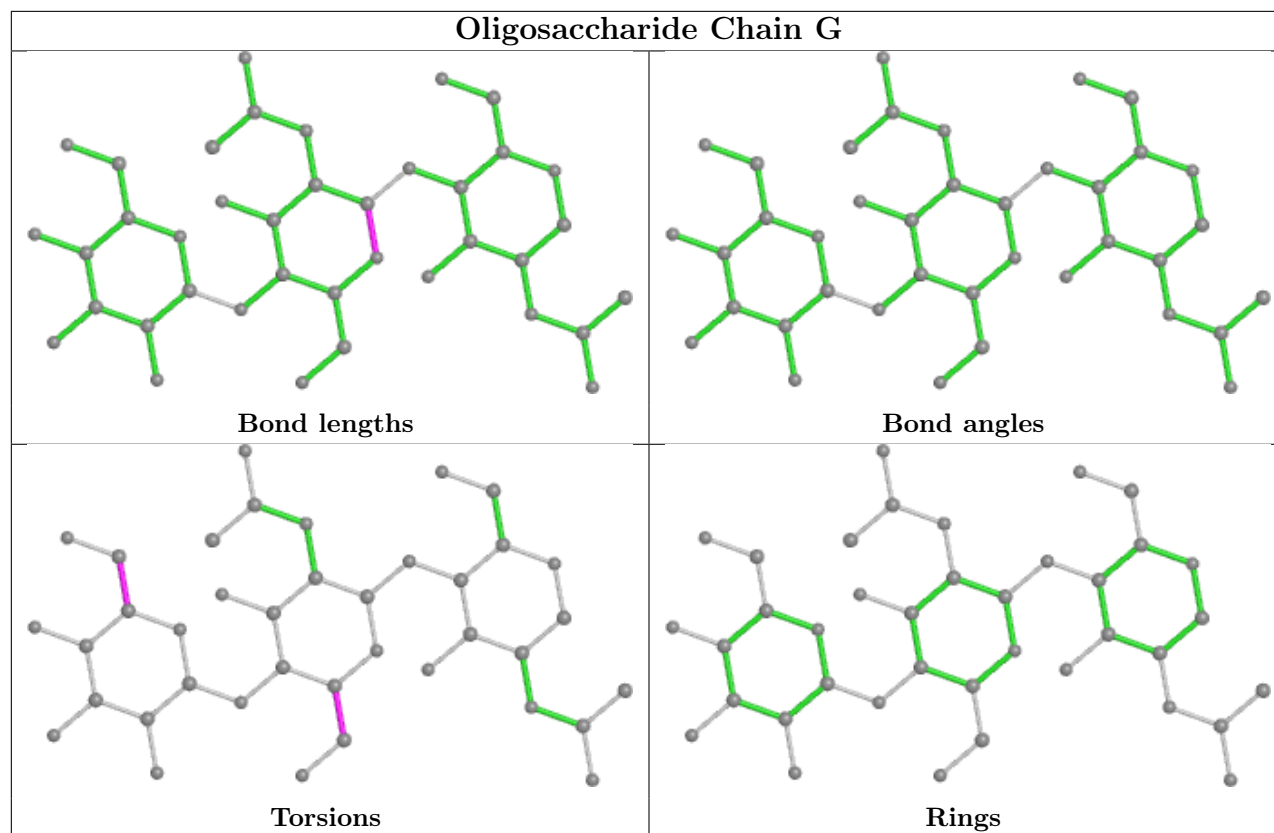
Mol	Chain	Res	Type	Atoms
4	H	2	SIA	O8-C8-C9-O9
4	I	2	SIA	O8-C8-C9-O9
4	H	2	SIA	C7-C8-C9-O9
6	K	1	NAG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
4	I	2	SIA	C7-C8-C9-O9
6	K	2	GAL	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
6	K	2	GAL	O5-C5-C6-O6

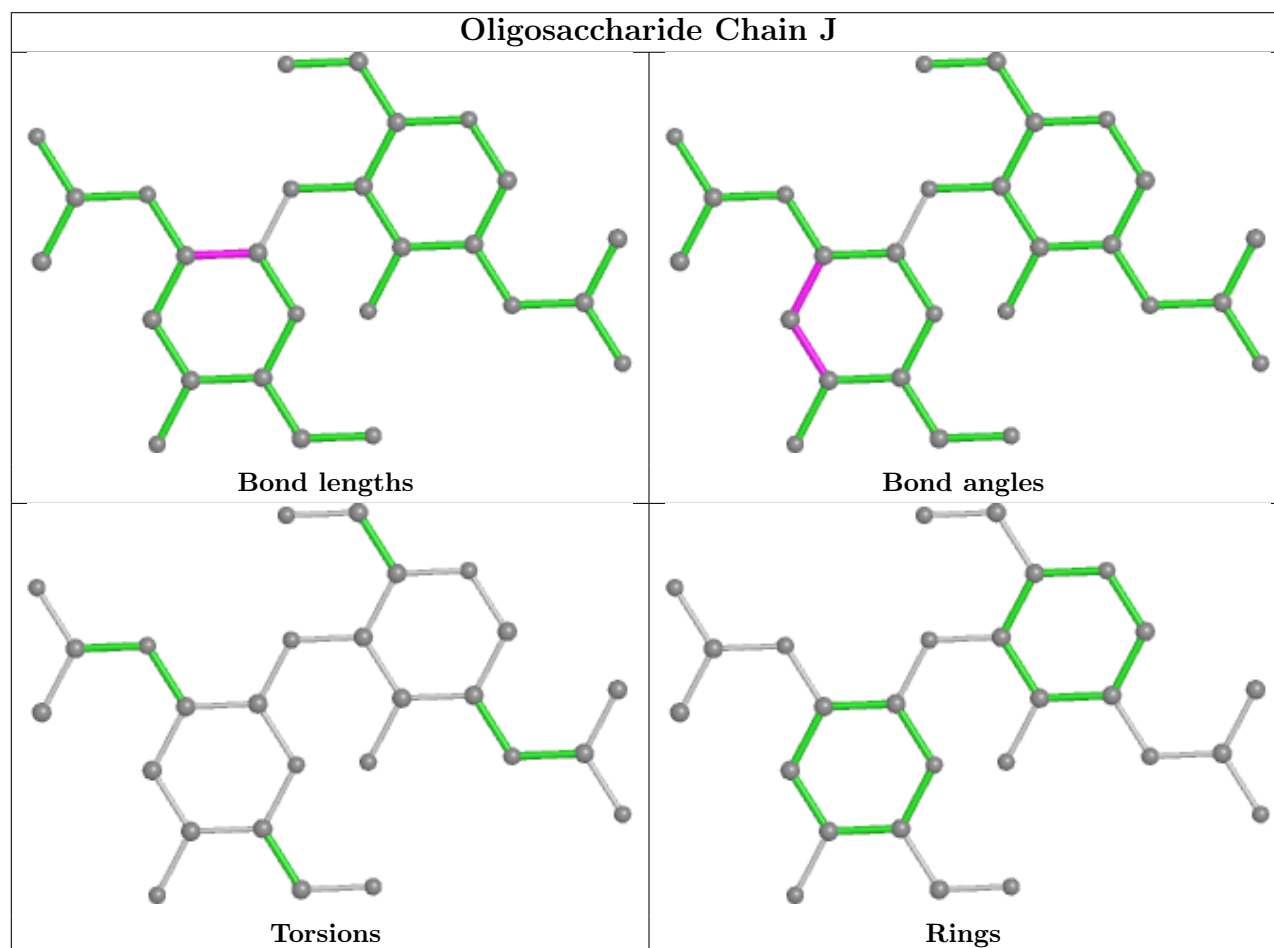
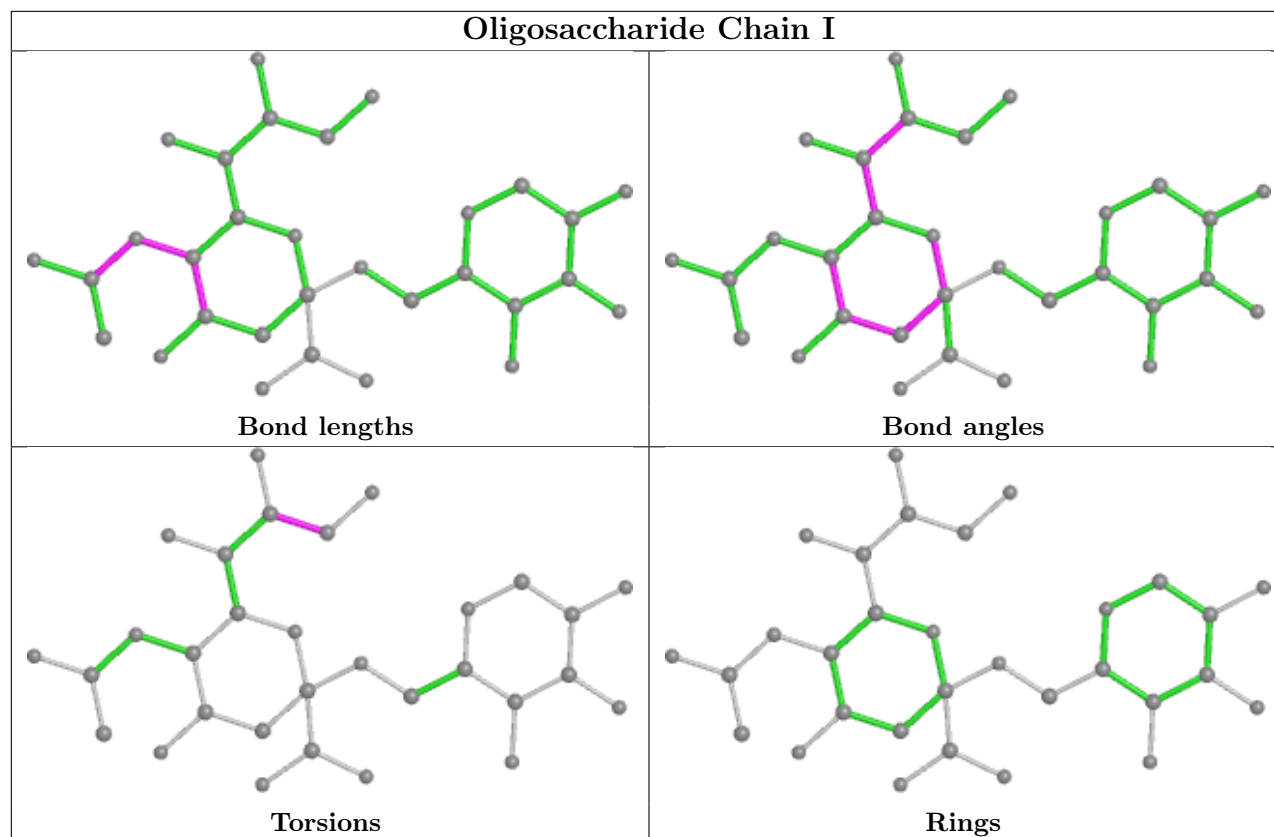
There are no ring outliers.

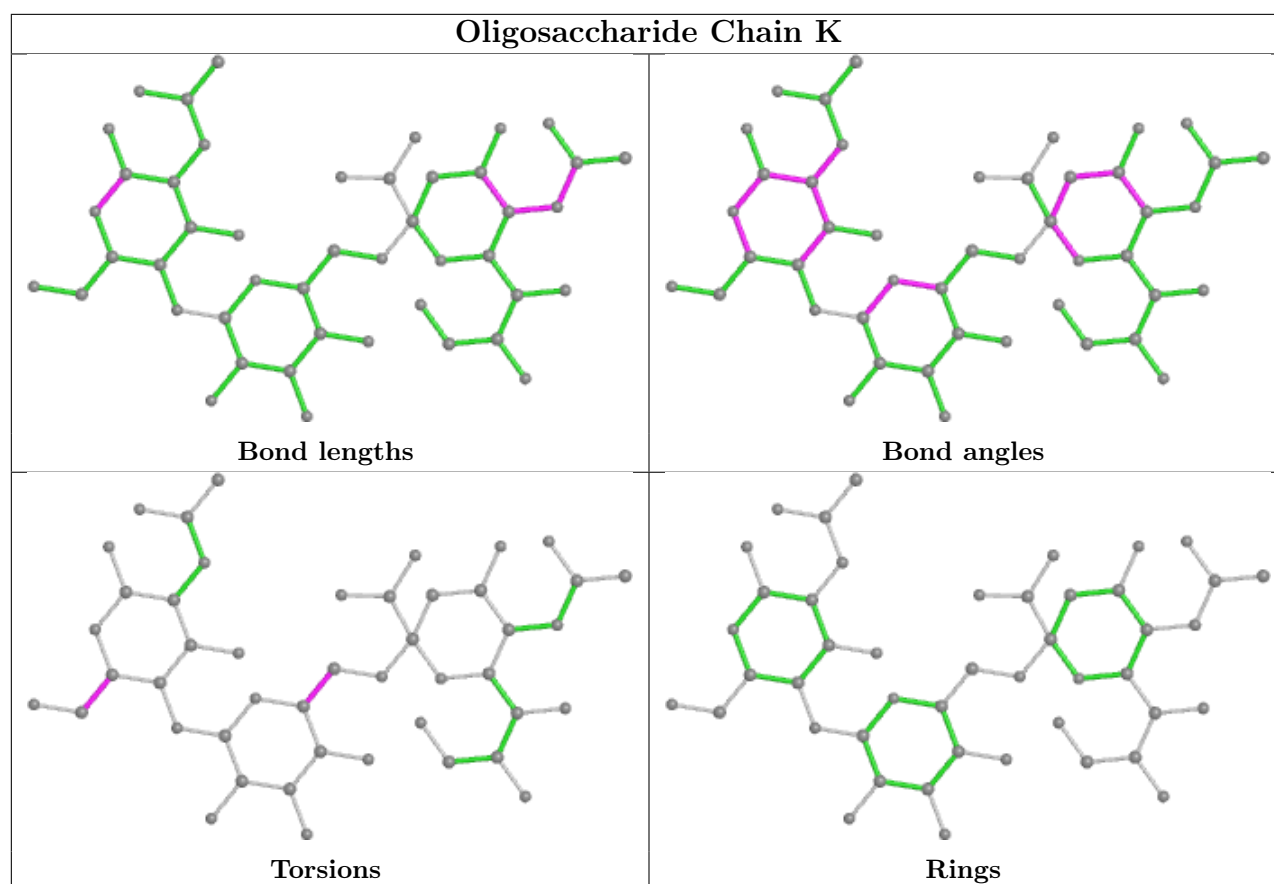
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0
6	K	2	GAL	1	0
3	G	3	BMA	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](#)

3 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	NAG	C	1002	1	14,14,15	0.77	1 (7%)	17,19,21	1.01	1 (5%)
7	NAG	A	1004	1	14,14,15	1.01	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	C	1001	1	14,14,15	0.81	1 (7%)	17,19,21	0.64	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	NAG	C	1002	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1001	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	NAG	C1-C2	3.47	1.57	1.52
7	C	1001	NAG	O5-C1	-2.50	1.39	1.43
7	C	1002	NAG	C1-C2	2.30	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1002	NAG	C1-O5-C5	3.60	117.08	112.19
7	A	1004	NAG	C1-O5-C5	3.15	116.46	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1002	NAG	O5-C5-C6-O6
7	C	1002	NAG	C4-C5-C6-O6
7	C	1001	NAG	C1-C2-N2-C7
7	C	1002	NAG	C1-C2-N2-C7
7	C	1001	NAG	C3-C2-N2-C7
7	C	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1002	NAG	2	0
7	A	1004	NAG	3	0
7	C	1001	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/326 (98%)	0.11	15 (4%) 31 29	16, 30, 49, 87	0
1	C	321/326 (98%)	0.09	6 (1%) 66 64	21, 35, 53, 69	0
1	E	321/326 (98%)	-0.17	1 (0%) 94 94	17, 25, 41, 56	0
2	B	164/191 (85%)	0.91	31 (18%) 1 0	18, 44, 83, 96	0
2	D	164/191 (85%)	0.56	17 (10%) 6 4	18, 44, 77, 90	0
2	F	164/191 (85%)	0.28	3 (1%) 68 65	16, 36, 50, 58	0
All	All	1455/1551 (93%)	0.20	73 (5%) 28 26	16, 32, 67, 96	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	6.2
2	B	29	GLU	5.3
2	D	31	GLY	4.9
2	B	143	LYS	4.8
1	A	1	ASP	4.7
2	B	160	PRO	4.7
1	A	69	LEU	4.2
2	B	140	PHE	4.1
2	B	148	CYS	4.1
2	B	163	SER	4.0
2	B	158	ASP	3.9
2	B	162	TYR	3.8
2	B	133	ILE	3.8
2	D	144	CYS	3.7
2	B	138	PHE	3.7
2	D	30	GLN	3.7
2	B	144	CYS	3.6
1	C	195	ASP	3.6
1	A	72	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	156	THR	3.5
2	B	141	TYR	3.5
2	D	29	GLU	3.4
2	B	151	SER	3.4
2	B	27	GLN	3.4
2	B	157	TYR	3.4
2	D	147	ALA	3.4
2	B	161	LYS	3.3
2	D	140	PHE	3.3
1	C	192	GLN	3.0
2	B	147	ALA	3.0
1	C	2	THR	3.0
2	B	159	TYR	3.0
1	A	71	LEU	2.8
2	D	16	GLY	2.8
2	B	126	LEU	2.8
2	B	142	HIS	2.7
1	A	120	THR	2.7
2	F	134	GLY	2.7
1	C	191	TYR	2.7
2	F	31	GLY	2.6
2	B	145	ASP	2.6
1	A	2	THR	2.6
2	D	160	PRO	2.6
2	B	156	THR	2.5
1	E	109	SER	2.5
2	B	31	GLY	2.5
2	B	149	MET	2.5
1	A	156	SER	2.4
1	A	154	GLY	2.4
2	D	163	SER	2.4
1	A	3	ILE	2.4
2	B	38	GLN	2.4
2	B	18	ILE	2.4
1	C	185	THR	2.4
1	A	155	SER	2.4
2	B	129	ASN	2.3
2	D	161	LYS	2.3
2	D	145	ASP	2.3
2	B	30	GLN	2.3
1	A	83	SER	2.3
2	B	146	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	135	ASN	2.3
2	D	146	ASP	2.3
1	A	188	GLN	2.2
2	D	33	GLY	2.2
2	D	143	LYS	2.1
2	D	28	ASN	2.1
1	A	261	GLY	2.1
2	B	33	GLY	2.1
1	A	192	GLN	2.1
2	D	38	GLN	2.1
1	C	156	SER	2.0
2	B	128	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

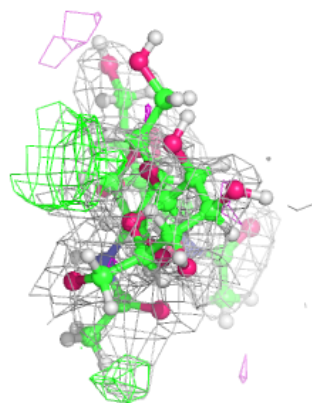
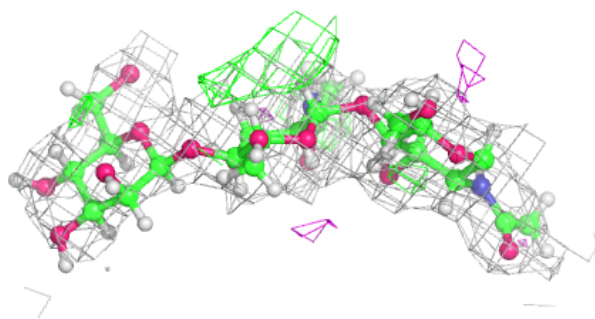
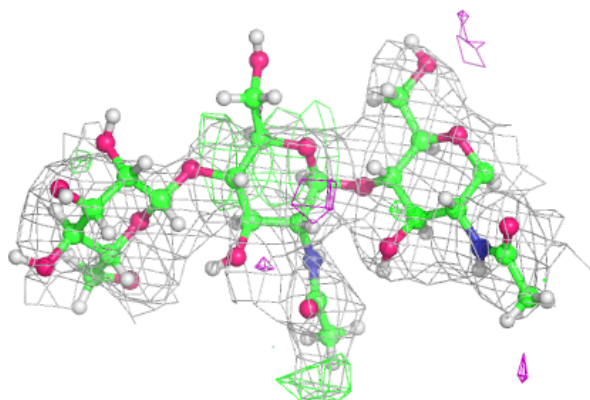
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.69	0.30	61,73,88,91	0
3	BMA	G	3	11/12	0.78	0.26	67,74,87,89	0
6	NAG	K	1	15/15	0.81	0.35	54,65,81,82	0
4	GAL	I	1	11/12	0.85	0.22	46,66,79,85	0
4	GAL	H	1	11/12	0.87	0.16	43,63,76,82	0
6	GAL	K	2	11/12	0.91	0.17	35,52,63,69	0
5	NAG	J	2	13/15	0.93	0.18	33,36,44,44	0
4	SIA	H	2	20/21	0.95	0.16	31,37,43,44	0
3	NAG	G	1	14/15	0.95	0.12	30,41,55,56	0
4	SIA	I	2	20/21	0.95	0.20	37,41,49,49	0
5	NAG	J	1	14/15	0.96	0.16	25,34,41,47	0
6	SIA	K	3	20/21	0.96	0.12	19,24,31,34	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.

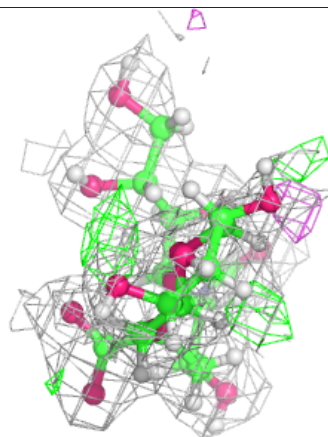
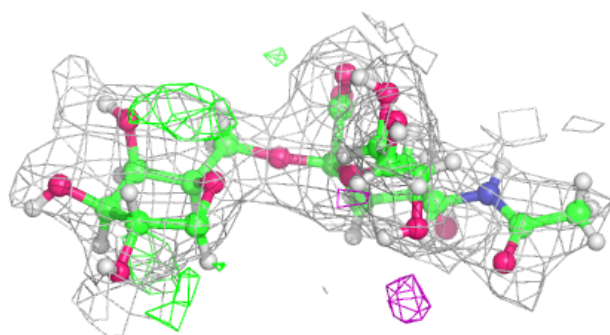
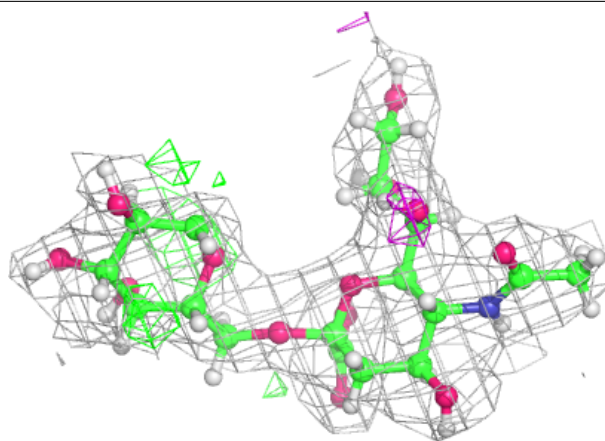
Electron density around Chain G:

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



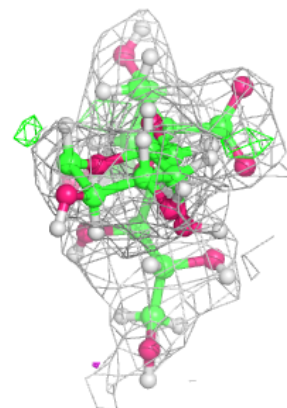
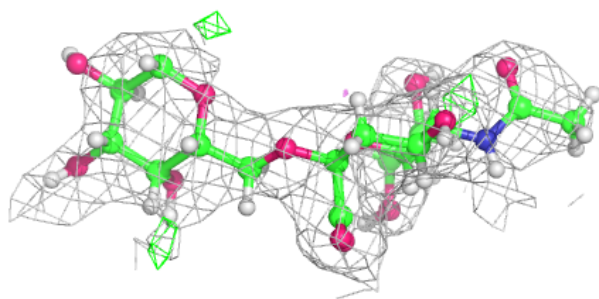
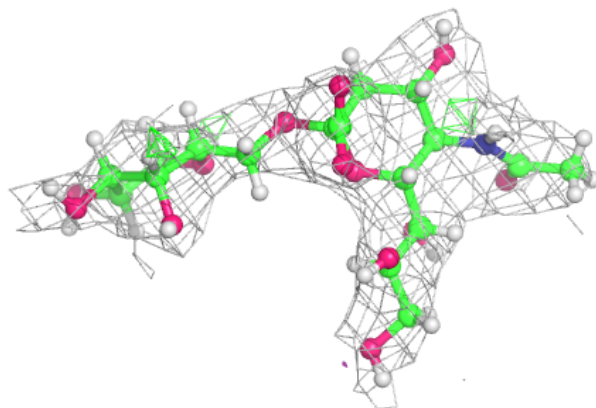
Electron density around Chain H:

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



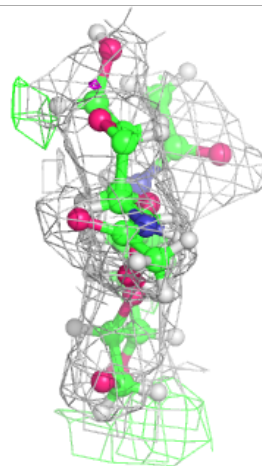
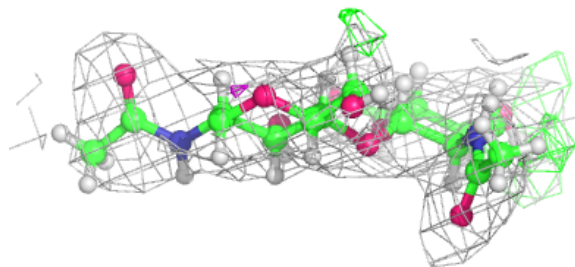
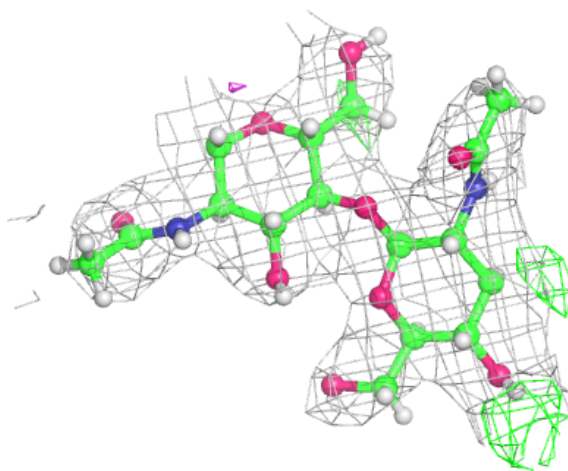
Electron density around Chain I:

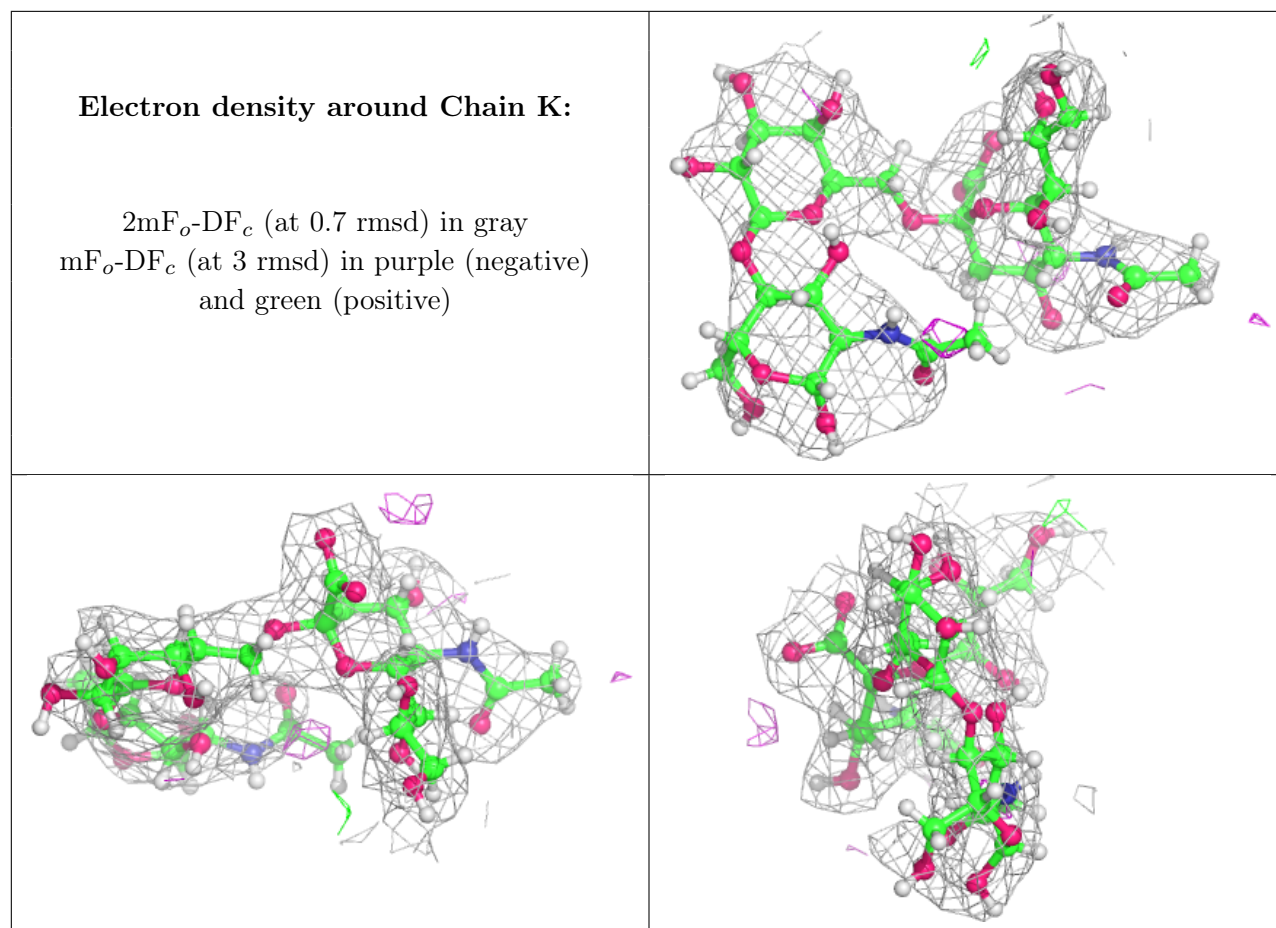
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
7	NAG	A	1004	14/15	0.52	0.46	59,71,83,86	0
7	NAG	C	1001	14/15	0.79	0.30	45,54,63,65	0
7	NAG	C	1002	14/15	0.82	0.28	44,53,64,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.