



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:50 AM BST

PDB ID : 6B3S
Title : Crystal structure of the Fab fragment of necitumumab (Fab11F8) in complex with domain III from a cetuximab resistant variant of EGFR (sEGFRd3-S468R)
Authors : Ferguson, K.M.; Bagchi, A.
Deposited on : 2017-09-23
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

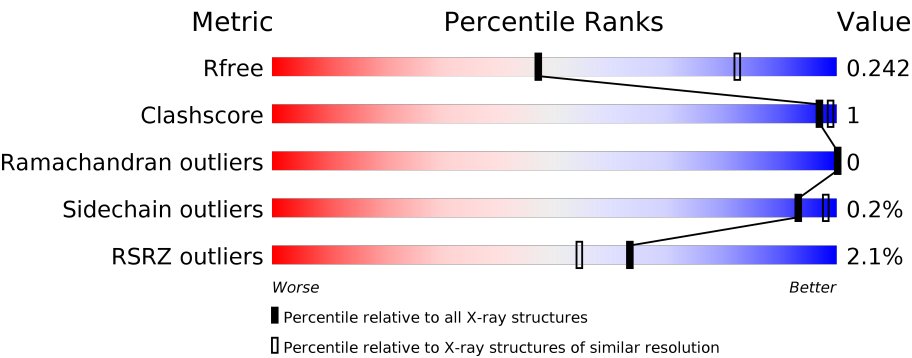
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	214	<div><div>9%</div><div><div></div><div>86%</div><div></div><div>11%</div></div><div></div></div>
1	B	214	<div><div>7%</div><div><div></div><div>88%</div><div></div><div>9%</div></div><div></div></div>
1	E	214	<div><div>3%</div><div><div></div><div>88%</div><div></div><div>9%</div></div><div></div></div>
1	I	214	<div><div>3%</div><div><div></div><div>90%</div><div></div><div>9%</div></div><div></div></div>
2	C	222	<div><div></div><div><div></div><div>95%</div><div></div><div></div></div><div></div></div>
2	F	222	<div><div></div><div><div></div><div>92%</div><div></div><div>5%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	222	 92%
2	J	222	 95%
3	D	213	 98%
3	G	213	 96%
3	K	213	 96%
3	L	213	 98%
4	M	2	 100%
4	O	2	 100%
4	Q	2	 100%
4	S	2	 100%
4	T	2	 100%
5	N	3	 100%
6	P	4	 50% 50%
6	R	4	 75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18965 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1426	898	252	268	8			
1	B	194	Total	C	N	O	S	0	0	0
			1434	899	248	278	9			
1	E	194	Total	C	N	O	S	0	0	0
			1469	921	257	282	9			
1	I	194	Total	C	N	O	S	0	0	0
			1457	916	256	276	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	expression tag	UNP P00533
A	308	GLU	-	expression tag	UNP P00533
A	309	GLU	-	expression tag	UNP P00533
A	310	LYS	-	expression tag	UNP P00533
A	468	ARG	SER	engineered mutation	UNP P00533
A	515	HIS	-	expression tag	UNP P00533
A	516	HIS	-	expression tag	UNP P00533
A	517	HIS	-	expression tag	UNP P00533
A	518	HIS	-	expression tag	UNP P00533
A	519	HIS	-	expression tag	UNP P00533
A	520	HIS	-	expression tag	UNP P00533
B	307	LEU	-	expression tag	UNP P00533
B	308	GLU	-	expression tag	UNP P00533
B	309	GLU	-	expression tag	UNP P00533
B	310	LYS	-	expression tag	UNP P00533
B	468	ARG	SER	engineered mutation	UNP P00533
B	515	HIS	-	expression tag	UNP P00533
B	516	HIS	-	expression tag	UNP P00533
B	517	HIS	-	expression tag	UNP P00533
B	518	HIS	-	expression tag	UNP P00533
B	519	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	expression tag	UNP P00533
E	307	LEU	-	expression tag	UNP P00533
E	308	GLU	-	expression tag	UNP P00533
E	309	GLU	-	expression tag	UNP P00533
E	310	LYS	-	expression tag	UNP P00533
E	468	ARG	SER	engineered mutation	UNP P00533
E	515	HIS	-	expression tag	UNP P00533
E	516	HIS	-	expression tag	UNP P00533
E	517	HIS	-	expression tag	UNP P00533
E	518	HIS	-	expression tag	UNP P00533
E	519	HIS	-	expression tag	UNP P00533
E	520	HIS	-	expression tag	UNP P00533
I	307	LEU	-	expression tag	UNP P00533
I	308	GLU	-	expression tag	UNP P00533
I	309	GLU	-	expression tag	UNP P00533
I	310	LYS	-	expression tag	UNP P00533
I	468	ARG	SER	engineered mutation	UNP P00533
I	515	HIS	-	expression tag	UNP P00533
I	516	HIS	-	expression tag	UNP P00533
I	517	HIS	-	expression tag	UNP P00533
I	518	HIS	-	expression tag	UNP P00533
I	519	HIS	-	expression tag	UNP P00533
I	520	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Necitumumab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1571	1004	252	310	5			
2	C	213	Total	C	N	O	S	0	0	0
			1583	1009	254	315	5			
2	F	214	Total	C	N	O	S	0	0	0
			1590	1013	255	317	5			
2	J	213	Total	C	N	O	S	0	0	0
			1589	1011	257	316	5			

- Molecule 3 is a protein called Necitumumab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1601	1002	266	328	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	213	Total	C	N	O	S	0	0	0
			1599	1000	268	326	5			
3	G	213	Total	C	N	O	S	0	0	0
			1603	1002	268	328	5			
3	K	213	Total	C	N	O	S	0	0	0
			1597	999	265	328	5			

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



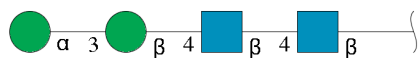
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



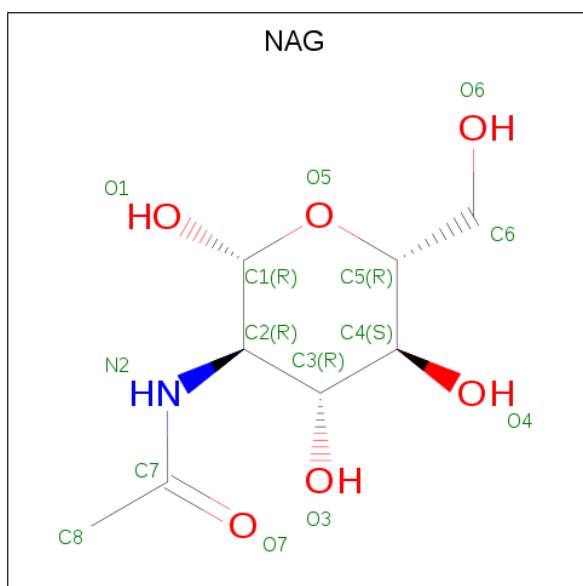
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
6	P	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

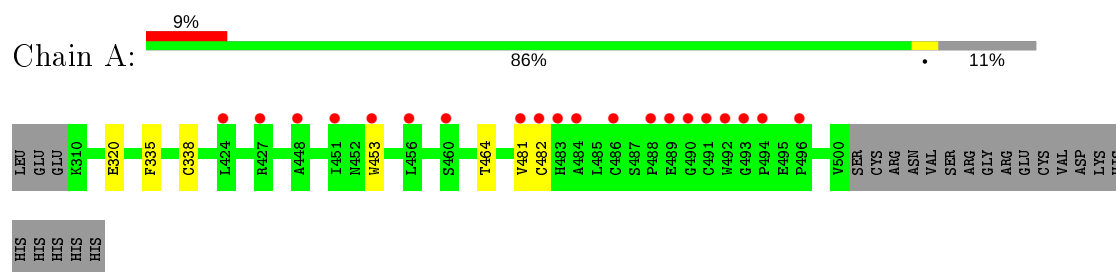
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	H	8	Total O 8 8	0	0
8	L	10	Total O 10 10	0	0
8	B	4	Total O 4 4	0	0
8	C	1	Total O 1 1	0	0
8	D	12	Total O 12 12	0	0
8	E	4	Total O 4 4	0	0
8	F	5	Total O 5 5	0	0
8	G	7	Total O 7 7	0	0
8	I	4	Total O 4 4	0	0
8	J	6	Total O 6 6	0	0
8	K	7	Total O 7 7	0	0

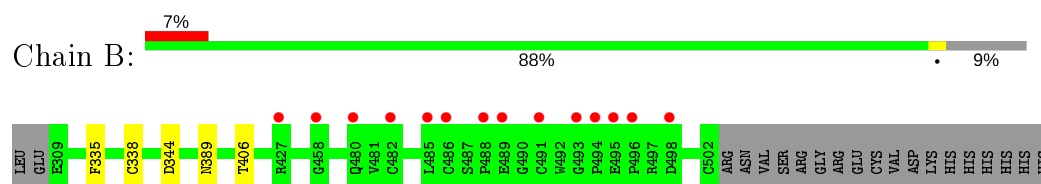
3 Residue-property plots

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.

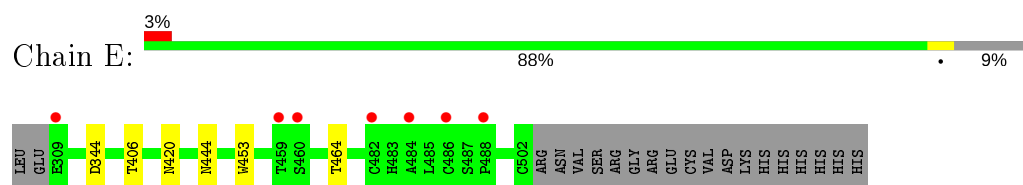
- Molecule 1: Epidermal growth factor receptor



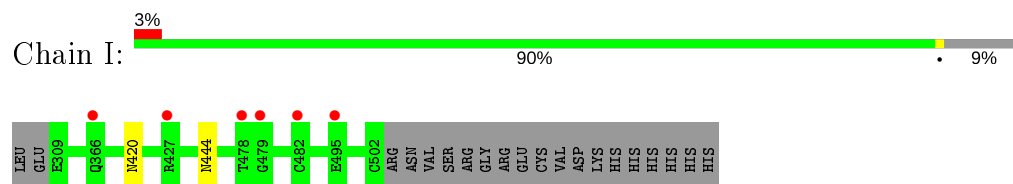
- Molecule 1: Epidermal growth factor receptor



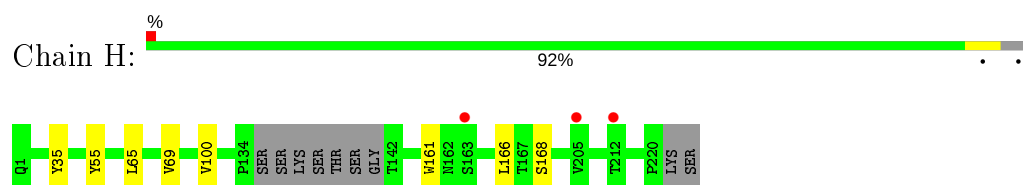
- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor

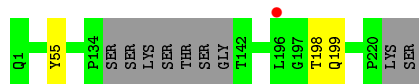


- Molecule 2: Necitumumab Fab Heavy chain



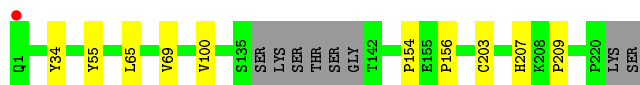
- Molecule 2: Necitumumab Fab Heavy chain

Chain C:  95%



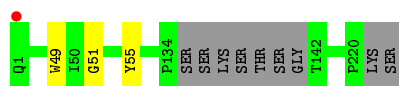
- Molecule 2: Necitumumab Fab Heavy chain

Chain F:  92%



- Molecule 2: Necitumumab Fab Heavy chain

Chain J:  95%



- Molecule 3: Necitumumab Fab Light chain

Chain L:  98%



- Molecule 3: Necitumumab Fab Light chain

Chain D:  98%



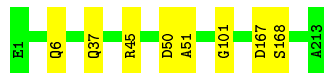
- Molecule 3: Necitumumab Fab Light chain

Chain G:  96%



- Molecule 3: Necitumumab Fab Light chain

Chain K:  96%



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

Chain M:  100%

HA01
HA02

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

Chain O:  100%

HA01
HA02

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

Chain Q:  100%

HA01
HA02

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

Chain S:  100%

HA01
HA02

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

Chain T:  100%

HA01
HA02

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

Chain N:  100%

HA01
HA02
BX03

- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.94Å 80.76Å 172.90Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	47.00 – 2.80 47.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.00-2.80) 96.0 (47.00-2.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.208 , 0.245 0.207 , 0.242	Depositor DCC
R_{free} test set	4977 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18965	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, MAN

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	0.26	0/1454	0.45	0/1974
1	B	0.26	0/1461	0.46	0/1989
1	E	0.26	0/1497	0.46	0/2030
1	I	0.25	0/1485	0.45	0/2015
2	C	0.28	0/1625	0.47	0/2228
2	F	0.28	0/1632	0.47	0/2237
2	H	0.29	0/1613	0.49	0/2213
2	J	0.28	0/1630	0.48	0/2232
3	D	0.27	0/1635	0.45	0/2228
3	G	0.28	0/1639	0.46	0/2233
3	K	0.28	0/1633	0.45	0/2226
3	L	0.27	0/1637	0.46	0/2230
All	All	0.27	0/18941	0.46	0/25835

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1426	0	1380	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1434	0	1359	4	0
1	E	1469	0	1426	3	0
1	I	1457	0	1413	1	0
2	C	1583	0	1529	1	0
2	F	1590	0	1536	4	0
2	H	1571	0	1512	4	0
2	J	1589	0	1550	1	0
3	D	1599	0	1526	2	0
3	G	1603	0	1530	4	0
3	K	1597	0	1519	4	0
3	L	1601	0	1530	2	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
4	Q	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
5	N	39	0	34	0	0
6	P	50	0	43	0	0
6	R	50	0	43	0	0
7	A	28	0	26	0	0
7	B	28	0	26	2	0
7	E	28	0	26	0	0
7	I	14	0	13	0	0
8	A	1	0	0	0	0
8	B	4	0	0	0	0
8	C	1	0	0	0	0
8	D	12	0	0	0	0
8	E	4	0	0	0	0
8	F	5	0	0	0	0
8	G	7	0	0	0	0
8	H	8	0	0	0	0
8	I	4	0	0	0	0
8	J	6	0	0	0	0
8	K	7	0	0	0	0
8	L	10	0	0	0	0
All	All	18965	0	18146	34	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 1.

All (34) 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)
3:L:108:ARG:NH1	3:L:109:THR:O	2.27	0.68
3:D:108:ARG:NH1	3:D:109:THR:O	2.38	0.56
3:K:37:GLN:OE1	3:K:45:ARG:NH1	2.40	0.55
1:B:344:ASP:OD1	1:B:406:THR:OG1	2.22	0.53
3:L:167:ASP:OD1	3:L:168:SER:N	2.45	0.50
1:A:453:TRP:CG	1:A:464:THR:HG21	2.48	0.49
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.48	0.49
3:G:149:LYS:NZ	3:G:195:GLU:OE1	2.32	0.49
2:H:65:LEU:HD22	2:H:69:VAL:HG21	1.97	0.47
2:C:198:THR:OG1	2:C:199:GLN:N	2.47	0.47
3:K:167:ASP:OD1	3:K:168:SER:N	2.48	0.47
1:E:420:ASN:OD1	1:E:444:ASN:ND2	2.49	0.46
3:G:167:ASP:OD1	3:G:168:SER:N	2.49	0.46
1:E:344:ASP:OD1	1:E:406:THR:OG1	2.32	0.46
2:F:65:LEU:HD22	2:F:69:VAL:HG21	1.97	0.45
2:F:154:PRO:HG2	2:F:209:PRO:HG2	1.99	0.45
1:B:389:ASN:HD21	7:B:602:NAG:H83	1.82	0.44
1:B:335:PHE:HA	1:B:338:CYS:SG	2.58	0.44
3:G:108:ARG:NH1	3:G:109:THR:O	2.51	0.43
2:J:49:TRP:CZ2	2:J:51:GLY:HA2	2.53	0.43
1:A:320:GLU:OE1	1:A:320:GLU:N	2.40	0.43
2:H:161:TRP:HB3	2:H:166:LEU:HD12	1.99	0.43
3:K:50:ASP:O	3:K:51:ALA:HB3	2.20	0.42
3:D:50:ASP:O	3:D:51:ALA:HB3	2.20	0.42
1:I:420:ASN:OD1	1:I:444:ASN:ND2	2.52	0.42
1:E:453:TRP:CG	1:E:464:THR:HG21	2.55	0.42
2:H:166:LEU:O	2:H:168:SER:N	2.47	0.42
1:B:389:ASN:ND2	7:B:602:NAG:H83	2.34	0.41
2:F:156:PRO:O	2:F:207:HIS:HD2	2.04	0.41
2:H:35:TYR:HB2	2:H:100:VAL:HB	2.03	0.41
1:A:335:PHE:HA	1:A:338:CYS:SG	2.61	0.41
1:A:481:VAL:HG12	1:A:482:CYS:N	2.36	0.40
3:K:6:GLN:OE1	3:K:101:GLY:N	2.54	0.40
2:F:34:TYR:HA	2:F:100:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	189/214 (88%)	185 (98%)	4 (2%)	0	100	100
1	B	192/214 (90%)	189 (98%)	3 (2%)	0	100	100
1	E	192/214 (90%)	185 (96%)	7 (4%)	0	100	100
1	I	192/214 (90%)	186 (97%)	6 (3%)	0	100	100
2	C	209/222 (94%)	198 (95%)	11 (5%)	0	100	100
2	F	210/222 (95%)	199 (95%)	11 (5%)	0	100	100
2	H	209/222 (94%)	197 (94%)	12 (6%)	0	100	100
2	J	209/222 (94%)	202 (97%)	7 (3%)	0	100	100
3	D	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
3	G	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
3	K	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
3	L	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
All	All	2446/2596 (94%)	2356 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	154/188 (82%)	154 (100%)	0	100	100
1	B	155/188 (82%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	163/188 (87%)	163 (100%)	0	100	100
1	I	159/188 (85%)	159 (100%)	0	100	100
2	C	180/192 (94%)	179 (99%)	1 (1%)	86	96
2	F	181/192 (94%)	179 (99%)	2 (1%)	73	92
2	H	176/192 (92%)	175 (99%)	1 (1%)	86	96
2	J	182/192 (95%)	181 (100%)	1 (0%)	88	96
3	D	176/181 (97%)	176 (100%)	0	100	100
3	G	177/181 (98%)	177 (100%)	0	100	100
3	K	176/181 (97%)	176 (100%)	0	100	100
3	L	177/181 (98%)	177 (100%)	0	100	100
All	All	2056/2244 (92%)	2051 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	55	TYR
2	C	55	TYR
2	F	55	TYR
2	F	203	CYS
2	J	55	TYR

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

Mol	Chain	Res	Type
1	I	408	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 ⓘ

21 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
4	NAG	M	1	1,4	14,14,15	0.39	0	17,19,21	0.52	0
4	NAG	M	2	4	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	N	1	1,5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	N	2	5	14,14,15	0.33	0	17,19,21	0.41	0
5	BMA	N	3	5	11,11,12	0.67	0	15,15,17	0.70	0
4	NAG	O	1	1,4	14,14,15	0.39	0	17,19,21	0.45	0
4	NAG	O	2	4	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	P	1	1,6	14,14,15	0.33	0	17,19,21	0.40	0
6	NAG	P	2	6	14,14,15	0.38	0	17,19,21	0.36	0
6	BMA	P	3	6	11,11,12	0.89	1 (9%)	15,15,17	0.84	0
6	MAN	P	4	6	11,11,12	0.91	1 (9%)	15,15,17	1.88	4 (26%)
4	NAG	Q	1	1,4	14,14,15	0.36	0	17,19,21	0.41	0
4	NAG	Q	2	4	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	R	1	1,6	14,14,15	0.29	0	17,19,21	0.41	0
6	NAG	R	2	6	14,14,15	0.39	0	17,19,21	0.40	0
6	BMA	R	3	6	11,11,12	0.75	0	15,15,17	0.87	0
6	MAN	R	4	6	11,11,12	0.85	0	15,15,17	1.85	4 (26%)
4	NAG	S	1	1,4	14,14,15	0.50	0	17,19,21	0.47	0
4	NAG	S	2	4	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	T	1	1,4	14,14,15	0.32	0	17,19,21	0.37	0
4	NAG	T	2	4	14,14,15	0.31	0	17,19,21	0.43	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
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	2/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	4	MAN	C1-C2	2.20	1.57	1.52
6	P	3	BMA	O5-C1	-2.10	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	4	MAN	C1-O5-C5	3.74	117.27	112.19
6	R	4	MAN	O5-C1-C2	3.74	116.54	110.77
6	P	4	MAN	O5-C1-C2	3.66	116.43	110.77
6	P	4	MAN	C1-O5-C5	3.66	117.15	112.19
6	P	4	MAN	C1-C2-C3	3.47	113.93	109.67
6	R	4	MAN	C1-C2-C3	3.21	113.61	109.67
6	P	4	MAN	O2-C2-C3	-2.73	104.66	110.14
6	R	4	MAN	O2-C2-C3	-2.54	105.04	110.14

There are no chirality outliers.

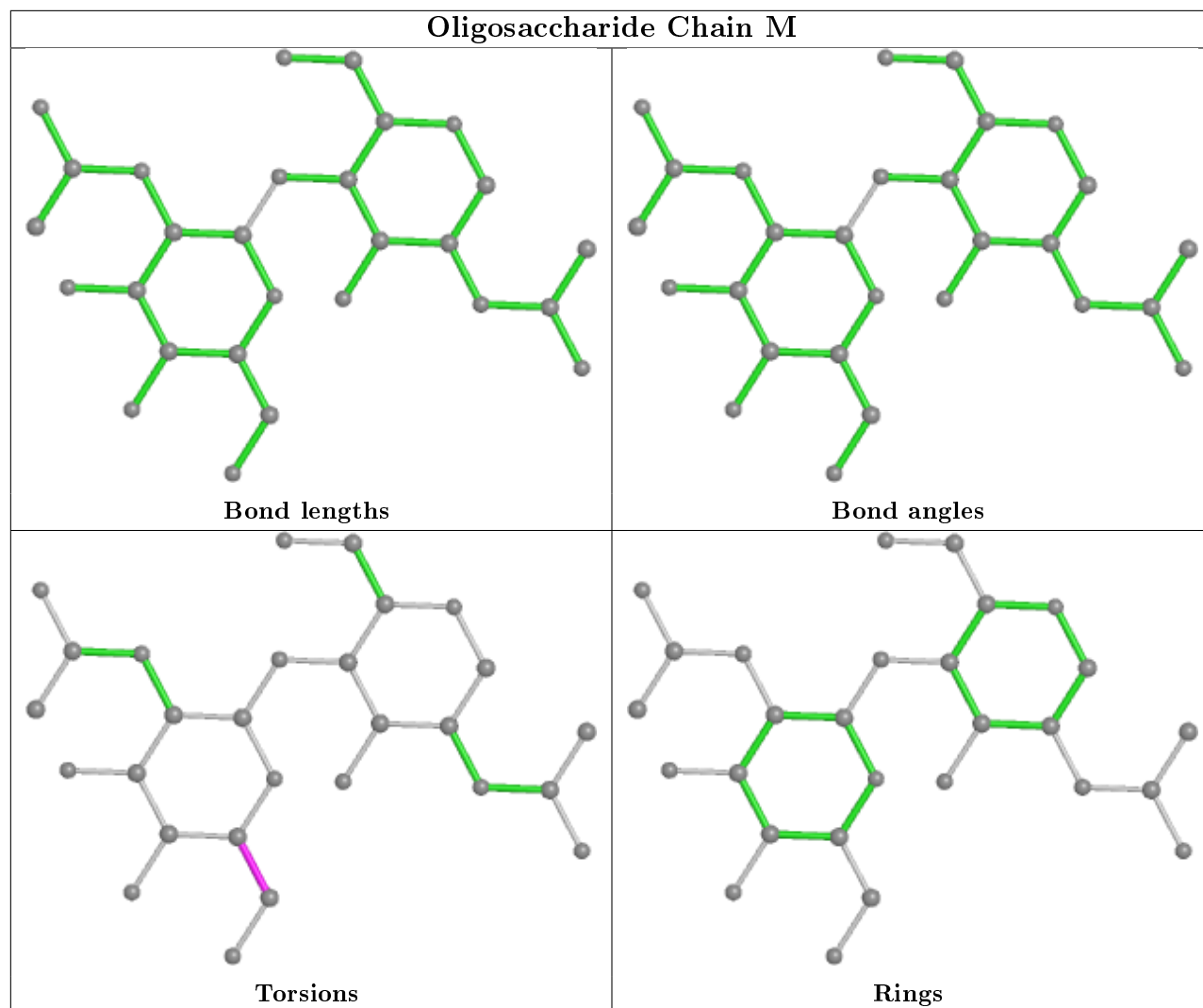
All (11) torsion outliers are listed below:

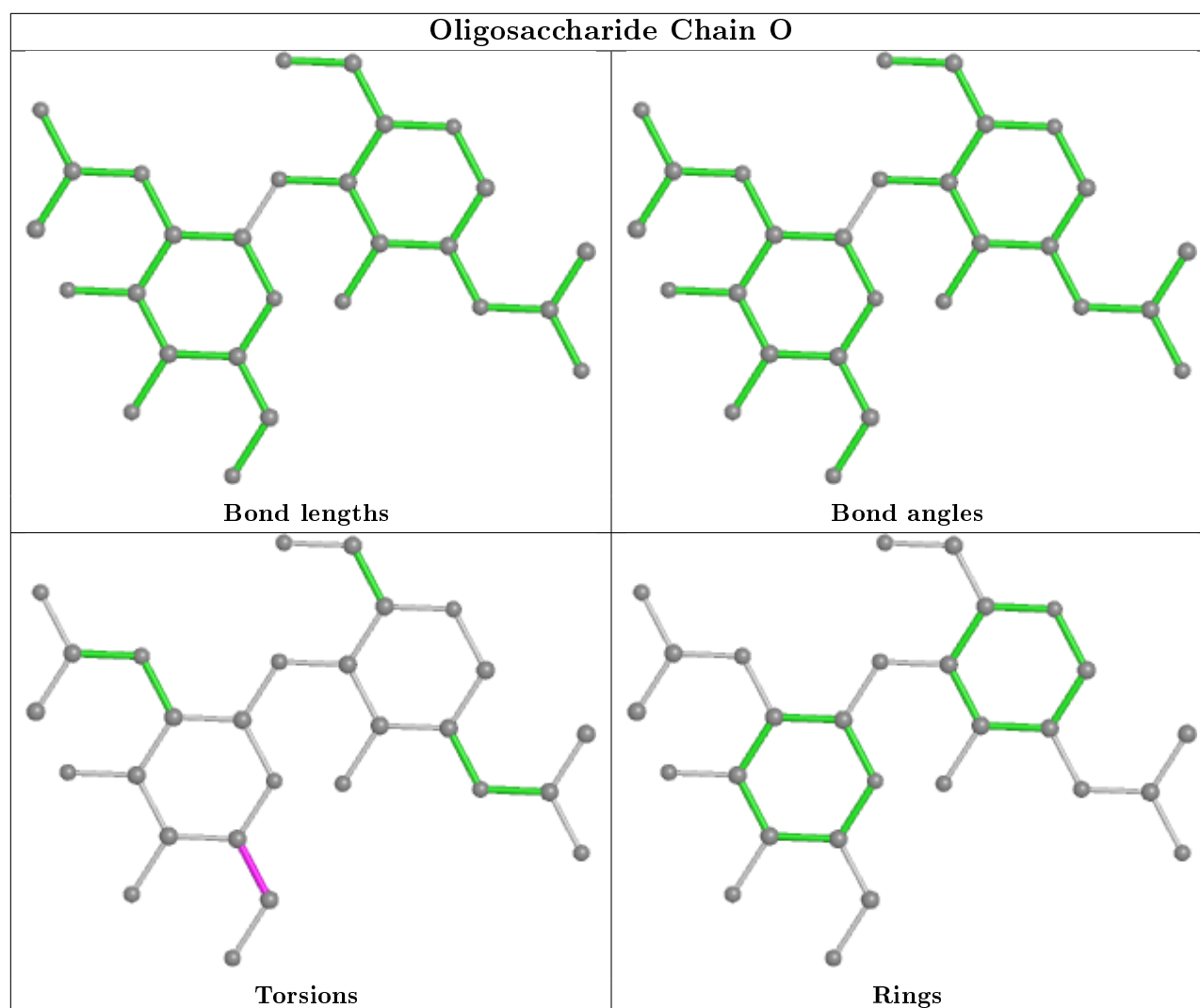
Mol	Chain	Res	Type	Atoms
4	O	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
6	P	4	MAN	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
6	R	4	MAN	C4-C5-C6-O6

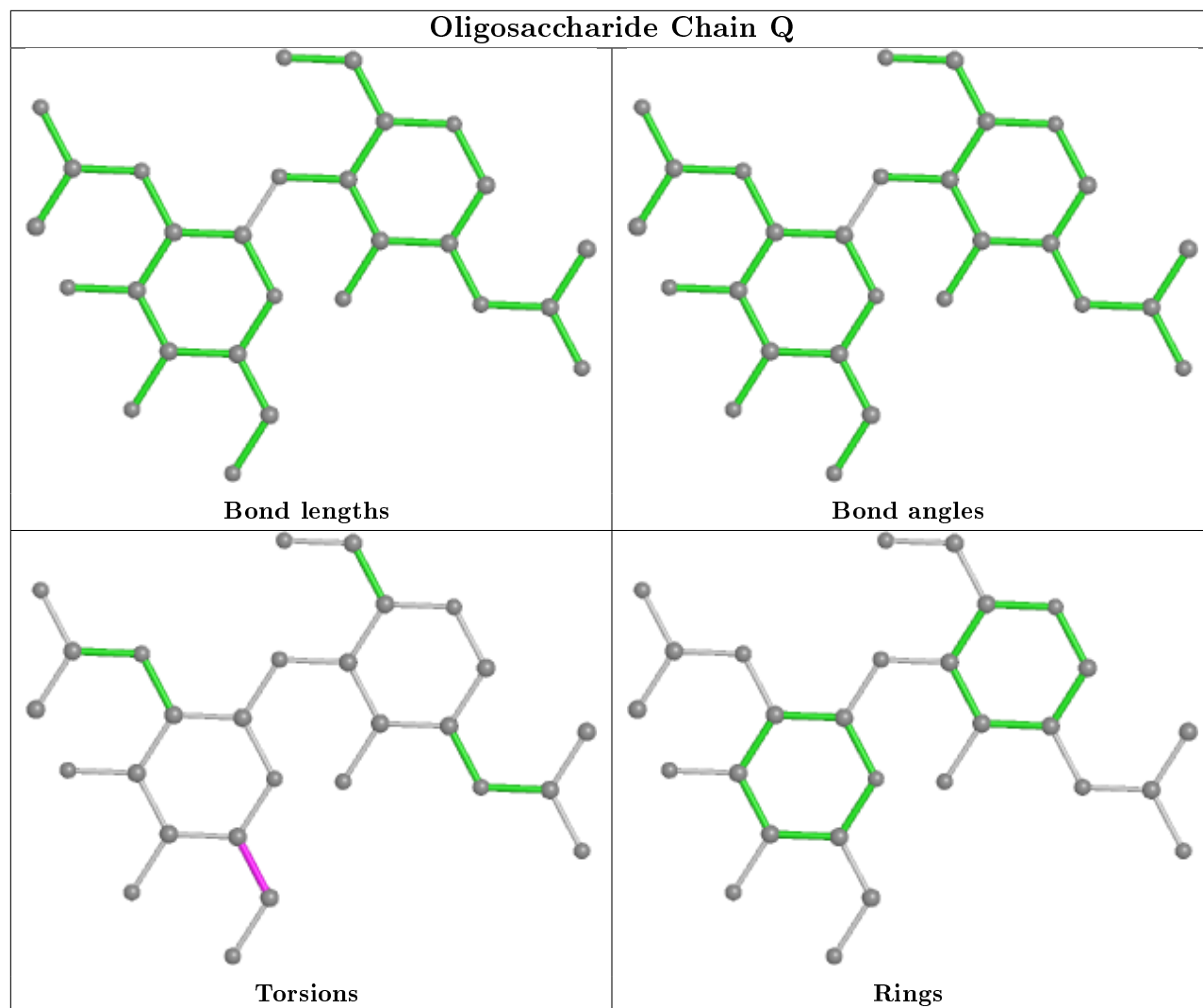
There are no ring outliers.

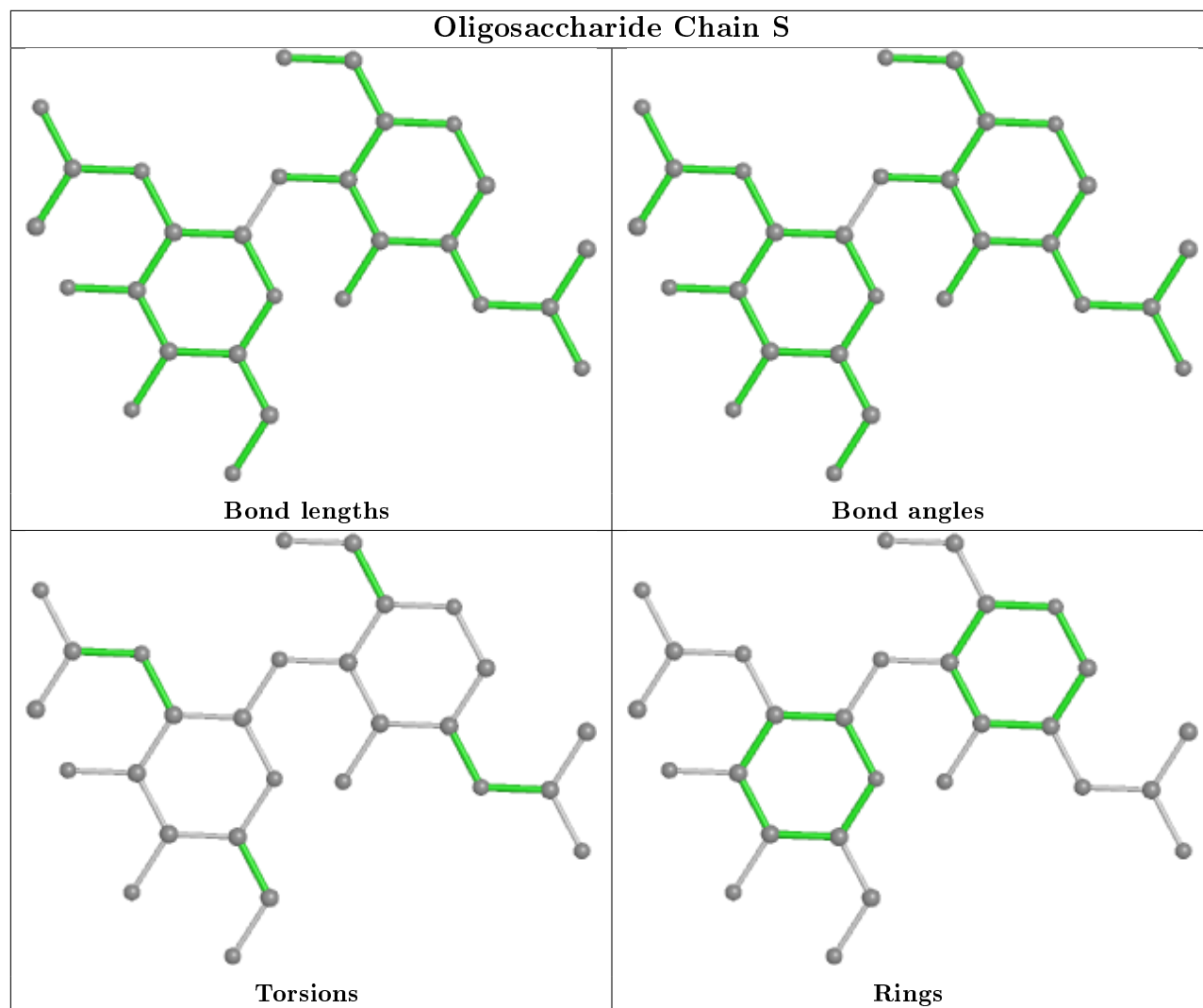
No monomer is involved in short contacts.

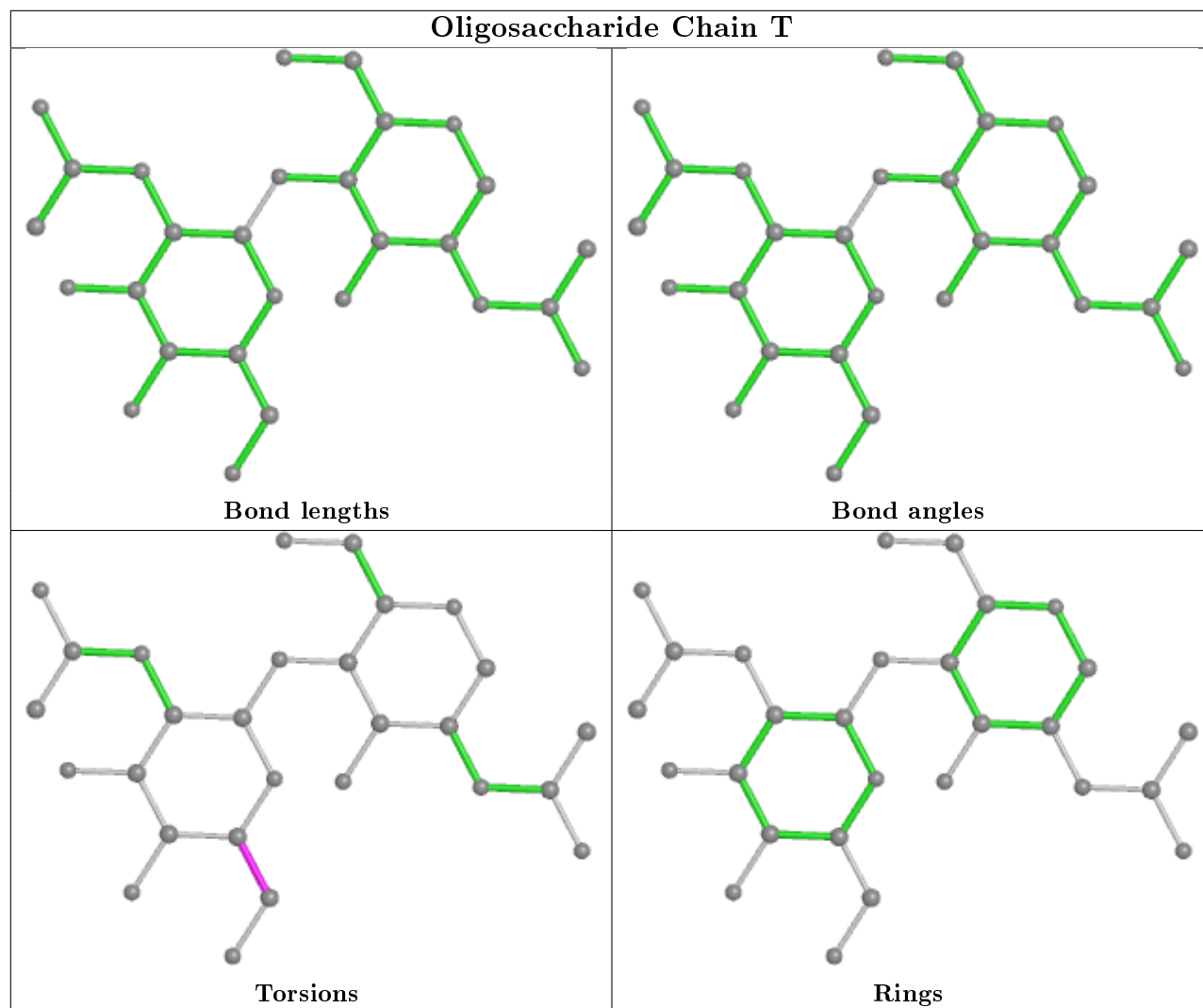
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

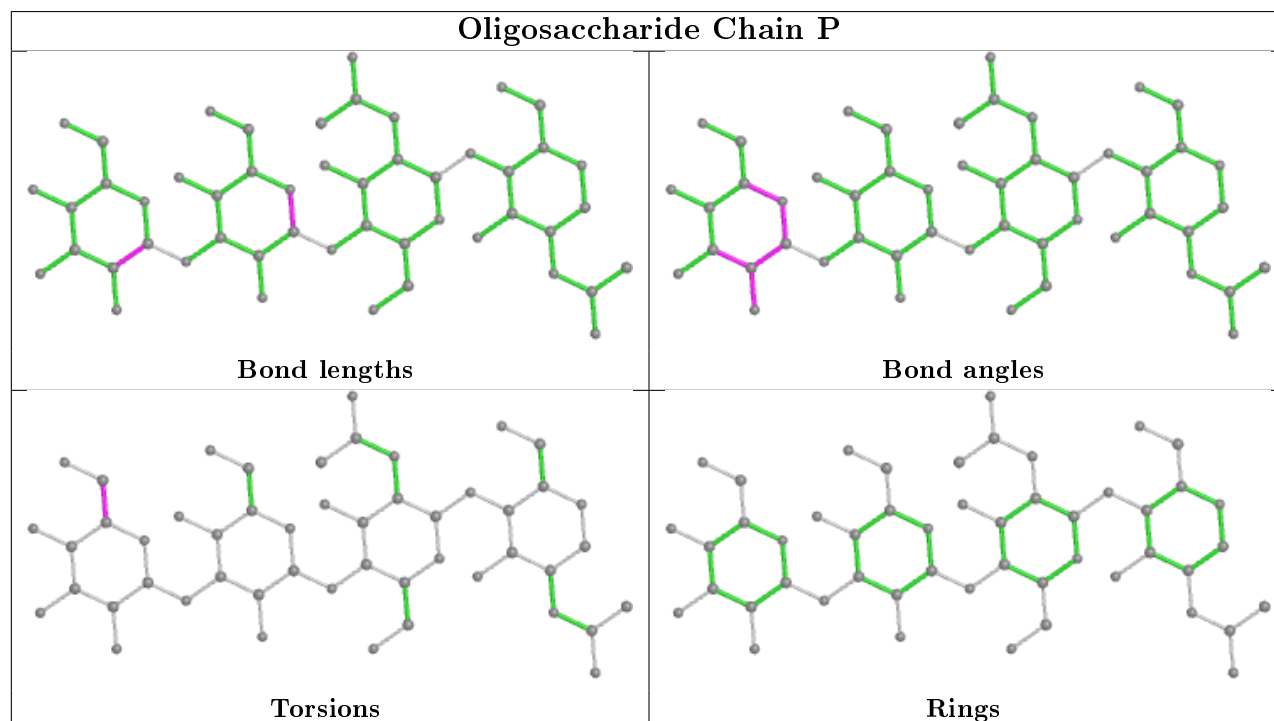
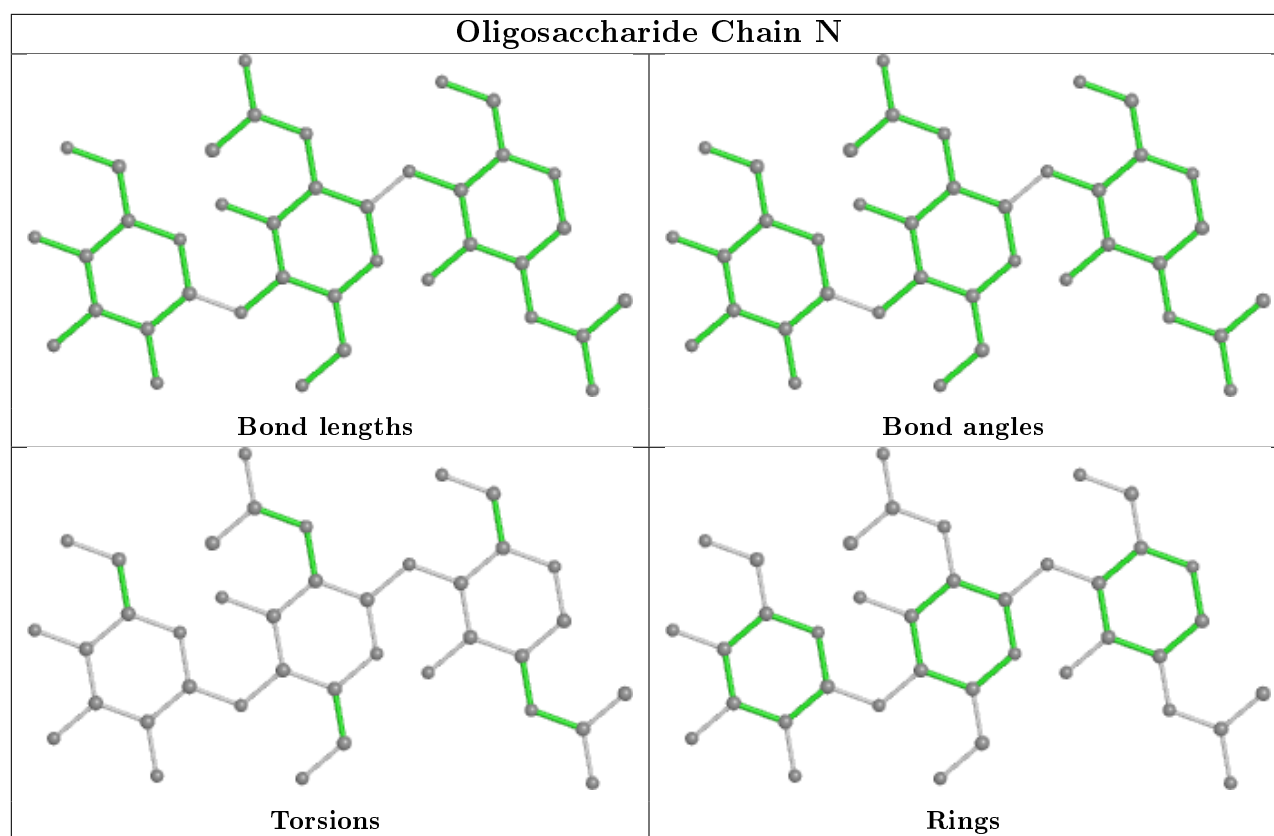


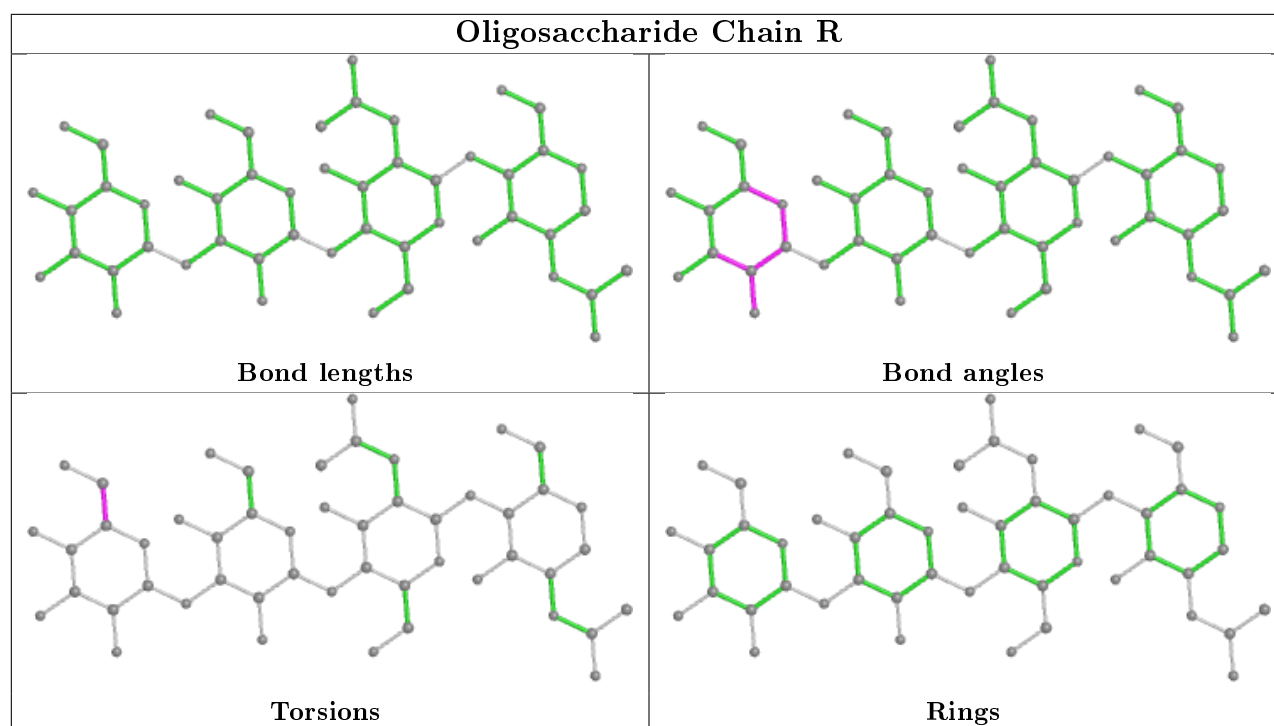












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	B	602	1	14,14,15	0.52	0	17,19,21	1.06	2 (11%)
7	NAG	E	604	1	14,14,15	0.18	0	17,19,21	0.77	1 (5%)
7	NAG	A	601	1	14,14,15	0.20	0	17,19,21	0.46	0
7	NAG	B	601	1	14,14,15	0.32	0	17,19,21	0.69	0
7	NAG	I	605	1	14,14,15	0.53	0	17,19,21	0.73	0
7	NAG	A	602	1	14,14,15	0.47	0	17,19,21	0.72	0
7	NAG	E	601	1	14,14,15	0.22	0	17,19,21	0.44	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	B	602	1	-	4/6/23/26	0/1/1/1
7	NAG	E	604	1	-	3/6/23/26	0/1/1/1
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	B	601	1	-	4/6/23/26	0/1/1/1
7	NAG	I	605	1	-	4/6/23/26	0/1/1/1
7	NAG	A	602	1	-	4/6/23/26	0/1/1/1
7	NAG	E	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	602	NAG	C1-O5-C5	3.36	116.74	112.19
7	E	604	NAG	C1-O5-C5	2.36	115.39	112.19
7	B	602	NAG	C2-N2-C7	2.10	125.89	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	602	NAG	O5-C5-C6-O6
7	I	605	NAG	O5-C5-C6-O6
7	A	602	NAG	O5-C5-C6-O6
7	B	602	NAG	C8-C7-N2-C2
7	B	602	NAG	O7-C7-N2-C2
7	E	604	NAG	C8-C7-N2-C2
7	E	604	NAG	O7-C7-N2-C2
7	B	601	NAG	C8-C7-N2-C2
7	B	601	NAG	O7-C7-N2-C2
7	I	605	NAG	C8-C7-N2-C2
7	I	605	NAG	O7-C7-N2-C2
7	A	602	NAG	C8-C7-N2-C2
7	A	602	NAG	O7-C7-N2-C2
7	A	602	NAG	C4-C5-C6-O6
7	B	602	NAG	C4-C5-C6-O6
7	I	605	NAG	C4-C5-C6-O6
7	E	604	NAG	O5-C5-C6-O6
7	B	601	NAG	O5-C5-C6-O6
7	B	601	NAG	C4-C5-C6-O6
7	A	601	NAG	C1-C2-N2-C7
7	E	601	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	A	601	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	602	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	191/214 (89%)	0.34	20 (10%) 6 3	47, 86, 146, 166	0
1	B	194/214 (90%)	0.18	14 (7%) 15 8	47, 78, 133, 146	0
1	E	194/214 (90%)	-0.04	7 (3%) 42 32	46, 75, 117, 132	0
1	I	194/214 (90%)	0.07	6 (3%) 49 39	48, 78, 127, 135	0
2	C	213/222 (95%)	-0.04	1 (0%) 91 88	44, 70, 111, 136	0
2	F	214/222 (96%)	-0.21	1 (0%) 91 88	43, 66, 99, 116	0
2	H	213/222 (95%)	-0.12	3 (1%) 75 70	50, 71, 119, 126	0
2	J	213/222 (95%)	-0.23	1 (0%) 91 88	45, 64, 93, 106	0
3	D	213/213 (100%)	-0.24	0 100 100	43, 66, 88, 101	0
3	G	213/213 (100%)	-0.31	0 100 100	45, 61, 83, 96	0
3	K	213/213 (100%)	-0.23	0 100 100	48, 64, 85, 102	0
3	L	213/213 (100%)	-0.26	0 100 100	45, 66, 89, 106	0
All	All	2478/2596 (95%)	-0.10	53 (2%) 63 54	43, 69, 114, 166	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	CYS	6.0
1	A	496	PRO	5.3
1	A	484	ALA	4.6
1	A	448	ALA	4.5
1	A	488	PRO	4.5
1	B	495	GLU	4.4
1	A	494	PRO	4.0
1	A	486	CYS	4.0
1	I	427	ARG	4.0
1	B	498	ASP	3.9
1	B	493	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	491	CYS	3.4
1	B	494	PRO	3.4
1	A	483	HIS	3.4
1	E	460	SER	3.4
2	H	163	SER	3.1
1	A	492	TRP	3.0
1	A	453	TRP	2.9
2	J	1	GLN	2.8
1	E	482	CYS	2.8
1	A	493	GLY	2.8
1	B	482	CYS	2.7
1	B	485	LEU	2.7
2	F	1	GLN	2.7
1	I	482	CYS	2.7
2	C	196	LEU	2.6
1	B	488	PRO	2.6
1	B	427	ARG	2.5
1	E	459	THR	2.4
1	E	309	GLU	2.4
1	E	486	CYS	2.4
1	A	460	SER	2.4
1	A	481	VAL	2.3
1	B	480	GLN	2.3
1	A	490	GLY	2.3
1	A	424	LEU	2.3
1	I	366	GLN	2.3
1	B	489	GLU	2.3
1	B	491	CYS	2.2
1	A	427	ARG	2.1
2	H	205	VAL	2.1
1	A	489	GLU	2.1
1	B	486	CYS	2.1
1	B	458	GLY	2.1
1	B	496	PRO	2.1
2	H	212	THR	2.1
1	A	451	ILE	2.1
1	A	456	LEU	2.1
1	E	484	ALA	2.1
1	I	478	THR	2.0
1	E	488	PRO	2.0
1	I	495	GLU	2.0
1	I	479	GLY	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 ⓘ

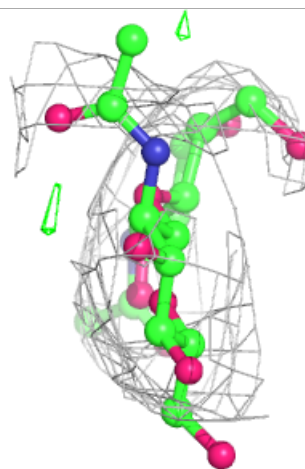
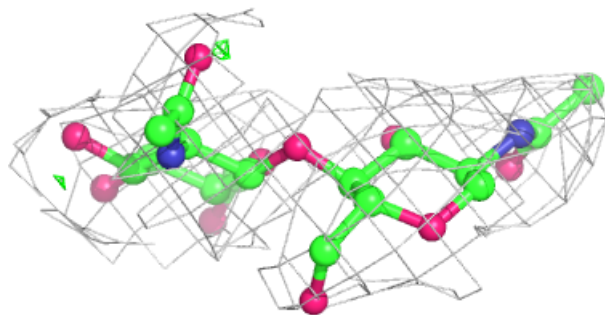
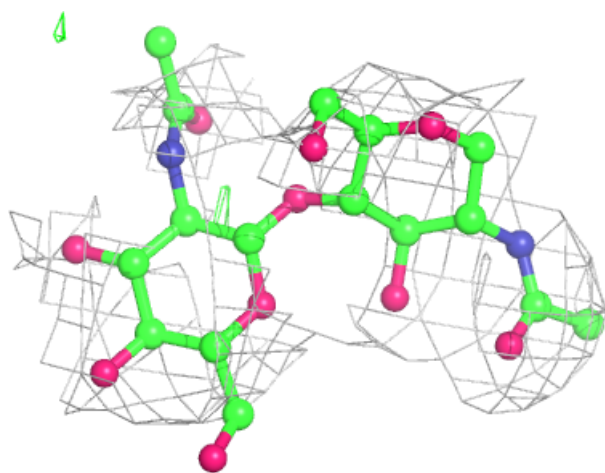
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	N	3	11/12	0.64	0.26	97,126,140,140	0
6	MAN	P	4	11/12	0.75	0.30	107,130,143,144	0
6	BMA	R	3	11/12	0.76	0.22	110,121,138,143	0
6	BMA	P	3	11/12	0.82	0.20	108,119,126,131	0
4	NAG	M	2	14/15	0.85	0.17	112,121,124,124	0
6	MAN	R	4	11/12	0.86	0.22	122,130,136,136	0
4	NAG	Q	2	14/15	0.89	0.15	76,103,125,127	0
4	NAG	O	2	14/15	0.89	0.15	91,102,120,120	0
4	NAG	S	2	14/15	0.90	0.17	74,91,102,103	0
4	NAG	T	2	14/15	0.92	0.16	89,106,117,120	0
4	NAG	Q	1	14/15	0.92	0.13	58,77,94,102	0
4	NAG	O	1	14/15	0.92	0.17	63,84,95,104	0
4	NAG	T	1	14/15	0.93	0.15	74,85,99,110	0
6	NAG	P	2	14/15	0.93	0.10	69,84,102,120	0
5	NAG	N	2	14/15	0.94	0.14	67,82,98,109	0
4	NAG	M	1	14/15	0.94	0.14	67,97,111,124	0
6	NAG	R	2	14/15	0.95	0.14	65,82,102,104	0
5	NAG	N	1	14/15	0.96	0.13	50,61,69,71	0
6	NAG	P	1	14/15	0.97	0.16	54,59,69,79	0
4	NAG	S	1	14/15	0.97	0.15	59,68,75,83	0
6	NAG	R	1	14/15	0.97	0.15	53,57,76,77	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.

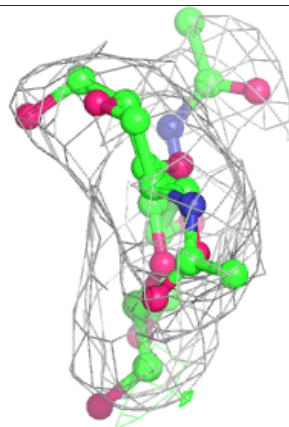
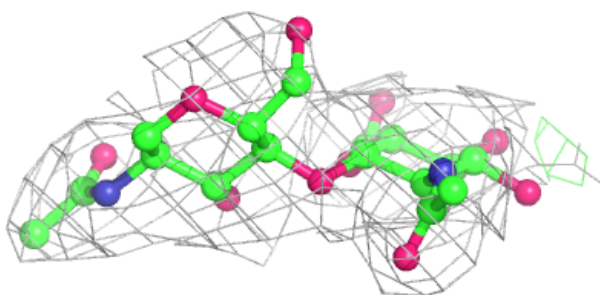
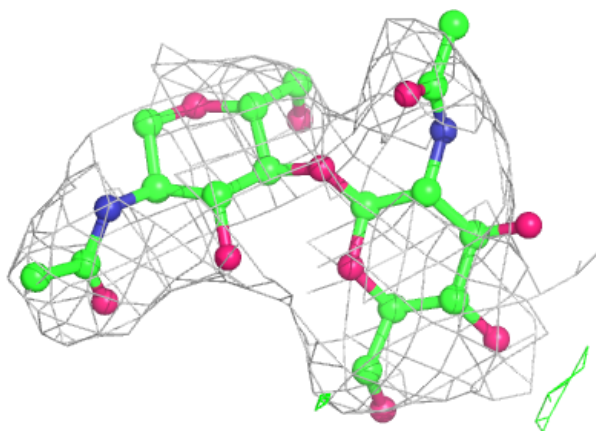
Electron density around Chain M:

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



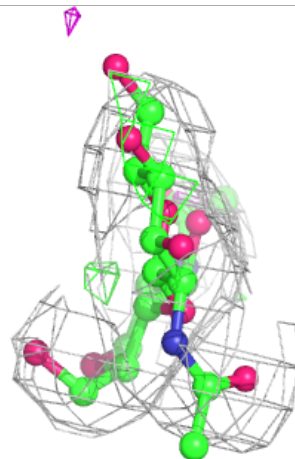
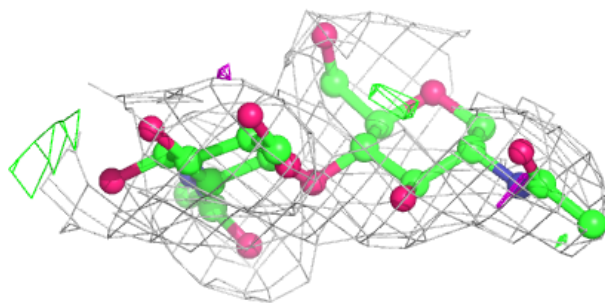
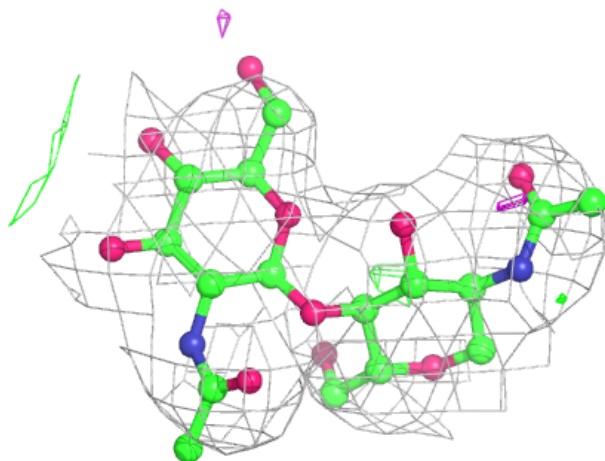
Electron density around Chain O:

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



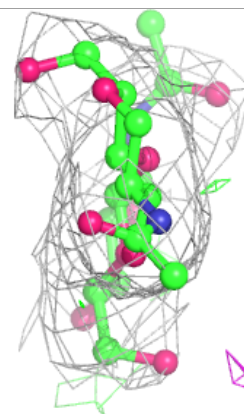
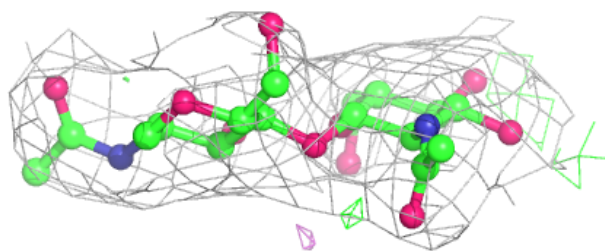
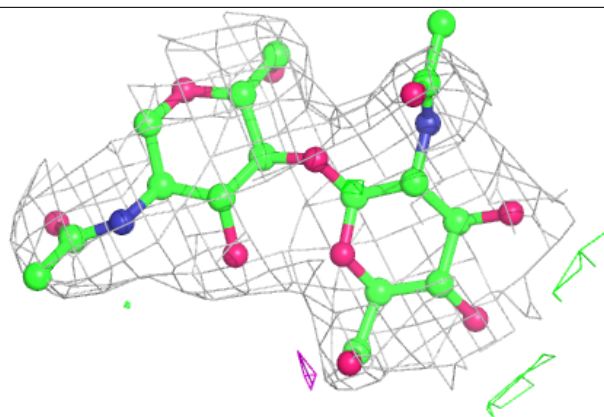
Electron density around Chain Q:

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

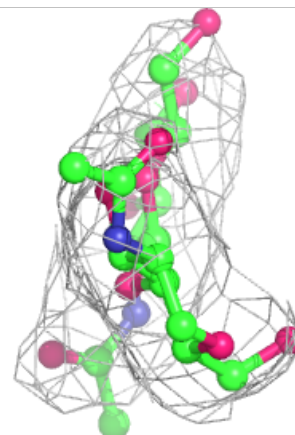
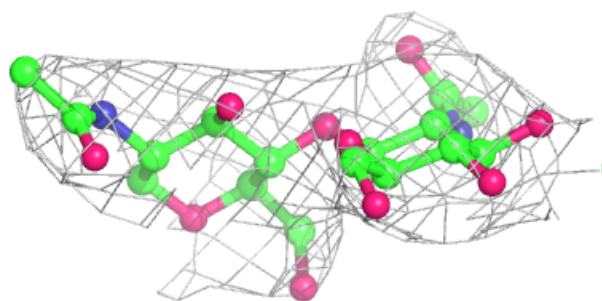
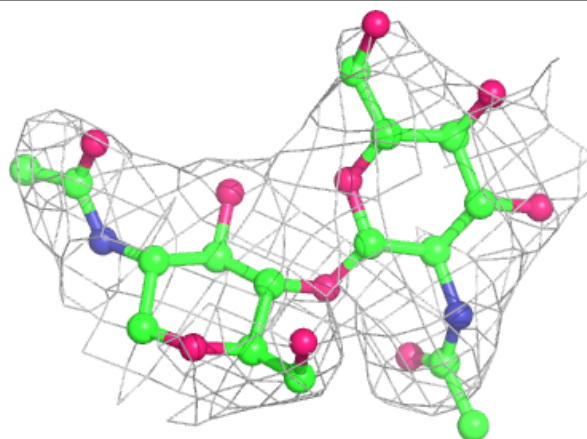


Electron density around Chain S:

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

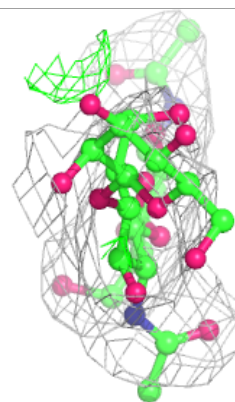
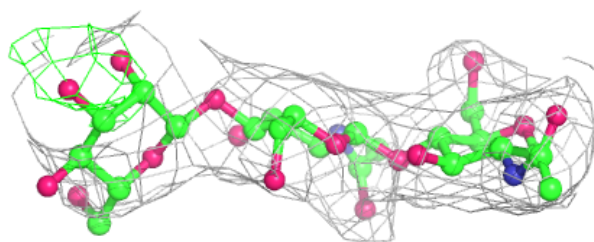
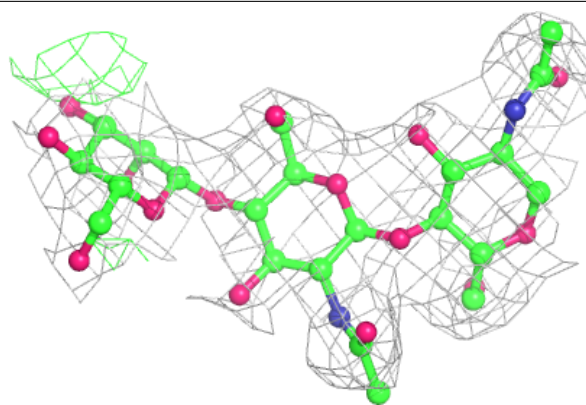
**Electron density around Chain T:**

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

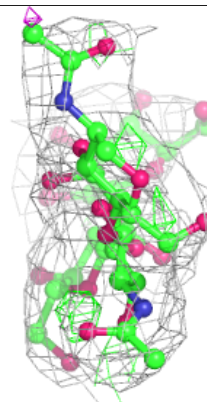
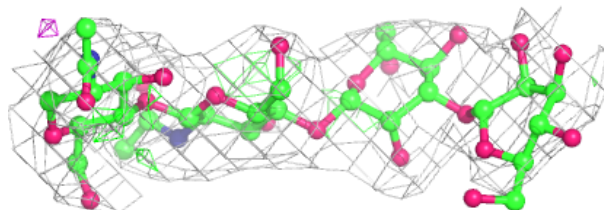
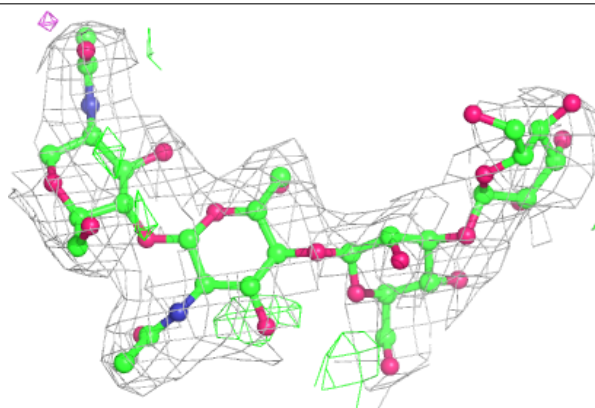


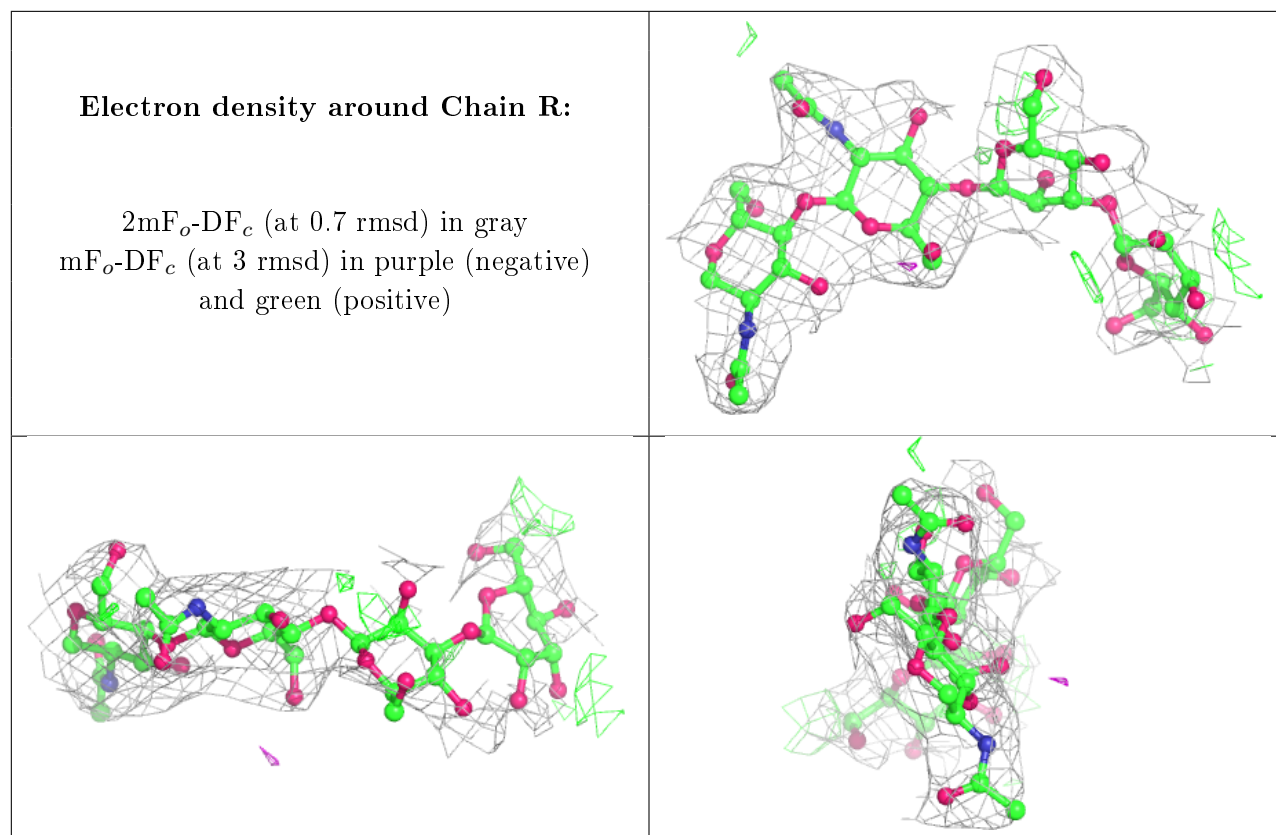
Electron density around Chain N:

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

**Electron density around Chain P:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
7	NAG	A	602	14/15	0.77	0.20	103,115,126,130	0
7	NAG	E	604	14/15	0.78	0.16	72,87,102,104	0
7	NAG	B	601	14/15	0.83	0.40	108,140,149,151	0
7	NAG	E	601	14/15	0.84	0.32	110,123,134,135	0
7	NAG	I	605	14/15	0.85	0.18	75,111,121,127	0
7	NAG	A	601	14/15	0.85	0.32	101,126,134,135	0
7	NAG	B	602	14/15	0.85	0.15	77,96,109,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.