



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 11:25 PM BST

PDB ID : 3SKU
Title : Herpes simplex virus glycoprotein D bound to the human receptor nectin-1
Authors : Di Giovine, P.; Settembre, E.C.; Bhargava, A.K.; Luftig, M.A.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Krummenacher, C.; Carfi, A.
Deposited on : 2011-06-23
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

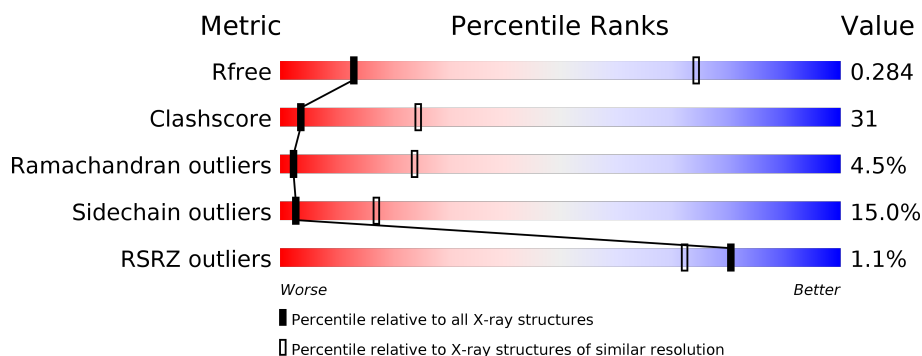
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.





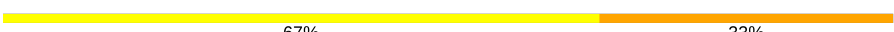
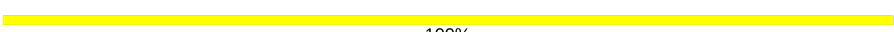


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	285	<div> <div>45%</div> <div>31%</div> <div>5%</div> <div>19%</div> </div>
1	B	285	<div> <div>45%</div> <div>29%</div> <div>5%</div> <div>22%</div> </div>
1	C	285	<div> <div>42%</div> <div>32%</div> <div>5%</div> <div>20%</div> </div>
2	D	319	<div> <div>23%</div> <div>24%</div> <div>8%</div> <div>43%</div> </div>
2	E	319	<div> <div>22%</div> <div>22%</div> <div>11%</div> <div>43%</div> </div>
2	F	319	<div> <div>22%</div> <div>26%</div> <div>6%</div> <div>45%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	3	
3	I	3	
3	K	3	
3	M	3	
4	H	2	
4	J	2	
4	L	2	

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
3	NAG	I	1	-	-	-	X
3	NAG	K	1	-	-	-	X
4	NAG	J	2	-	-	-	X
5	NAG	C	1307	-	-	X	-
5	NAG	D	350	-	-	-	X
5	NAG	F	350	X	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9902 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 Glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1806	1159	310	327	10			
1	B	223	Total	C	N	O	S	0	0	0
			1755	1127	302	316	10			
1	C	228	Total	C	N	O	S	0	0	0
			1794	1152	308	324	10			

- Molecule 2 is a protein called Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	181	Total	C	N	O	S	0	0	0
			1424	899	243	274	8			
2	D	181	Total	C	N	O	S	0	0	0
			1424	899	243	274	8			
2	F	176	Total	C	N	O	S	0	0	0
			1389	875	238	268	8			

There are 12 discrepancies between the modelled and reference sequences:

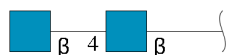
Chain	Residue	Modelled	Actual	Comment	Reference
E	346	HIS	-	expression tag	UNP Q15223
E	347	HIS	-	expression tag	UNP Q15223
E	348	HIS	-	expression tag	UNP Q15223
E	349	HIS	-	expression tag	UNP Q15223
D	346	HIS	-	expression tag	UNP Q15223
D	347	HIS	-	expression tag	UNP Q15223
D	348	HIS	-	expression tag	UNP Q15223
D	349	HIS	-	expression tag	UNP Q15223
F	346	HIS	-	expression tag	UNP Q15223
F	347	HIS	-	expression tag	UNP Q15223
F	348	HIS	-	expression tag	UNP Q15223
F	349	HIS	-	expression tag	UNP Q15223

- 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.



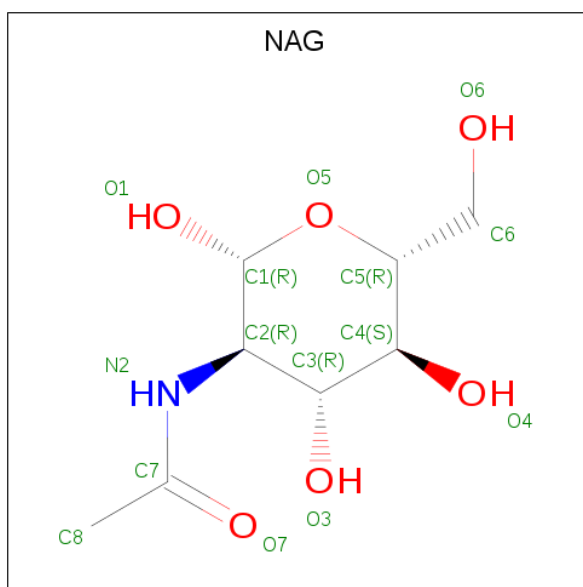
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

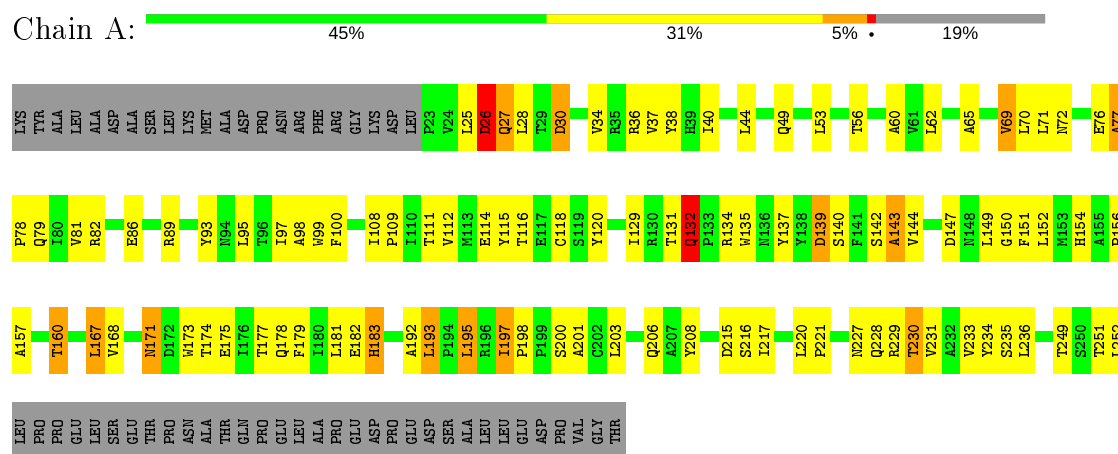


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

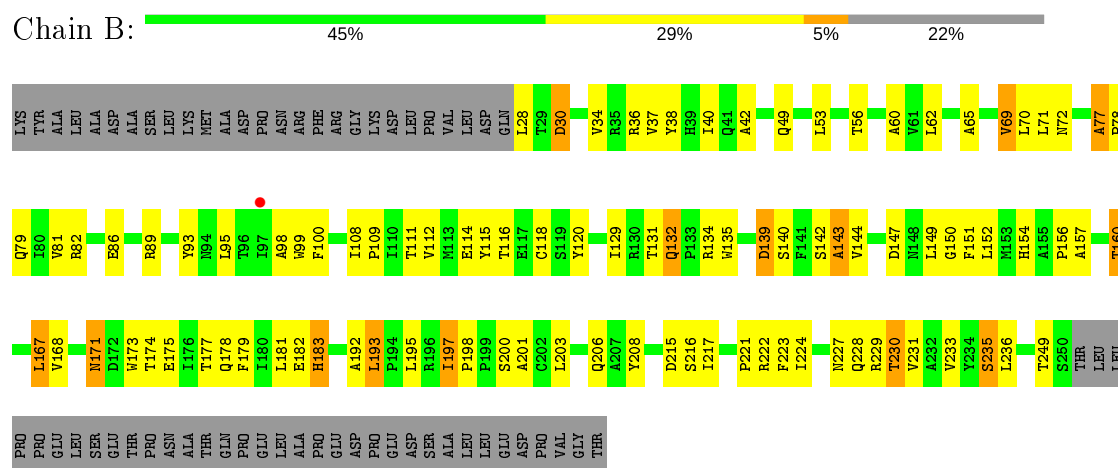
3 Residue-property plots

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.

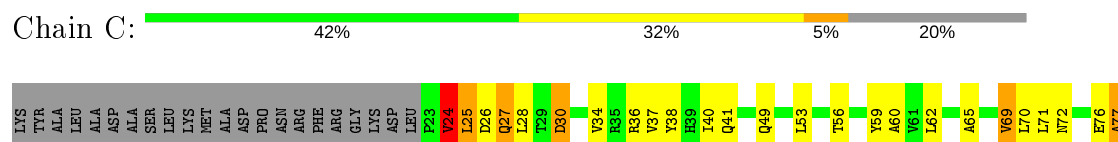
• Molecule 1: Glycoprotein D



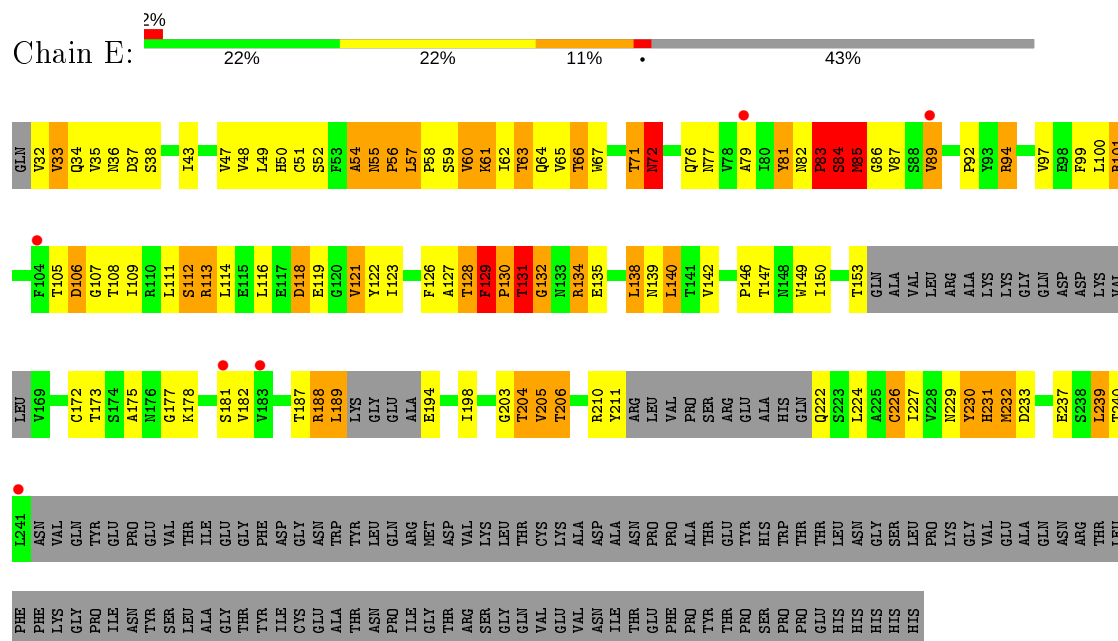
• Molecule 1: Glycoprotein D



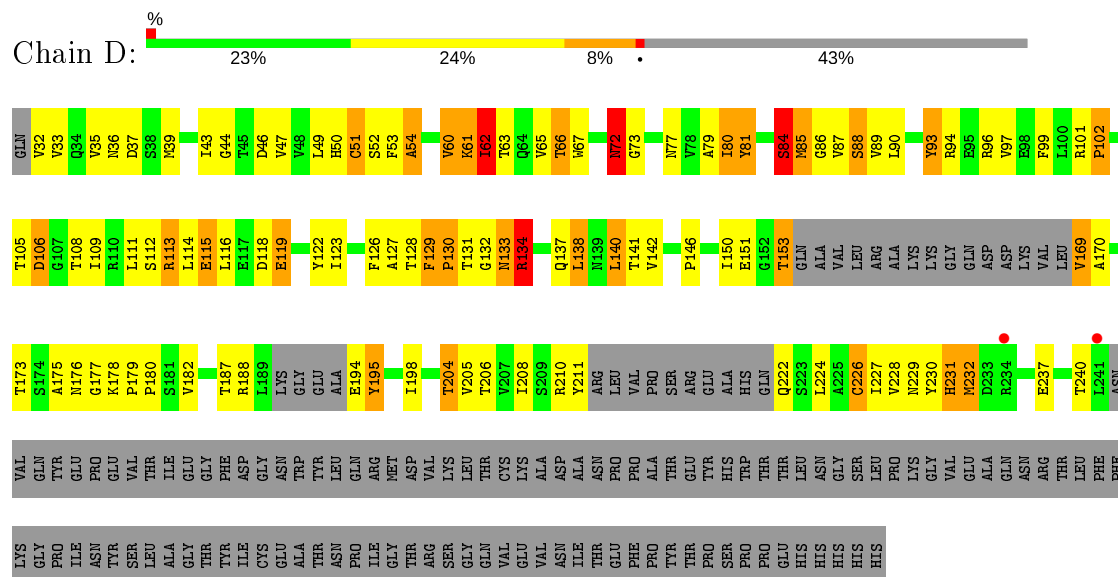
• Molecule 1: Glycoprotein D



- Molecule 2: Poliovirus receptor-related protein 1



- Molecule 2: Poliovirus receptor-related protein 1



- Molecule 2: Poliovirus receptor-related protein 1

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

Chain H:  100%

NAG1
NAG2

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

Chain J:  50% 50%

NAG1
NAG2

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

Chain L:  50% 50%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.00Å 188.00Å 185.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 49.16 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-4.00) 99.0 (49.16-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.266 , 0.287 0.266 , 0.284	Depositor DCC
R_{free} test set	1623 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	151.6	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 177.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l	Xtriage
Reported twinning fraction	0.502 for H, K, L 0.498 for -h,-k,l	Depositor
Outliers	0 of 31947 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9902	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: BMA, 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	0.62	1/1860 (0.1%)	0.67	0/2544
1	B	0.58	0/1808	0.68	0/2472
1	C	0.64	0/1848	0.71	0/2527
2	D	1.01	7/1452 (0.5%)	0.92	1/1974 (0.1%)
2	E	0.99	9/1452 (0.6%)	0.93	2/1974 (0.1%)
2	F	1.03	8/1414 (0.6%)	0.91	1/1918 (0.1%)
All	All	0.81	25/9834 (0.3%)	0.80	4/13409 (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
2	D	0	2
2	E	0	3
2	F	0	4
All	All	0	9

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	61	LYS	CD-CE	8.36	1.72	1.51
2	E	81	TYR	CE1-CZ	7.12	1.47	1.38
2	F	82	ASN	C-O	6.94	1.36	1.23
2	F	81	TYR	CE2-CZ	6.94	1.47	1.38
2	E	131	THR	CB-CG2	6.51	1.73	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	230	TYR	CB-CG-CD1	-6.17	117.30	121.00
2	F	85	MET	CB-CG-SD	5.97	130.30	112.40
2	E	230	TYR	CB-CG-CD2	5.70	124.42	121.00
2	D	86	GLY	N-CA-C	5.58	127.05	113.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	130	PRO	Peptide
2	D	84	SER	Peptide
2	E	132	GLY	Peptide
2	E	71	THR	Peptide
2	E	83	PRO	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	1806	0	1781	93	0
1	B	1755	0	1732	88	0
1	C	1794	0	1772	98	0
2	D	1424	0	1395	129	0
2	E	1424	0	1395	113	0
2	F	1389	0	1355	129	0
3	G	39	0	34	4	1
3	I	39	0	34	0	0
3	K	39	0	34	0	1
3	M	39	0	34	1	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
5	B	14	0	13	0	0
5	C	14	0	13	11	0
5	D	14	0	13	0	0
5	E	14	0	13	1	0
5	F	14	0	13	0	0
All	All	9902	0	9706	613	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 613 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:VAL:CG1	2:D:128:THR:HG23	1.59	1.32
2:D:60:VAL:CG1	2:D:128:THR:CG2	2.22	1.16
2:D:60:VAL:HG11	2:D:128:THR:HG23	1.17	1.13
2:D:60:VAL:HG11	2:D:128:THR:CG2	1.78	1.11
2:F:175:ALA:HA	2:F:206:THR:HG23	1.30	1.11

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:BMA:O2	3:K:3:BMA:O3[4_555]	2.13	0.07

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	228/285 (80%)	196 (86%)	27 (12%)	5 (2%)	6	37
1	B	221/285 (78%)	190 (86%)	26 (12%)	5 (2%)	6	37
1	C	226/285 (79%)	190 (84%)	30 (13%)	6 (3%)	5	34
2	D	173/319 (54%)	140 (81%)	20 (12%)	13 (8%)	1	15
2	E	173/319 (54%)	141 (82%)	18 (10%)	14 (8%)	1	13
2	F	166/319 (52%)	132 (80%)	24 (14%)	10 (6%)	1	19
All	All	1187/1812 (66%)	989 (83%)	145 (12%)	53 (4%)	2	24

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	C	24	VAL
2	E	56	PRO
2	E	57	LEU
2	E	60	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/243 (81%)	170 (87%)	26 (13%)	4	21
1	B	190/243 (78%)	167 (88%)	23 (12%)	5	23
1	C	195/243 (80%)	171 (88%)	24 (12%)	4	23
2	D	163/281 (58%)	135 (83%)	28 (17%)	2	13
2	E	163/281 (58%)	128 (78%)	35 (22%)	1	6
2	F	158/281 (56%)	134 (85%)	24 (15%)	3	16
All	All	1065/1572 (68%)	905 (85%)	160 (15%)	3	17

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	THR
2	E	118	ASP
2	F	111	LEU
2	E	37	ASP
2	E	83	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	HIS
2	E	77	ASN
2	F	148	ASN
1	C	206	GLN

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Mol	Chain	Res	Type
2	E	222	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 ⓘ

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$
3	NAG	G	1	1,3	14,14,15	0.66	0	17,19,21	1.59	3 (17%)
3	NAG	G	2	3	14,14,15	1.30	2 (14%)	17,19,21	2.87	7 (41%)
3	BMA	G	3	3	11,11,12	0.55	0	15,15,17	2.45	4 (26%)
4	NAG	H	1	2,4	14,14,15	0.49	0	17,19,21	1.21	2 (11%)
4	NAG	H	2	4	14,14,15	0.60	0	17,19,21	0.94	1 (5%)
3	NAG	I	1	3,2	14,14,15	0.57	0	17,19,21	1.98	4 (23%)
3	NAG	I	2	3	14,14,15	0.50	0	17,19,21	1.56	3 (17%)
3	BMA	I	3	3	11,11,12	0.75	0	15,15,17	1.51	5 (33%)
4	NAG	J	1	2,4	14,14,15	0.68	0	17,19,21	1.23	1 (5%)
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	0.79	0
3	NAG	K	1	3,2	14,14,15	0.62	0	17,19,21	1.92	2 (11%)
3	NAG	K	2	3	14,14,15	0.44	0	17,19,21	2.04	6 (35%)
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	2.07	3 (20%)
4	NAG	L	1	2,4	14,14,15	0.78	0	17,19,21	0.96	0
4	NAG	L	2	4	14,14,15	0.54	0	17,19,21	1.22	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	1	3,2	14,14,15	0.67	0	17,19,21	1.62	3 (17%)
3	NAG	M	2	3	14,14,15	0.65	0	17,19,21	1.76	4 (23%)
3	BMA	M	3	3	11,11,12	0.70	0	15,15,17	2.01	4 (26%)

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	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
4	NAG	L	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	-3.38	1.38	1.43
3	G	2	NAG	C1-C2	2.58	1.56	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	8.51	123.72	112.19
3	G	3	BMA	C1-O5-C5	7.16	121.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-O5-C5	6.63	121.17	112.19
3	I	1	NAG	C1-O5-C5	6.08	120.43	112.19
3	M	3	BMA	C1-O5-C5	5.71	119.93	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

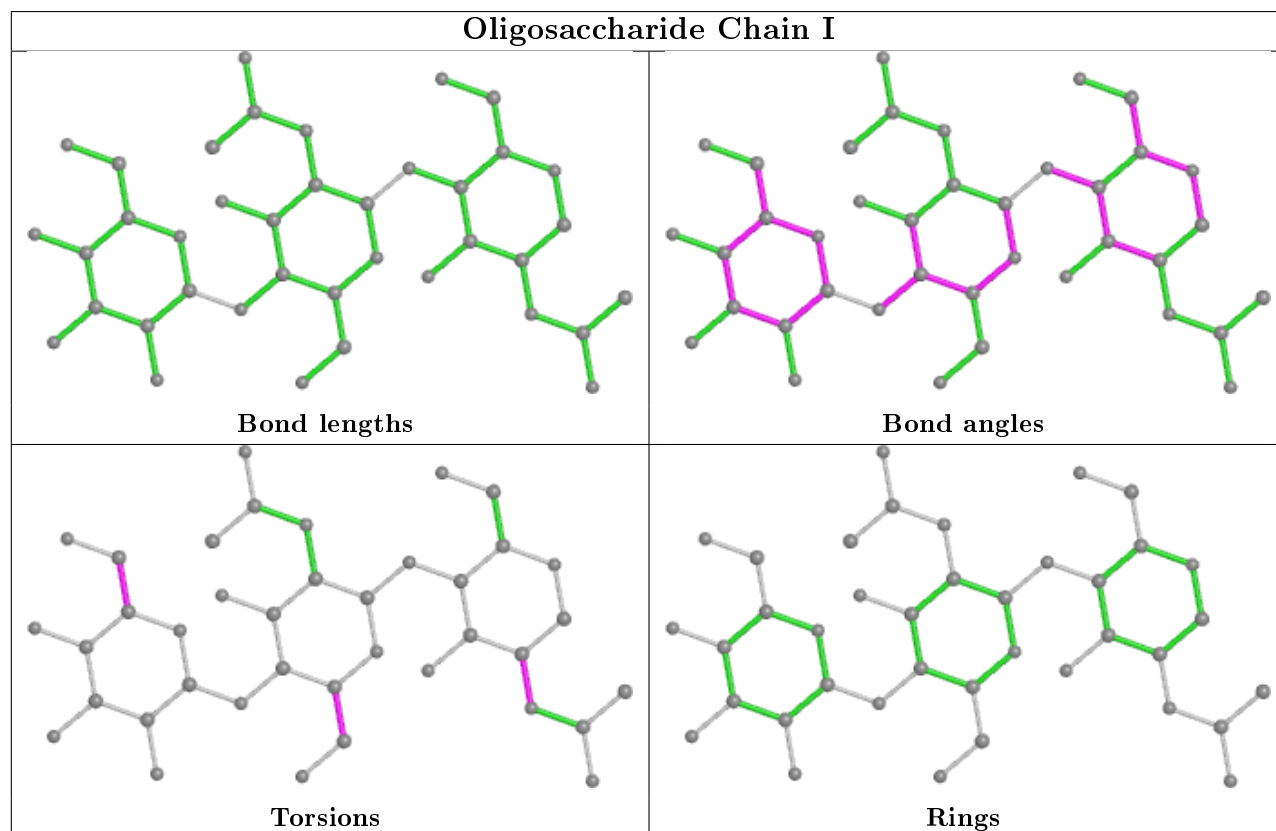
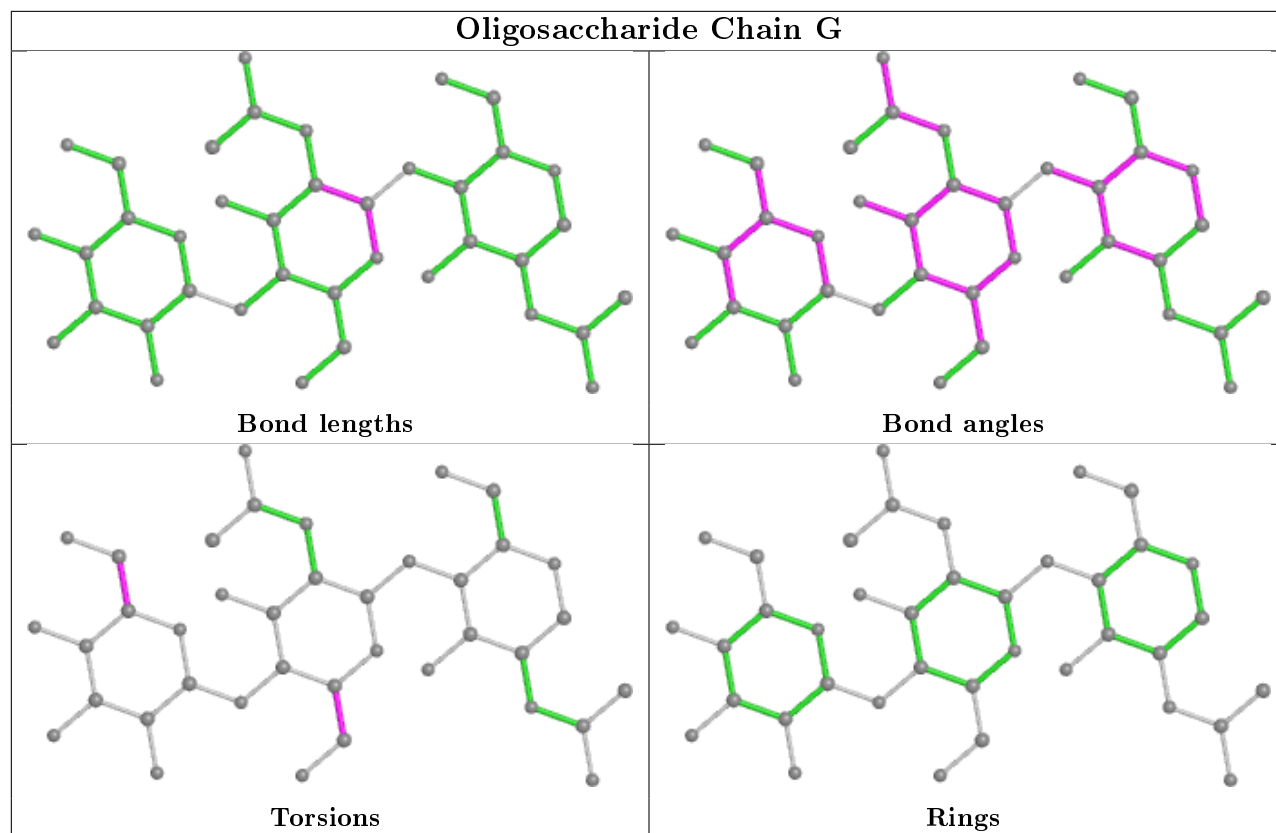
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6

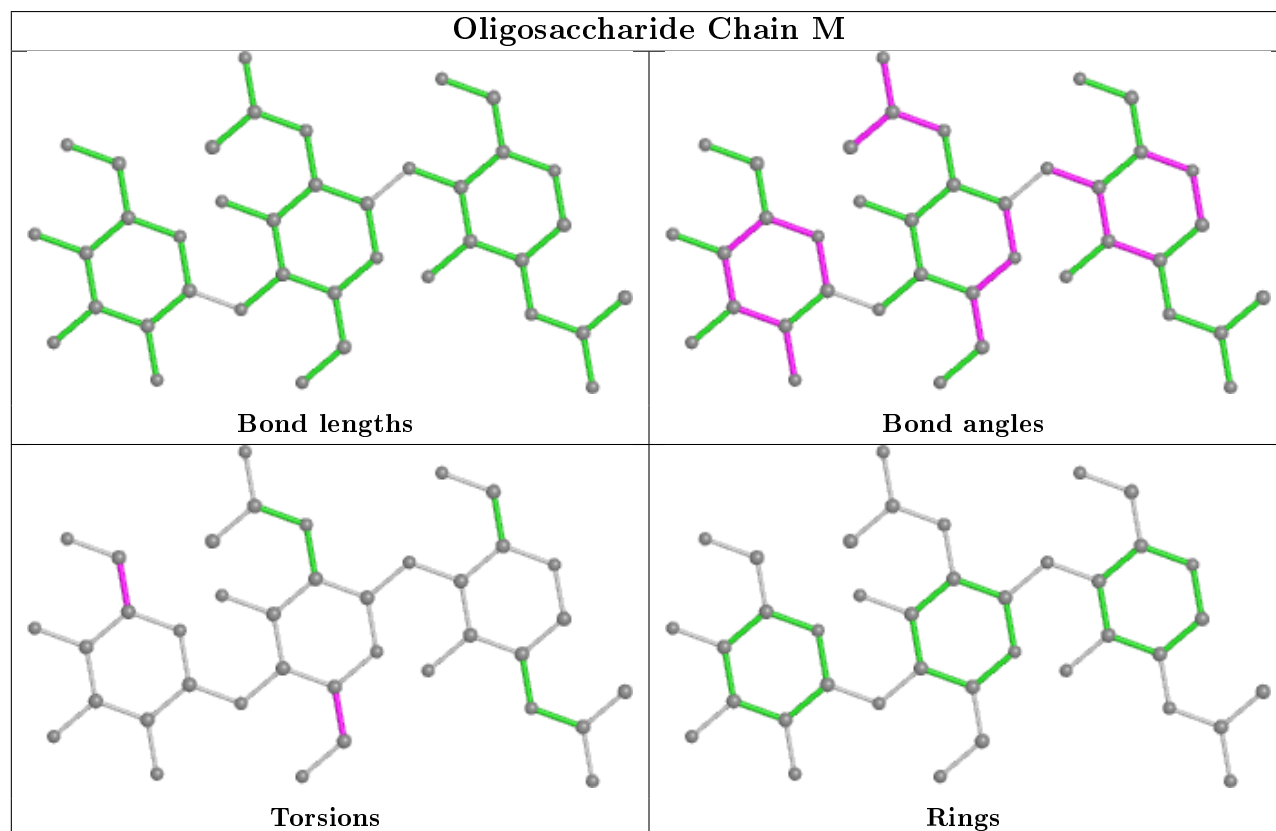
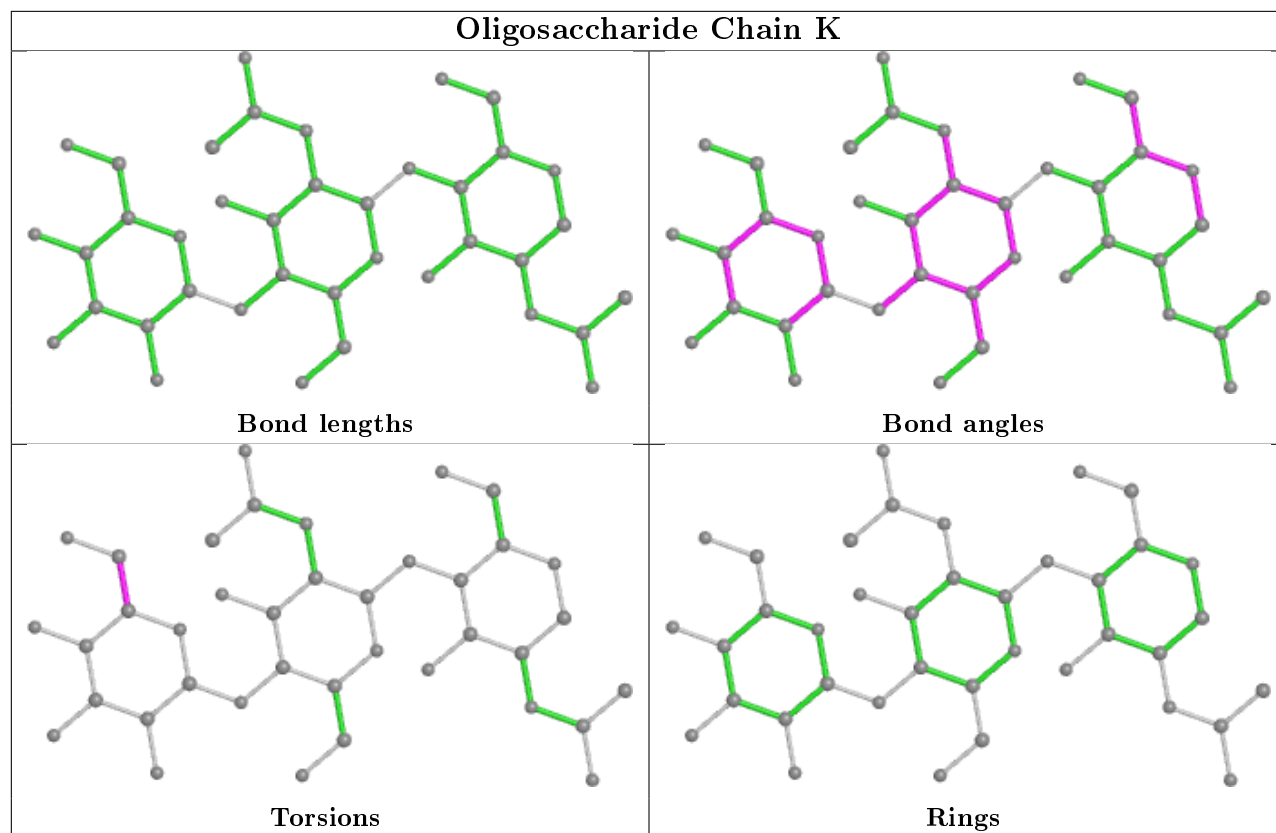
There are no ring outliers.

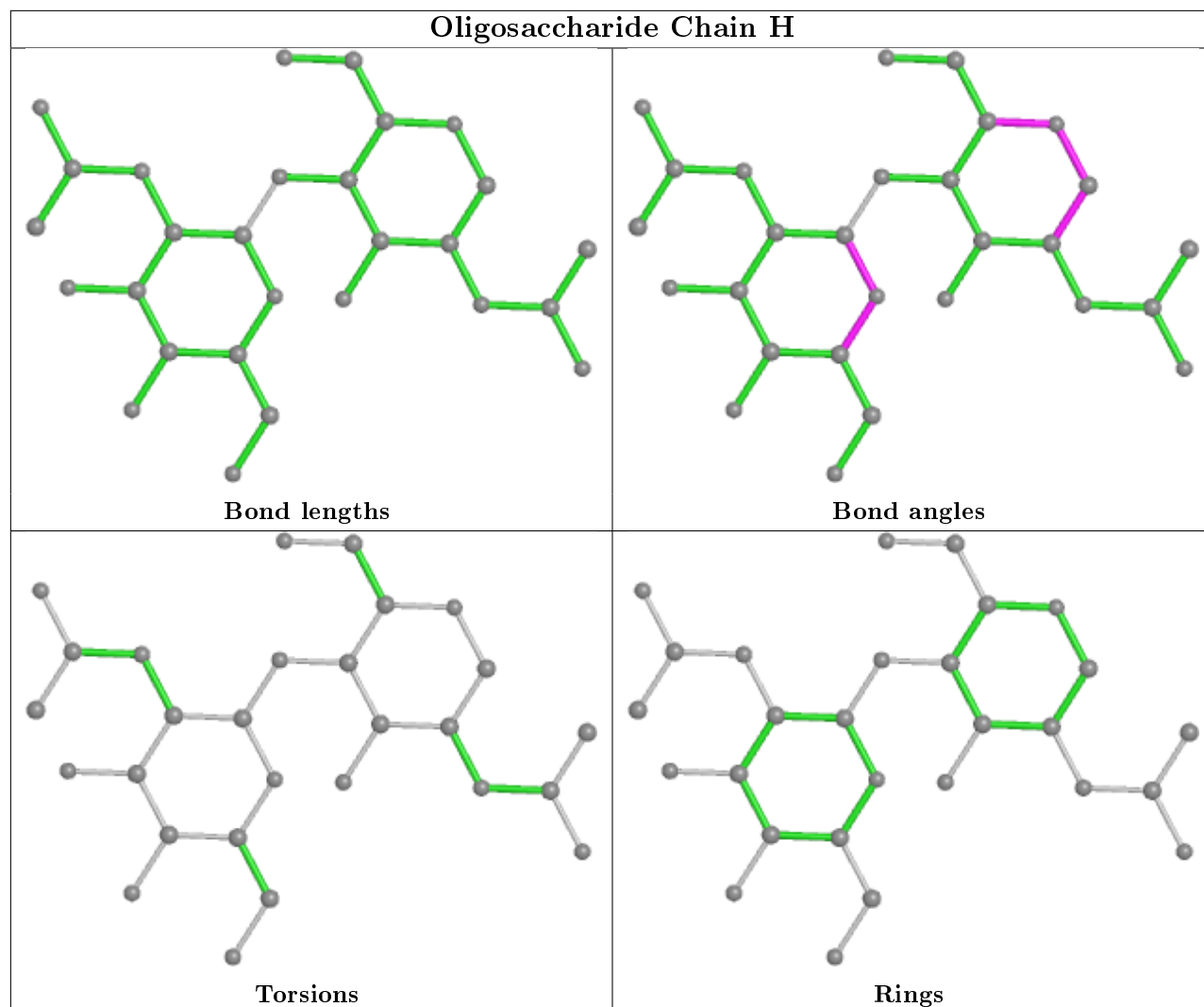
4 monomers are involved in 6 short contacts:

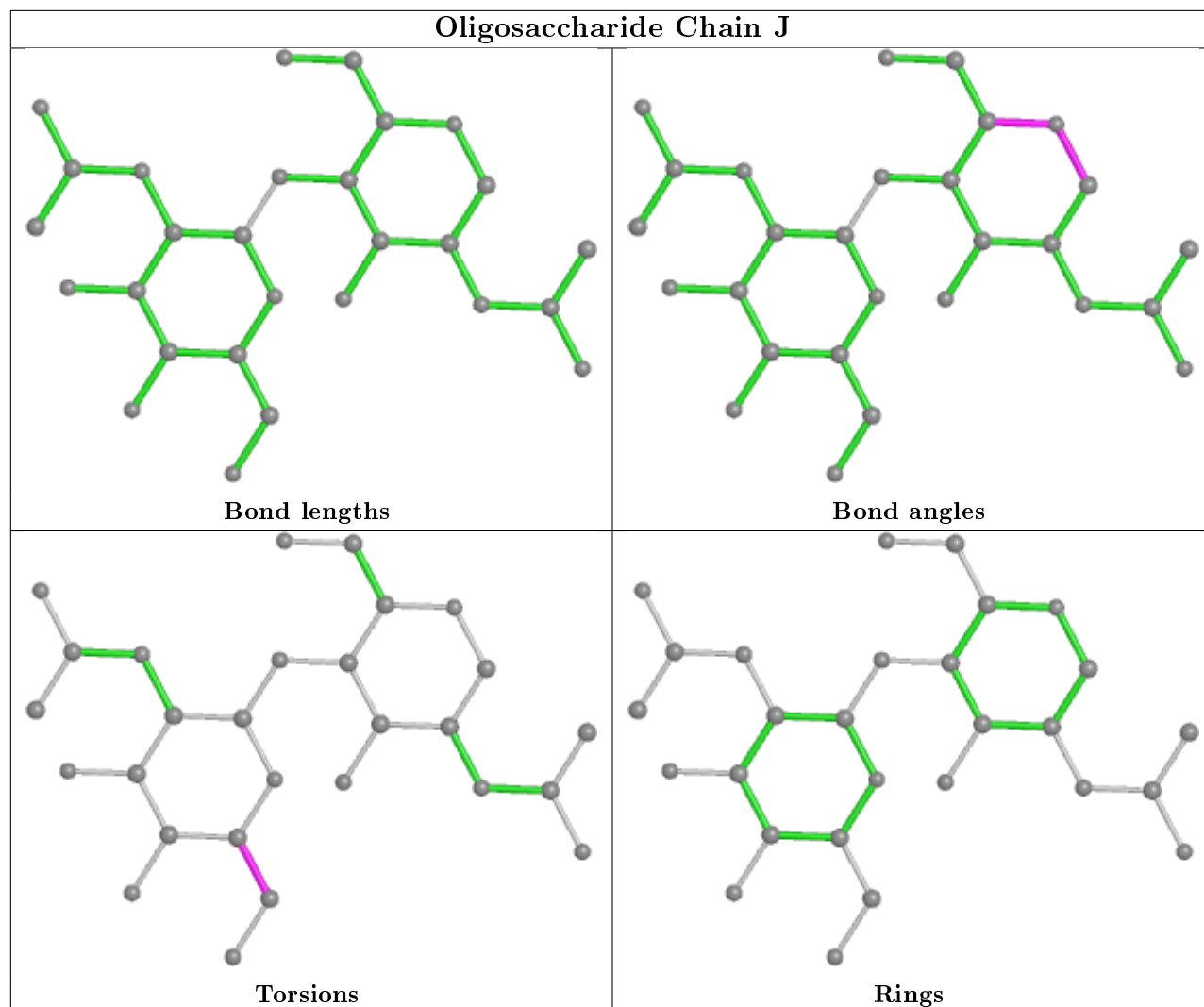
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	BMA	0	1
3	G	2	NAG	4	0
3	M	1	NAG	1	0
3	G	3	BMA	4	1

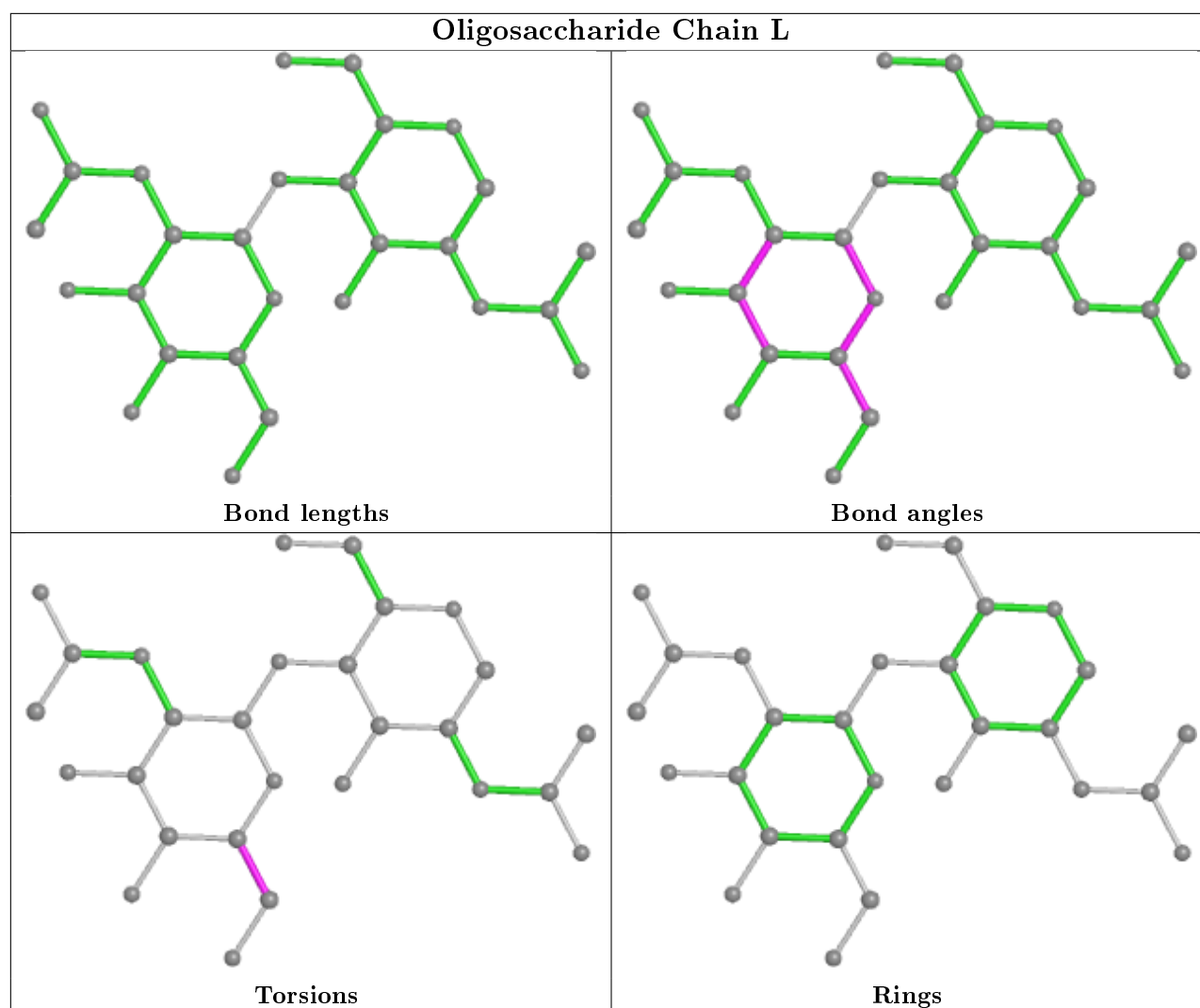
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
5	NAG	C	1307	1	14,14,15	1.48	3 (21%)	17,19,21	2.59	5 (29%)
5	NAG	D	350	2	14,14,15	0.62	0	17,19,21	2.14	2 (11%)
5	NAG	F	350	2	14,14,15	1.01	1 (7%)	17,19,21	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1307	1	14,14,15	2.05	6 (42%)	17,19,21	2.95	7 (41%)
5	NAG	E	350	2	14,14,15	0.45	0	17,19,21	1.42	1 (5%)

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	C	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	D	350	2	-	1/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	F	350	2	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	E	350	2	-	1/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	C1-C2	3.41	1.57	1.52
5	B	1307	NAG	C8-C7	3.11	1.57	1.50
5	C	1307	NAG	O7-C7	3.09	1.30	1.23
5	F	350	NAG	C1-C2	2.82	1.56	1.52
5	B	1307	NAG	C2-N2	2.44	1.50	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1307	NAG	C1-O5-C5	9.68	125.31	112.19
5	D	350	NAG	C1-O5-C5	6.89	121.53	112.19
5	C	1307	NAG	C8-C7-N2	-5.65	106.54	116.10
5	C	1307	NAG	C2-N2-C7	5.22	130.33	122.90
5	E	350	NAG	C1-O5-C5	4.71	118.58	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	350	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1307	NAG	C1-C2-N2-C7
5	F	350	NAG	C4-C5-C6-O6
5	F	350	NAG	O5-C5-C6-O6
5	E	350	NAG	O5-C5-C6-O6
5	D	350	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1307	NAG	11	0
5	E	350	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	230/285 (80%)	-0.08	0 100 100	114, 136, 165, 185	0
1	B	223/285 (78%)	-0.06	1 (0%) 92 87	119, 142, 177, 196	0
1	C	228/285 (80%)	-0.03	0 100 100	112, 134, 167, 188	0
2	D	181/319 (56%)	0.11	2 (1%) 80 72	86, 139, 216, 300	0
2	E	181/319 (56%)	0.10	6 (3%) 46 37	100, 148, 227, 320	0
2	F	176/319 (55%)	0.32	5 (2%) 53 42	106, 152, 222, 337	0
All	All	1219/1812 (67%)	0.05	14 (1%) 80 72	86, 140, 204, 337	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	241	LEU	5.3
2	D	241	LEU	4.7
2	F	222	GLN	3.2
2	F	239	LEU	3.0
2	E	183	VAL	2.5

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

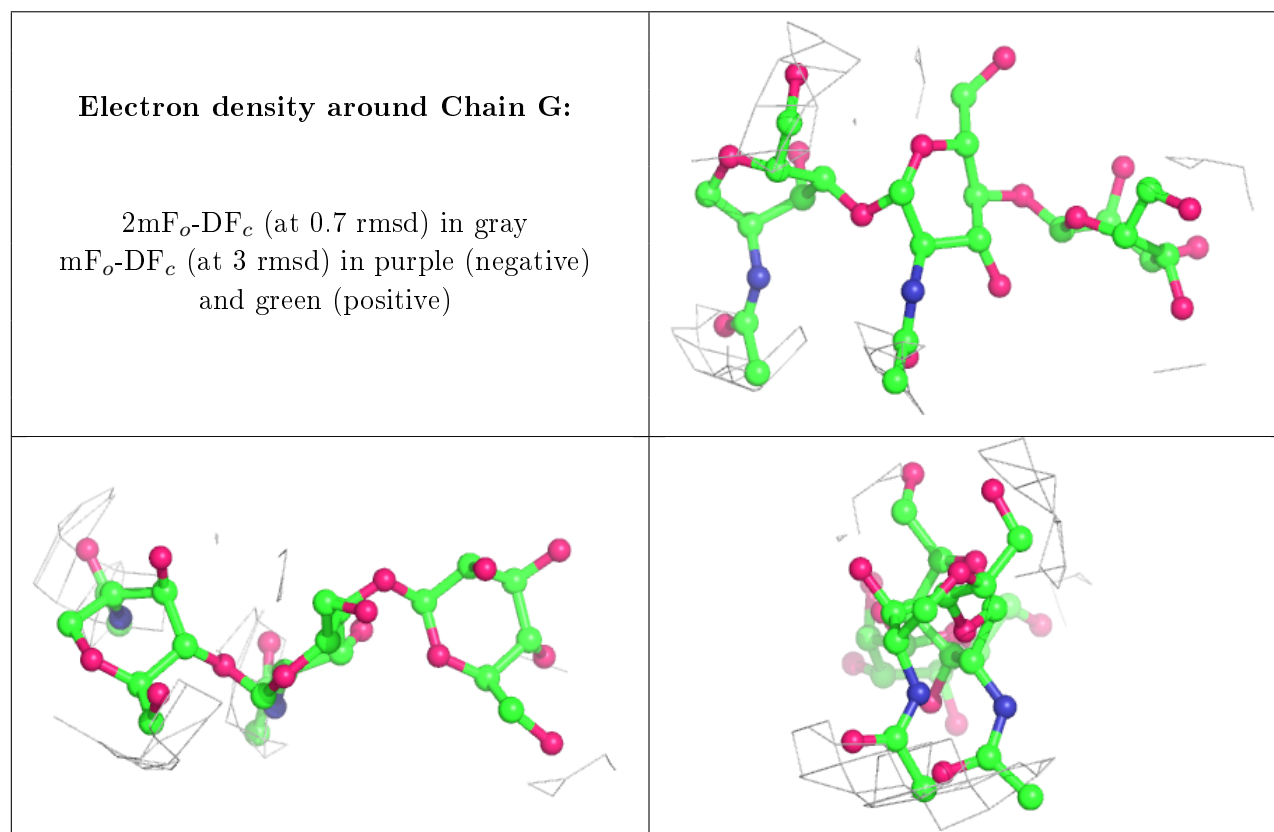
There are no non-standard protein/DNA/RNA residues in this entry.

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.

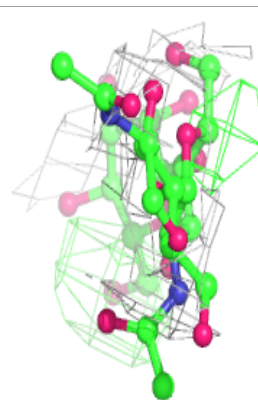
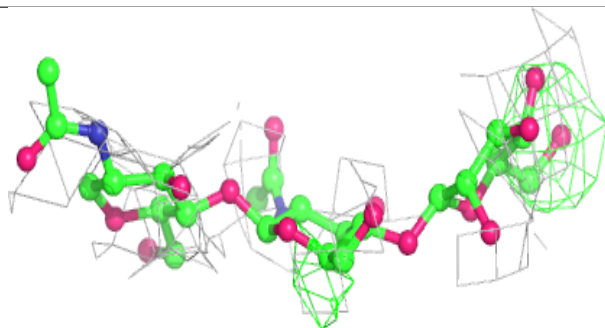
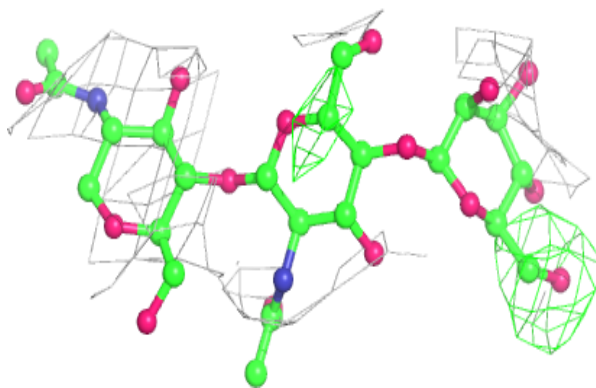
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	I	3	11/12	0.50	0.29	367,367,367,367	0
3	NAG	I	2	14/15	0.65	0.25	367,367,367,367	0
3	NAG	M	2	14/15	0.69	0.27	367,367,367,367	0
3	NAG	I	1	14/15	0.73	0.52	367,367,367,367	0
3	NAG	K	1	14/15	0.74	0.41	367,367,367,367	0
3	BMA	K	3	11/12	0.78	0.14	367,367,367,367	0
4	NAG	J	2	14/15	0.78	0.42	367,367,367,367	0
4	NAG	H	1	14/15	0.78	0.23	367,367,367,367	0
4	NAG	L	2	14/15	0.80	0.26	367,367,367,367	0
4	NAG	J	1	14/15	0.81	0.41	367,367,367,367	0
4	NAG	L	1	14/15	0.82	0.26	367,367,367,367	0
3	NAG	M	1	14/15	0.82	0.40	367,367,367,367	0
3	BMA	M	3	11/12	0.83	0.25	367,367,367,367	0
3	NAG	K	2	14/15	0.86	0.31	367,367,367,367	0
3	BMA	G	3	11/12	0.87	0.29	162,166,175,176	0
4	NAG	H	2	14/15	0.92	0.22	367,367,367,367	0
3	NAG	G	2	14/15	0.92	0.25	141,148,158,158	0
3	NAG	G	1	14/15	0.93	0.23	135,141,146,149	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.

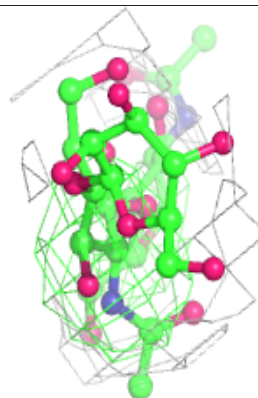
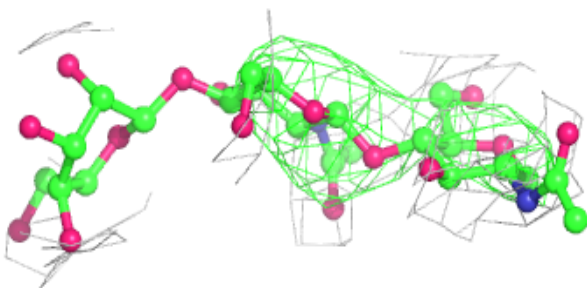
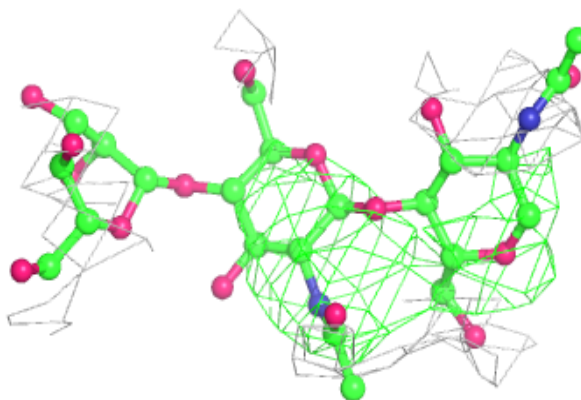


Electron density around Chain I:

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

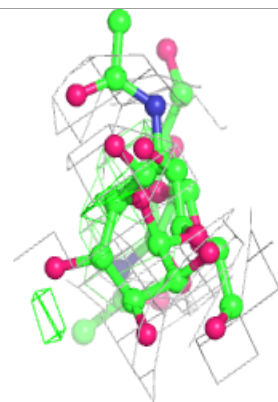
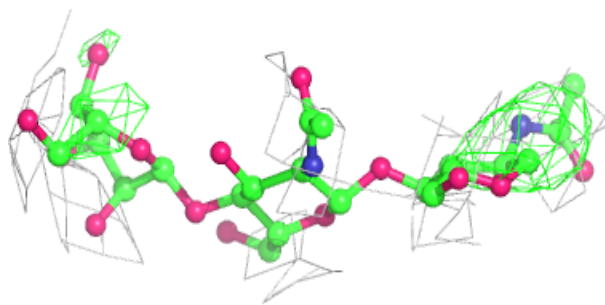
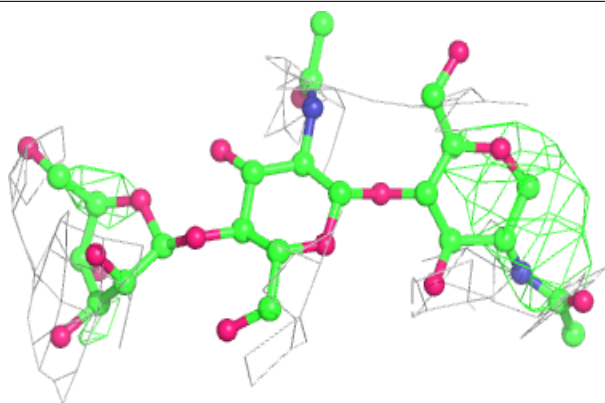
**Electron density around Chain K:**

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



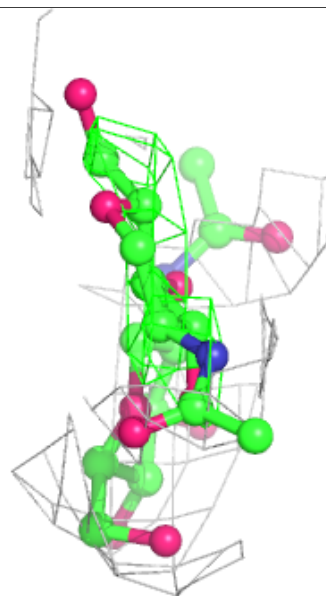
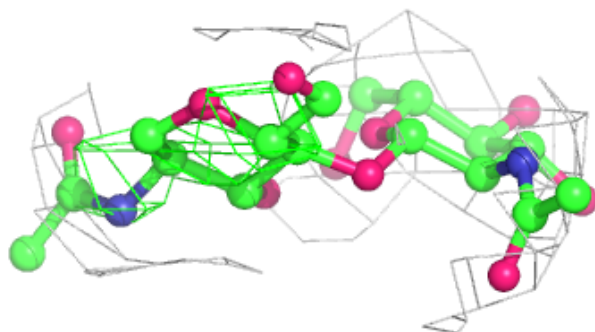
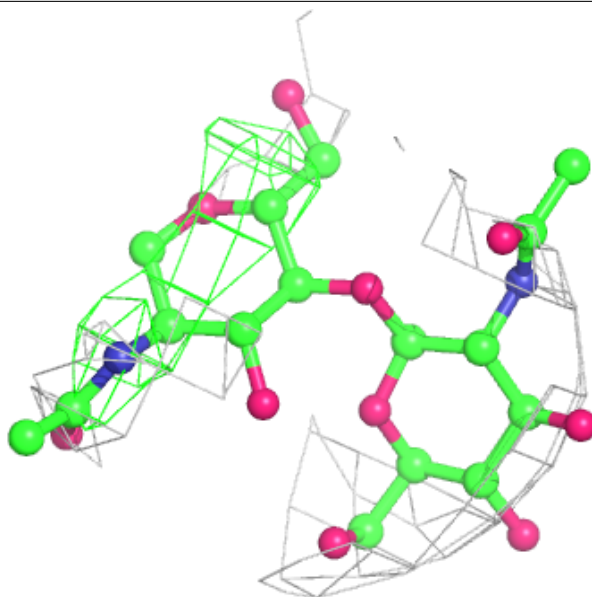
Electron density around Chain M:

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



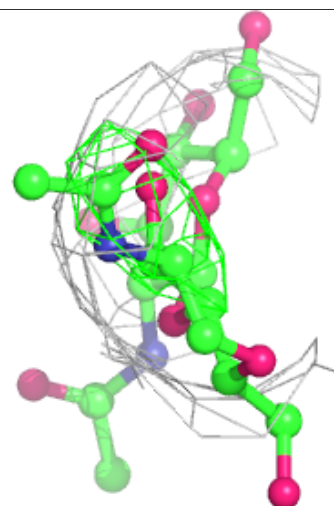
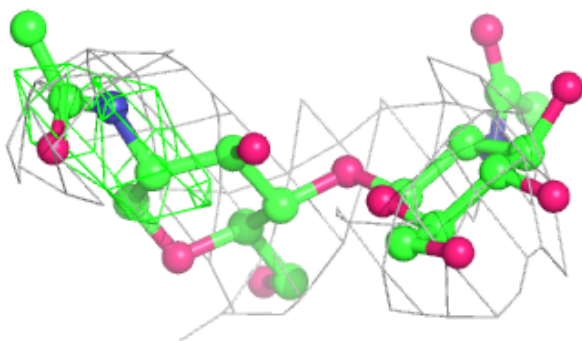
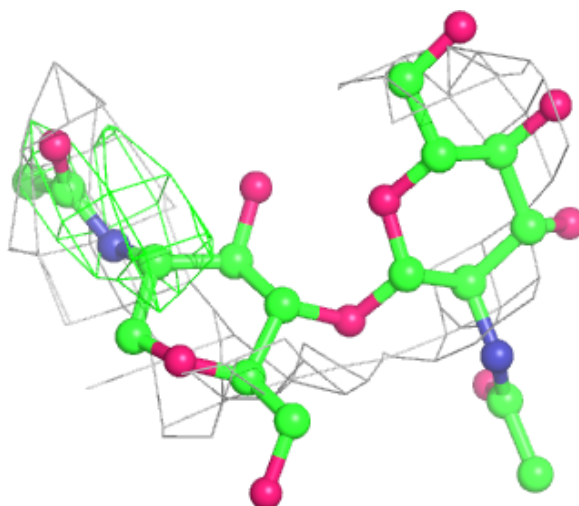
Electron density around Chain H:

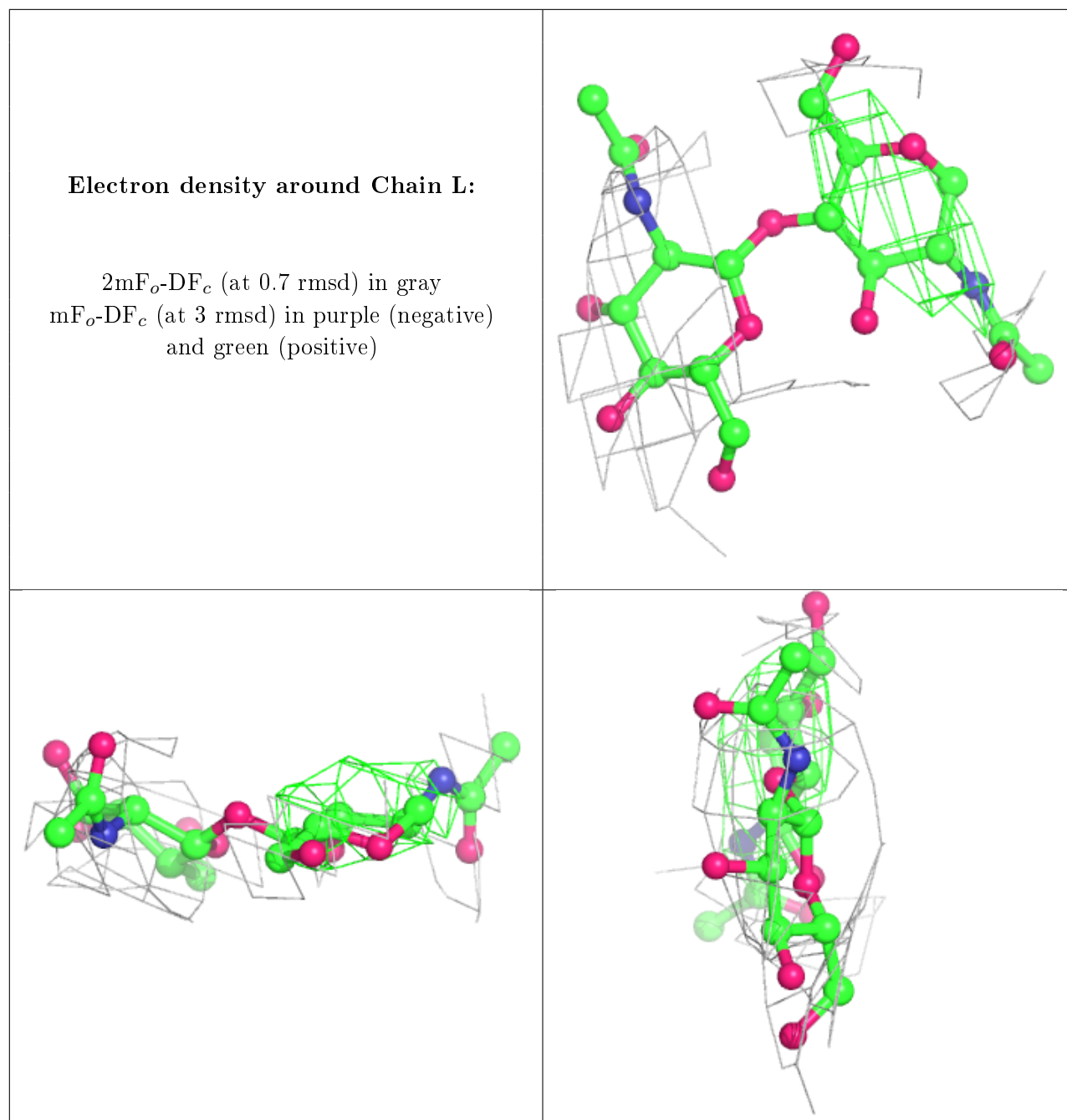
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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
5	NAG	F	350	14/15	0.41	0.56	367,367,367,367	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	C	1307	14/15	0.53	0.36	184,193,198,198	0
5	NAG	D	350	14/15	0.65	0.41	367,367,367,367	0
5	NAG	E	350	14/15	0.74	0.28	367,367,367,367	0
5	NAG	B	1307	14/15	0.86	0.29	188,194,200,203	0

6.5 Other polymers ⓘ

There are no such residues in this entry.