



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 07:47 PM BST

PDB ID : 6OPA
Title : Crystal structure of bovine Fab NC-Cow1 in complex with HIV-1 BG505
SOSIP.664, and human Fabs 35022 and PGT128
Authors : Stanfield, R.L.; Wilson, I.A.
Deposited on : 2019-04-24
Resolution : 4.08 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

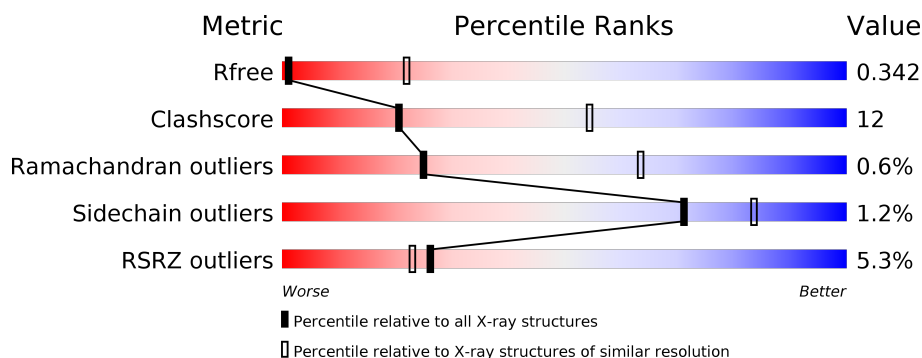
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 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	1133 (4.46-3.70)
Clashscore	141614	1013 (4.42-3.74)
Ramachandran outliers	138981	1151 (4.46-3.70)
Sidechain outliers	138945	1139 (4.46-3.70)
RSRZ outliers	127900	1012 (4.48-3.68)

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	G	475	<div> <div>55%</div> <div>34%</div> <div>10%</div> </div>
2	B	153	<div> <div>62%</div> <div>22%</div> <div>16%</div> </div>
3	F	240	<div> <div>37%</div> <div>17%</div> <div>46%</div> </div>
4	I	216	<div> <div>38%</div> <div>13%</div> <div>49%</div> </div>
5	J	211	<div> <div>43%</div> <div>6%</div> <div>52%</div> </div>
6	K	239	<div> <div>40%</div> <div>15%</div> <div>45%</div> </div>

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Mol	Chain	Length	Quality of chain
7	R	216	% 
8	S	272	
9	A	7	
10	C	2	
10	L	2	
11	D	3	
11	E	3	
11	Q	3	
12	H	4	
12	N	4	
13	M	5	
13	O	5	
13	P	5	
13	U	5	
14	T	4	

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
10	NAG	L	2	-	-	-	X
12	NAG	N	2	-	-	-	X
13	MAN	M	4	-	-	-	X
13	MAN	M	5	-	-	-	X
13	MAN	P	4	-	-	-	X
9	MAN	A	6	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10798 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	427	Total	C	N	O	S	0	0	0
			3360	2117	591	625	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			1026	647	178	195	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called Fab 35022 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	130	Total	C	N	O	S	0	0	0
			1015	649	171	190	5			

- Molecule 4 is a protein called Fab 35022 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	110	Total	C	N	O	S	0	0	0
			836	525	138	167	6			

- Molecule 5 is a protein called Fab PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	102	Total	C	N	O	S	0	0	0
			746	466	127	151	2			

- Molecule 6 is a protein called Fab PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	132	Total	C	N	O	S	0	0	0
			1028	659	175	190	4			

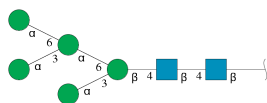
- Molecule 7 is a protein called Fab NC-Cow1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	R	112	Total	C	N	O	S	0	0	0
			807	492	137	176	2			

- Molecule 8 is a protein called Fab NC-Cow1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S	168	Total	C	N	O	S	0	0	0
			1302	801	227	263	11			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



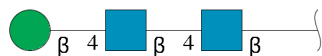
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

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

- Molecule 11 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.



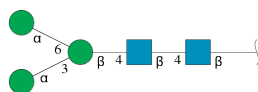
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
12	H	4	Total	C	N	O	0	0	0
			50	28	2	20			
12	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



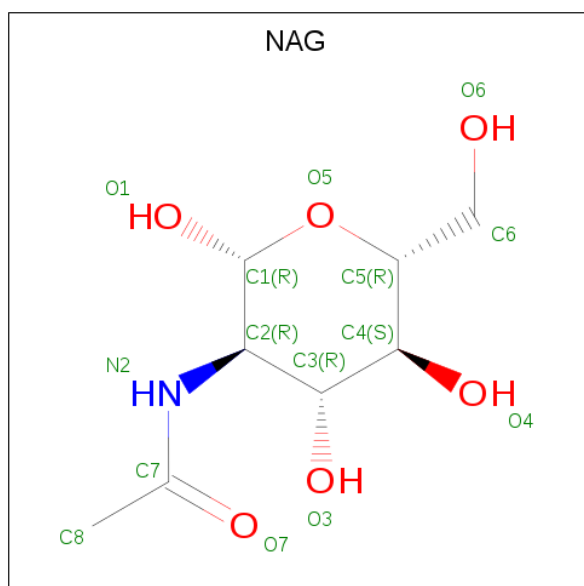
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
13	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
13	P	5	Total	C	N	O	0	0	0
			61	34	2	25			
13	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 14 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
14	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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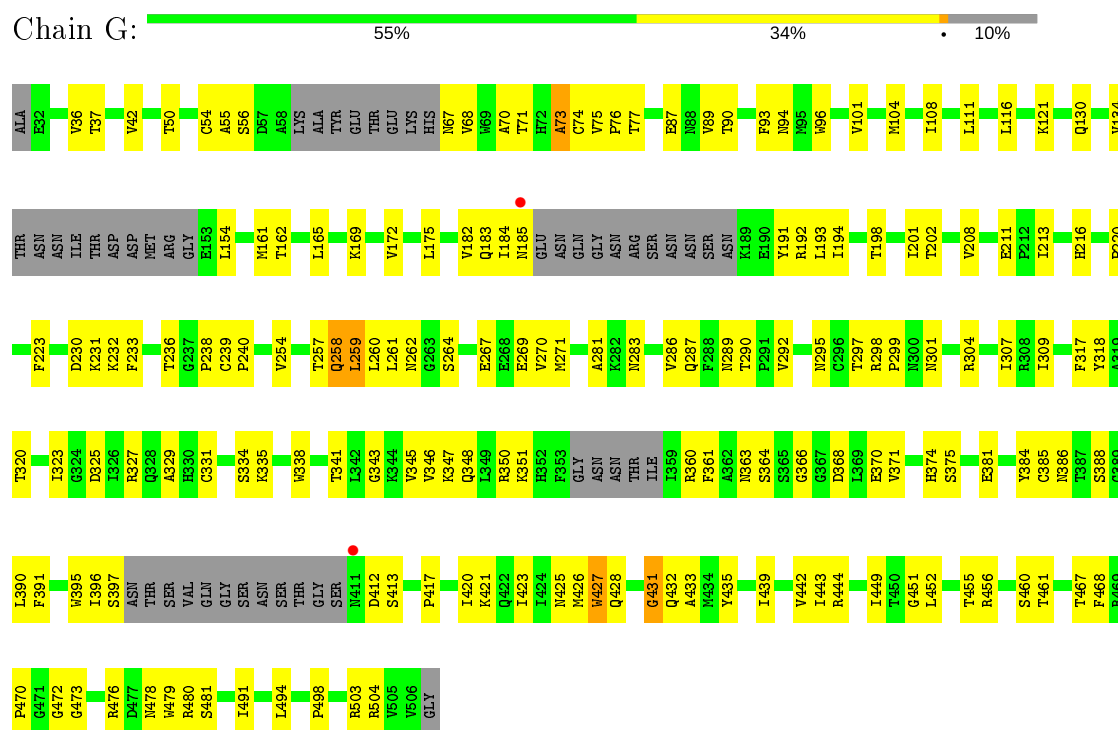
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	N	O	0	0
			14	8	1	5		

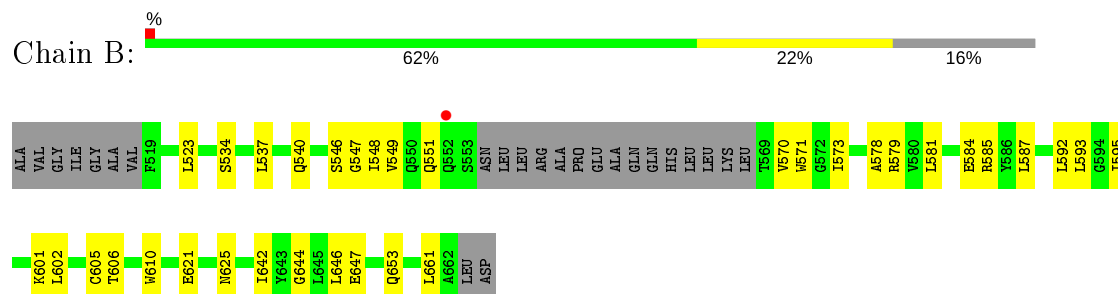
3 Residue-property plots

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.

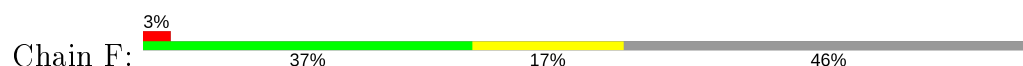
- Molecule 1: Envelope glycoprotein gp160



- Molecule 2: Envelope glycoprotein gp41



- Molecule 3: Fab 35022 heavy chain





- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



- Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



- Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



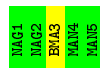
- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  80% 20%



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  20% 60% 20%



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  60% 40%



- Molecule 14: 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 T:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	215.24Å 215.24Å 438.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 4.08 48.76 – 4.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.76-4.08) 98.6 (48.76-4.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.332 , 0.343 0.332 , 0.342	Depositor DCC
R_{free} test set	1558 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	169.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 119.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10798	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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	G	0.31	0/3429	0.57	0/4653
2	B	0.26	0/1044	0.43	0/1415
3	F	0.29	0/1043	0.56	0/1416
4	I	0.32	0/860	0.56	0/1175
5	J	0.27	0/763	0.46	0/1040
6	K	0.28	0/1061	0.56	0/1455
7	R	0.28	0/822	0.49	0/1120
8	S	0.26	0/1331	0.50	0/1806
All	All	0.29	0/10353	0.53	0/14080

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	G	3360	0	3306	136	0
2	B	1026	0	1001	28	1
3	F	1015	0	985	30	0
4	I	836	0	785	24	0
5	J	746	0	721	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	1028	0	990	27	0
7	R	807	0	756	12	0
8	S	1302	0	1235	30	0
9	A	83	0	70	5	0
10	C	28	0	25	0	0
10	L	28	0	25	0	0
11	D	39	0	34	0	0
11	E	39	0	34	1	0
11	Q	39	0	34	0	0
12	H	50	0	43	3	0
12	N	50	0	43	0	0
13	M	61	0	52	0	0
13	O	61	0	52	0	0
13	P	61	0	52	1	0
13	U	61	0	52	0	0
14	T	50	0	43	0	0
15	B	28	0	26	2	0
All	All	10798	0	10364	260	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 12.

The worst 5 of 260 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:G:350:ARG:HH22	1:G:396:ILE:HA	1.38	0.87
1:G:54:CYS:SG	2:B:571:TRP:CD2	2.73	0.81
1:G:473:GLY:HA3	8:S:130:PHE:HA	1.63	0.78
4:I:47:ILE:HG22	4:I:48:ILE:HG12	1.64	0.78
1:G:281:ALA:O	8:S:129:ARG:HD3	1.87	0.74

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)
2:B:579:ARG:NH2	2:B:581:LEU:CA[3_455]	2.12	0.08

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	G	415/475 (87%)	390 (94%)	22 (5%)	3 (1%)	22	61
2	B	125/153 (82%)	114 (91%)	9 (7%)	2 (2%)	9	44
3	F	128/240 (53%)	124 (97%)	3 (2%)	1 (1%)	19	58
4	I	108/216 (50%)	102 (94%)	6 (6%)	0	100	100
5	J	100/211 (47%)	94 (94%)	6 (6%)	0	100	100
6	K	130/239 (54%)	119 (92%)	10 (8%)	1 (1%)	19	58
7	R	110/216 (51%)	103 (94%)	6 (6%)	1 (1%)	17	55
8	S	166/272 (61%)	159 (96%)	7 (4%)	0	100	100
All	All	1282/2022 (63%)	1205 (94%)	69 (5%)	8 (1%)	25	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	73	ALA
2	B	549	VAL
2	B	602	LEU
1	G	427	TRP
6	K	41	PRO

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	G	381/422 (90%)	377 (99%)	4 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	111/129 (86%)	109 (98%)	2 (2%)	59	77
3	F	108/203 (53%)	107 (99%)	1 (1%)	78	88
4	I	96/189 (51%)	96 (100%)	0	100	100
5	J	83/177 (47%)	83 (100%)	0	100	100
6	K	110/203 (54%)	110 (100%)	0	100	100
7	R	92/184 (50%)	91 (99%)	1 (1%)	73	84
8	S	148/238 (62%)	143 (97%)	5 (3%)	37	61
All	All	1129/1745 (65%)	1116 (99%)	13 (1%)	71	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	584	GLU
3	F	64	GLN
8	S	30	ASN
2	B	551	GLN
8	S	27	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	374	HIS
1	G	425	ASN

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 ⓘ

52 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	$\# Z > 2$
9	NAG	A	1	1,9	14,14,15	0.41	0	17,19,21	0.48	0
9	NAG	A	2	9	14,14,15	0.49	0	17,19,21	1.22	1 (5%)
9	BMA	A	3	9	11,11,12	1.01	1 (9%)	15,15,17	1.04	0
9	MAN	A	4	9	11,11,12	1.27	2 (18%)	15,15,17	1.83	3 (20%)
9	MAN	A	5	9	11,11,12	0.97	1 (9%)	15,15,17	0.83	1 (6%)
9	MAN	A	6	9	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
9	MAN	A	7	9	11,11,12	0.78	1 (9%)	15,15,17	1.29	2 (13%)
10	NAG	C	1	1,10	14,14,15	0.20	0	17,19,21	0.54	0
10	NAG	C	2	10	14,14,15	0.39	0	17,19,21	0.47	0
11	NAG	D	1	1,11	14,14,15	0.41	0	17,19,21	0.44	0
11	NAG	D	2	11	14,14,15	0.35	0	17,19,21	0.57	0
11	BMA	D	3	11	11,11,12	0.67	0	15,15,17	1.00	0
11	NAG	E	1	1,11	14,14,15	0.23	0	17,19,21	0.38	0
11	NAG	E	2	11	14,14,15	0.23	0	17,19,21	0.40	0
11	BMA	E	3	11	11,11,12	0.57	0	15,15,17	0.75	0
12	NAG	H	1	1,12	14,14,15	0.25	0	17,19,21	0.45	0
12	NAG	H	2	12	14,14,15	0.15	0	17,19,21	0.43	0
12	BMA	H	3	12	11,11,12	0.61	0	15,15,17	0.98	0
12	MAN	H	4	12	11,11,12	1.00	1 (9%)	15,15,17	1.28	3 (20%)
10	NAG	L	1	1,10	14,14,15	0.41	0	17,19,21	0.43	0
10	NAG	L	2	10	14,14,15	0.34	0	17,19,21	0.56	0
13	NAG	M	1	1,13	14,14,15	0.22	0	17,19,21	0.51	0
13	NAG	M	2	13	14,14,15	0.30	0	17,19,21	0.40	0
13	BMA	M	3	13	11,11,12	0.65	0	15,15,17	0.75	0
13	MAN	M	4	13	11,11,12	1.16	1 (9%)	15,15,17	0.96	0
13	MAN	M	5	13	11,11,12	0.91	1 (9%)	15,15,17	1.05	2 (13%)
12	NAG	N	1	1,12	14,14,15	0.34	0	17,19,21	0.49	0
12	NAG	N	2	12	14,14,15	0.35	0	17,19,21	0.45	0
12	BMA	N	3	12	11,11,12	0.77	0	15,15,17	0.83	0
12	MAN	N	4	12	11,11,12	0.77	1 (9%)	15,15,17	1.07	2 (13%)
13	NAG	O	1	1,13	14,14,15	0.33	0	17,19,21	0.35	0
13	NAG	O	2	13	14,14,15	0.28	0	17,19,21	0.85	0
13	BMA	O	3	13	11,11,12	0.29	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	O	4	13	11,11,12	0.24	0	15,15,17	0.96	0
13	MAN	O	5	13	11,11,12	0.26	0	15,15,17	0.94	0
13	NAG	P	1	1,13	14,14,15	0.47	0	17,19,21	1.22	1 (5%)
13	NAG	P	2	13	14,14,15	0.22	0	17,19,21	0.47	0
13	BMA	P	3	13	11,11,12	0.99	1 (9%)	15,15,17	1.05	1 (6%)
13	MAN	P	4	13	11,11,12	0.81	1 (9%)	15,15,17	1.35	2 (13%)
13	MAN	P	5	13	11,11,12	0.81	1 (9%)	15,15,17	1.25	2 (13%)
11	NAG	Q	1	1,11	14,14,15	0.76	1 (7%)	17,19,21	0.67	0
11	NAG	Q	2	11	14,14,15	0.28	0	17,19,21	0.34	0
11	BMA	Q	3	11	11,11,12	0.74	0	15,15,17	0.80	0
14	NAG	T	1	1,14	14,14,15	0.25	0	17,19,21	0.45	0
14	NAG	T	2	14	14,14,15	0.24	0	17,19,21	0.42	0
14	BMA	T	3	14	11,11,12	0.60	0	15,15,17	0.97	0
14	MAN	T	4	14	11,11,12	0.70	0	15,15,17	1.30	2 (13%)
13	NAG	U	1	1,13	14,14,15	0.23	0	17,19,21	0.52	0
13	NAG	U	2	13	14,14,15	0.29	0	17,19,21	0.43	0
13	BMA	U	3	13	11,11,12	0.62	0	15,15,17	0.76	0
13	MAN	U	4	13	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
13	MAN	U	5	13	11,11,12	0.92	1 (9%)	15,15,17	1.18	2 (13%)

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
9	NAG	A	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	2	9	-	5/6/23/26	0/1/1/1
9	BMA	A	3	9	-	0/2/19/22	0/1/1/1
9	MAN	A	4	9	-	0/2/19/22	0/1/1/1
9	MAN	A	5	9	-	0/2/19/22	0/1/1/1
9	MAN	A	6	9	-	0/2/19/22	0/1/1/1
9	MAN	A	7	9	-	0/2/19/22	0/1/1/1
10	NAG	C	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	C	2	10	-	0/6/23/26	0/1/1/1
11	NAG	D	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	D	2	11	-	1/6/23/26	0/1/1/1
11	BMA	D	3	11	-	1/2/19/22	0/1/1/1
11	NAG	E	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	E	2	11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	E	3	11	-	0/2/19/22	0/1/1/1
12	NAG	H	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	H	2	12	-	2/6/23/26	0/1/1/1
12	BMA	H	3	12	-	2/2/19/22	0/1/1/1
12	MAN	H	4	12	-	2/2/19/22	0/1/1/1
10	NAG	L	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	L	2	10	-	2/6/23/26	0/1/1/1
13	NAG	M	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	M	2	13	-	2/6/23/26	0/1/1/1
13	BMA	M	3	13	-	0/2/19/22	0/1/1/1
13	MAN	M	4	13	-	0/2/19/22	0/1/1/1
13	MAN	M	5	13	-	1/2/19/22	0/1/1/1
12	NAG	N	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	N	2	12	-	0/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	0/2/19/22	0/1/1/1
13	NAG	O	1	1,13	-	3/6/23/26	0/1/1/1
13	NAG	O	2	13	-	0/6/23/26	0/1/1/1
13	BMA	O	3	13	-	2/2/19/22	0/1/1/1
13	MAN	O	4	13	-	1/2/19/22	0/1/1/1
13	MAN	O	5	13	-	0/2/19/22	0/1/1/1
13	NAG	P	1	1,13	-	4/6/23/26	0/1/1/1
13	NAG	P	2	13	-	2/6/23/26	0/1/1/1
13	BMA	P	3	13	-	0/2/19/22	0/1/1/1
13	MAN	P	4	13	-	2/2/19/22	0/1/1/1
13	MAN	P	5	13	-	2/2/19/22	0/1/1/1
11	NAG	Q	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	Q	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Q	3	11	-	1/2/19/22	0/1/1/1
14	NAG	T	1	1,14	-	0/6/23/26	0/1/1/1
14	NAG	T	2	14	-	0/6/23/26	0/1/1/1
14	BMA	T	3	14	-	0/2/19/22	0/1/1/1
14	MAN	T	4	14	-	2/2/19/22	0/1/1/1
13	NAG	U	1	1,13	-	1/6/23/26	0/1/1/1
13	NAG	U	2	13	-	1/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	0/2/19/22	0/1/1/1
13	MAN	U	5	13	-	0/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	4	MAN	C1-C2	3.17	1.59	1.52
13	M	4	MAN	C2-C3	2.95	1.56	1.52
12	H	4	MAN	C1-C2	2.90	1.58	1.52
13	U	5	MAN	C1-C2	2.53	1.58	1.52
11	Q	1	NAG	C1-C2	2.51	1.56	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	4	MAN	C1-O5-C5	5.72	119.94	112.19
13	P	1	NAG	C2-N2-C7	4.21	128.90	122.90
9	A	2	NAG	C2-N2-C7	4.14	128.80	122.90
14	T	4	MAN	C1-O5-C5	3.80	117.34	112.19
9	A	7	MAN	C1-O5-C5	3.73	117.25	112.19

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

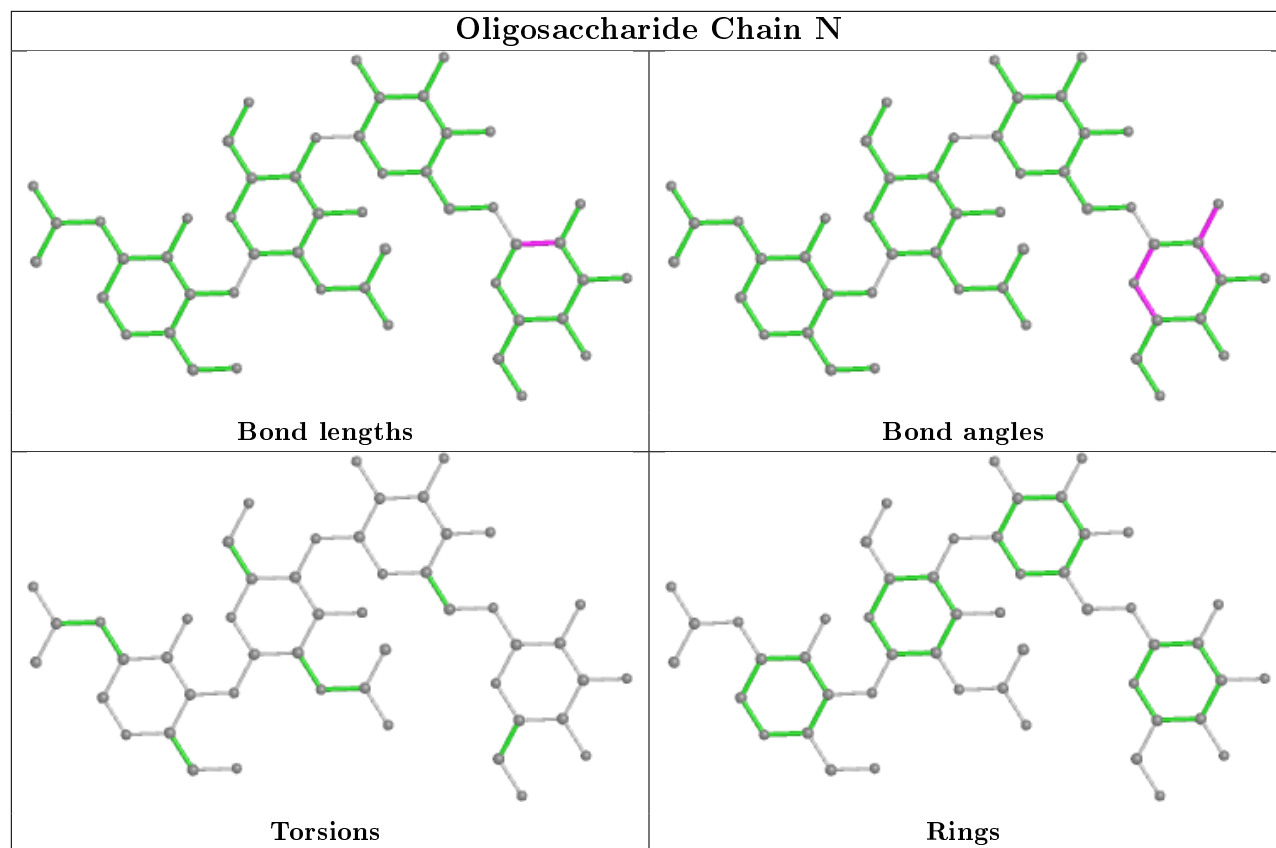
Mol	Chain	Res	Type	Atoms
11	D	1	NAG	O5-C5-C6-O6
12	H	4	MAN	O5-C5-C6-O6
9	A	2	NAG	O5-C5-C6-O6
13	O	1	NAG	C4-C5-C6-O6
9	A	2	NAG	C4-C5-C6-O6

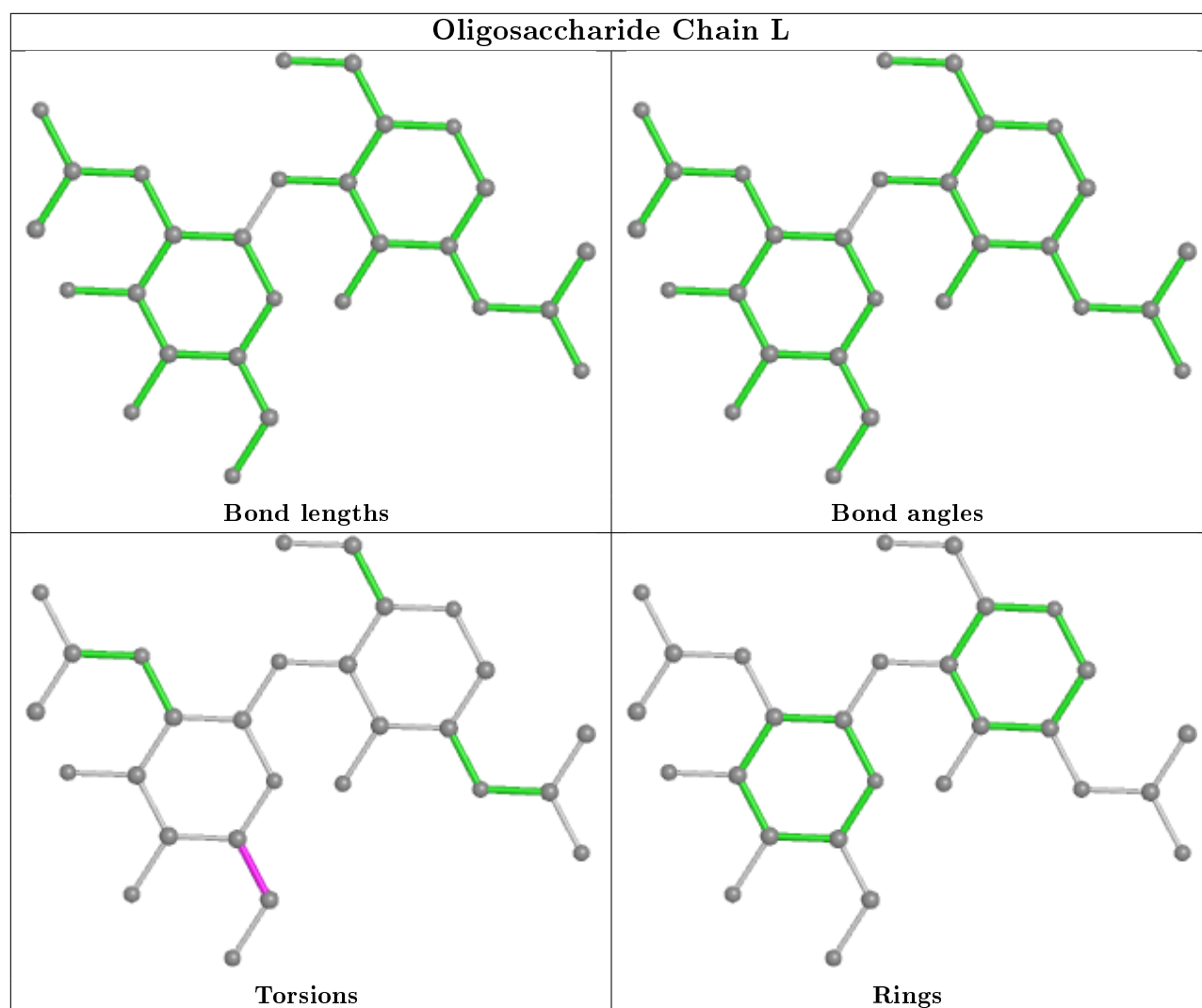
There are no ring outliers.

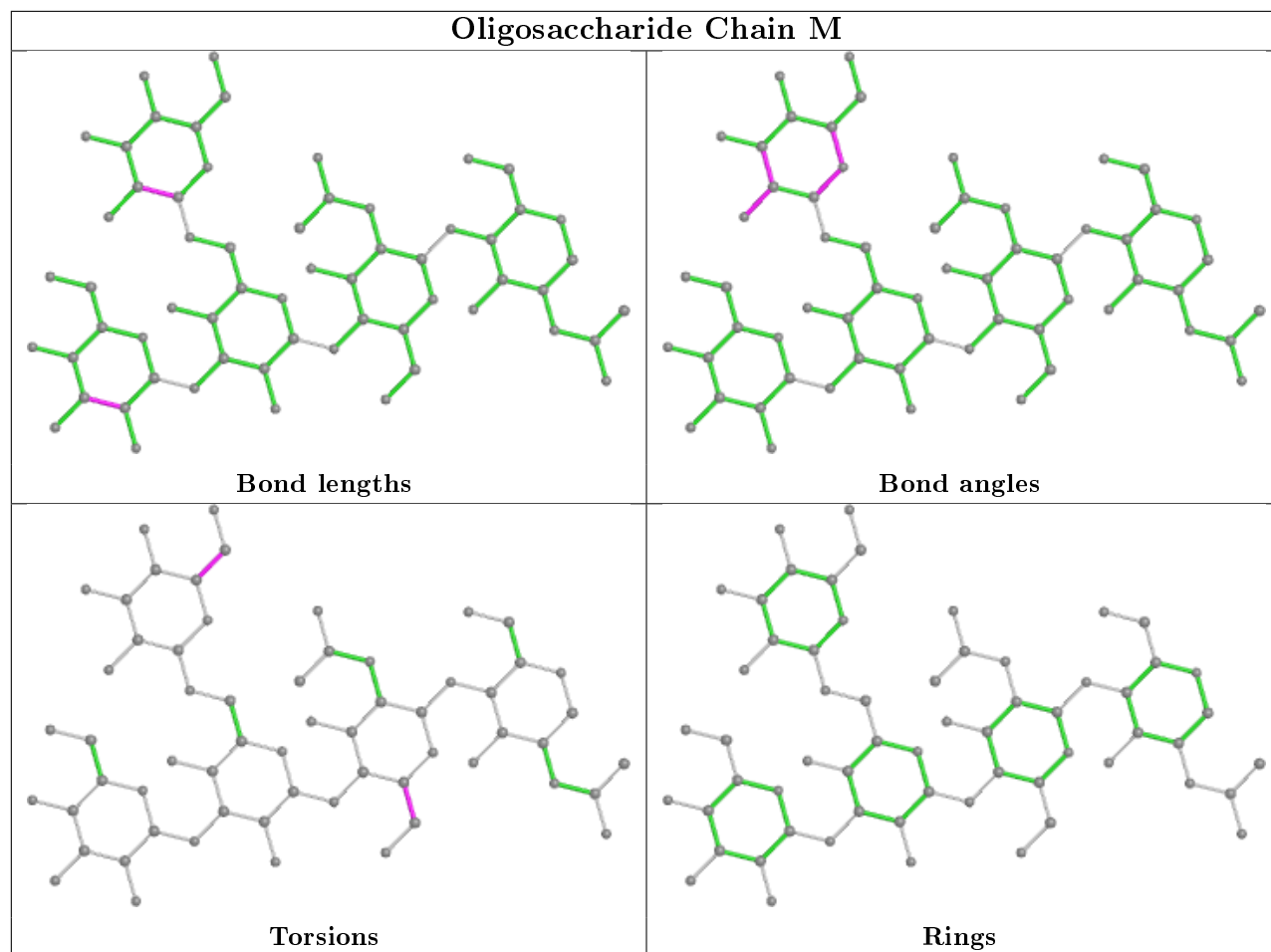
7 monomers are involved in 10 short contacts:

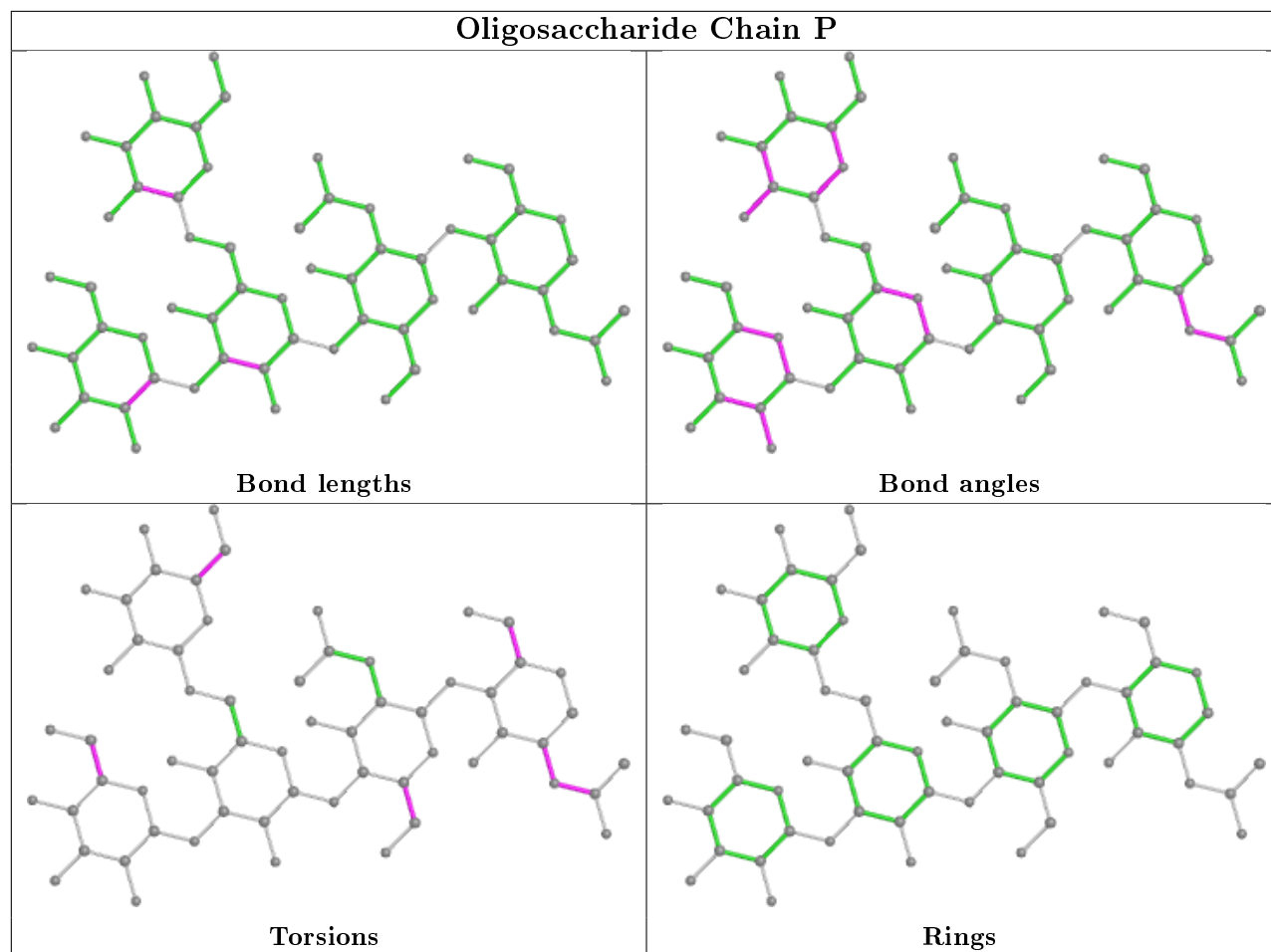
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	1	NAG	1	0
12	H	1	NAG	3	0
9	A	4	MAN	1	0
11	E	1	NAG	1	0
9	A	3	BMA	3	0
9	A	2	NAG	1	0
9	A	1	NAG	1	0

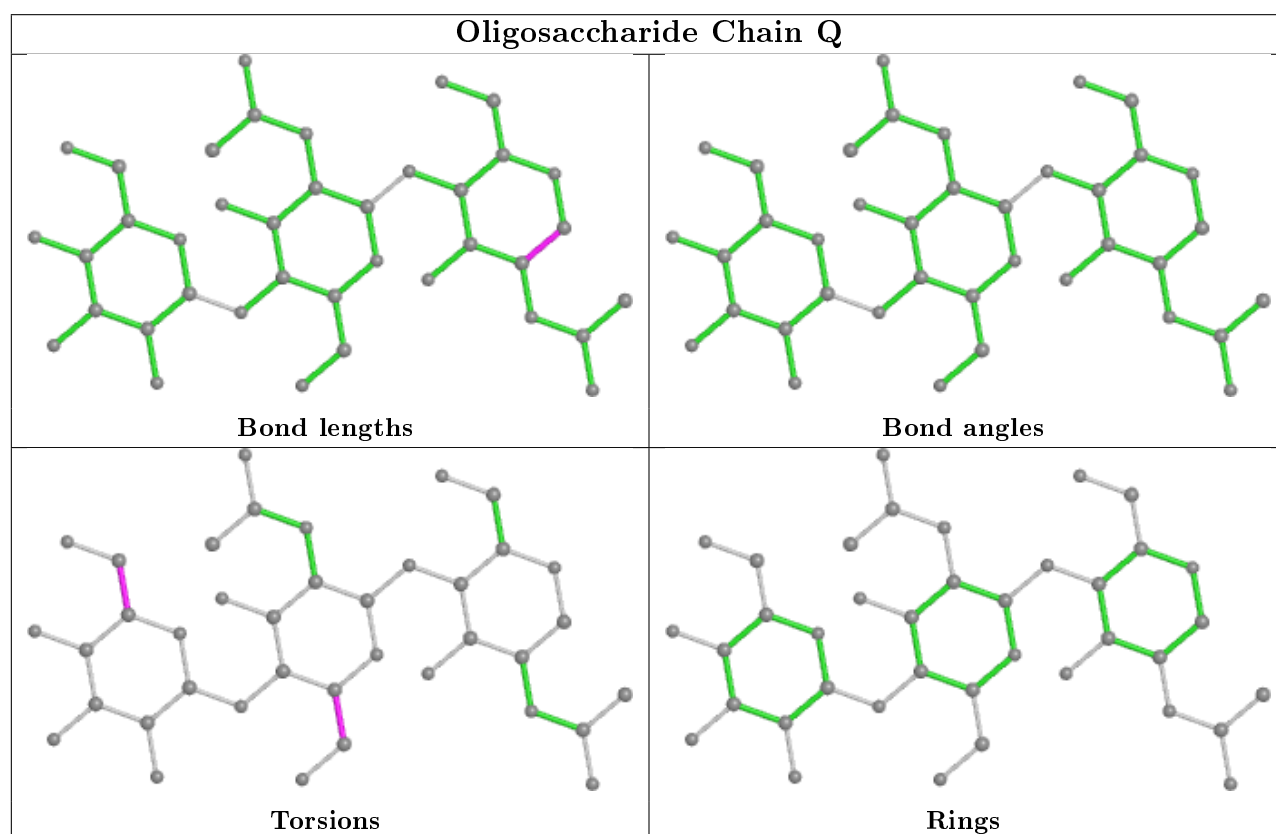
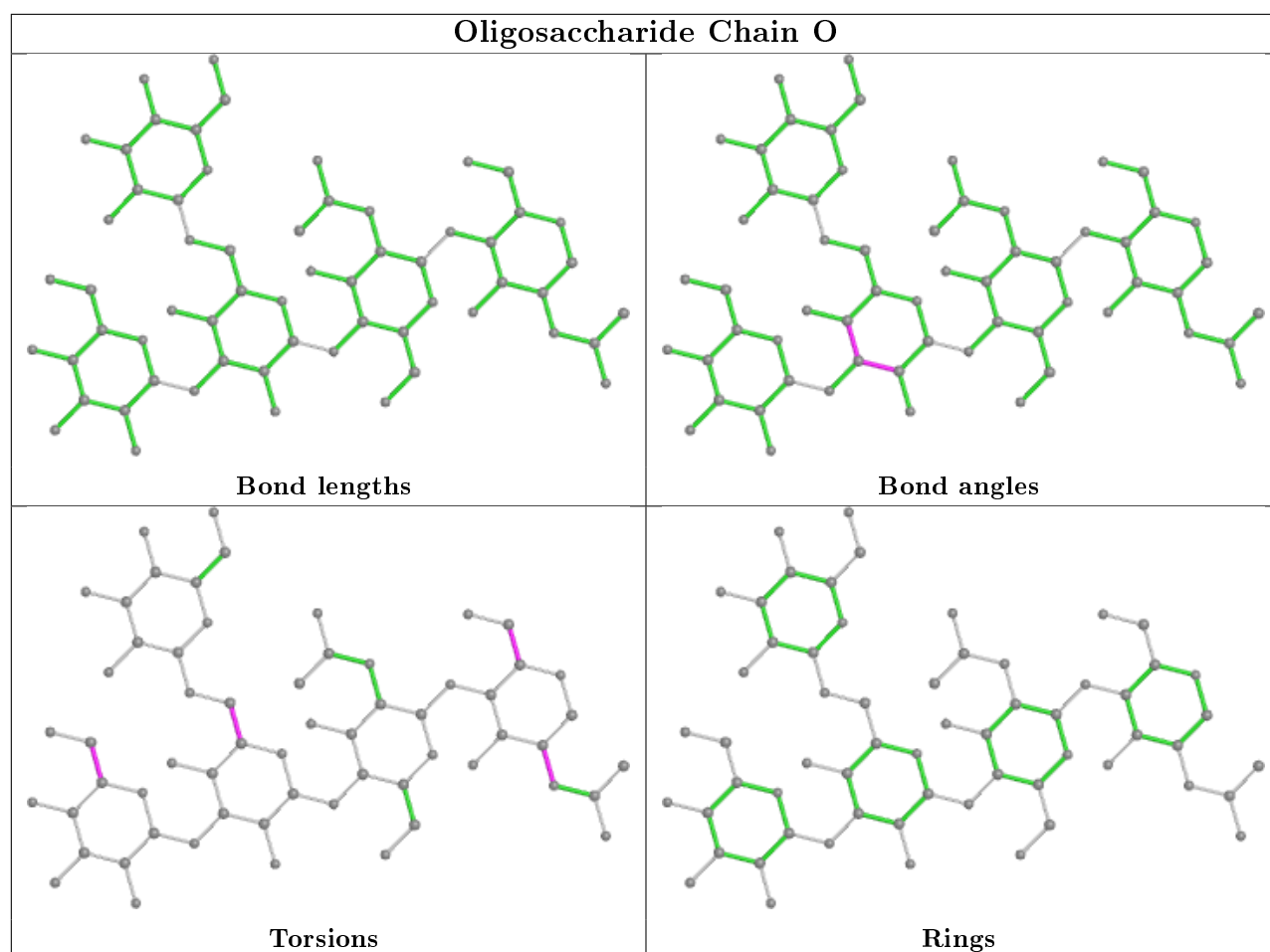
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



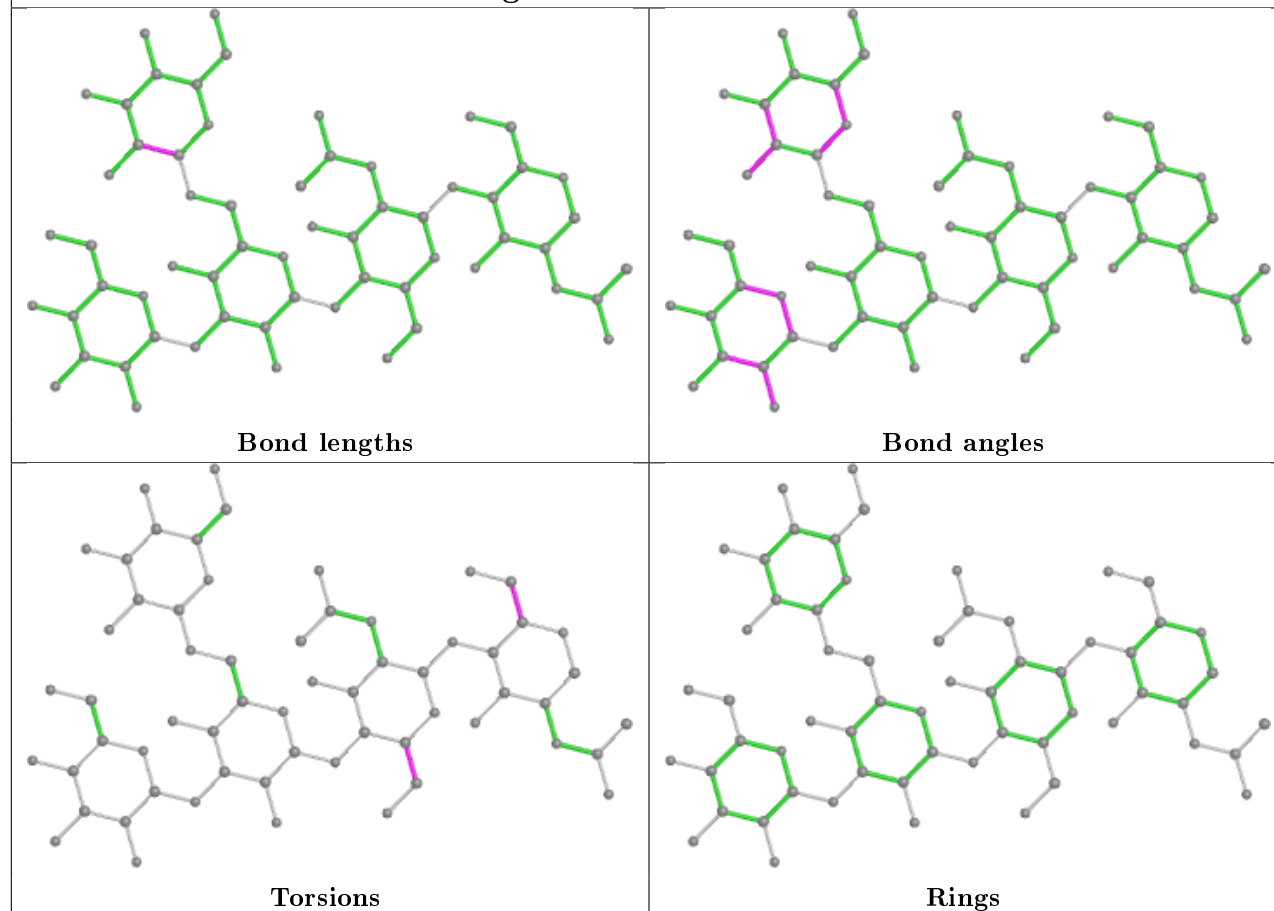




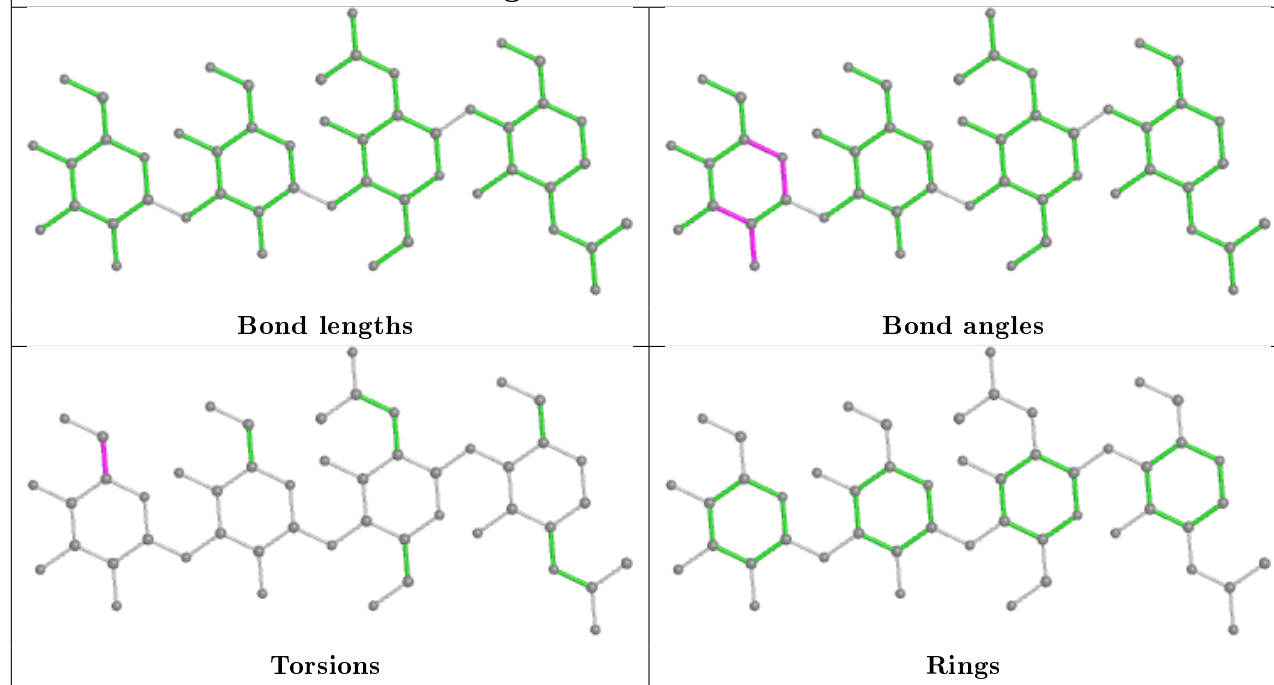




Oligosaccharide Chain U



Oligosaccharide Chain T



5.6 Ligand geometry

2 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$
15	NAG	B	801	2	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
15	NAG	B	802	2	14,14,15	0.58	0	17,19,21	1.25	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
15	NAG	B	801	2	-	5/6/23/26	0/1/1/1
15	NAG	B	802	2	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	801	NAG	C2-N2-C7	4.32	129.05	122.90
15	B	802	NAG	C2-N2-C7	4.28	128.99	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	801	NAG	C8-C7-N2-C2
15	B	801	NAG	O7-C7-N2-C2
15	B	802	NAG	C8-C7-N2-C2
15	B	802	NAG	O7-C7-N2-C2
15	B	802	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	801	NAG	1	0
15	B	802	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	427/475 (89%)	0.02	2 (0%) 91 85	152, 184, 215, 243	0
2	B	129/153 (84%)	-0.01	1 (0%) 86 79	158, 176, 213, 235	0
3	F	130/240 (54%)	0.24	8 (6%) 20 17	180, 211, 232, 237	0
4	I	110/216 (50%)	0.12	4 (3%) 42 34	187, 210, 222, 225	0
5	J	102/211 (48%)	0.47	11 (10%) 5 6	246, 283, 297, 298	0
6	K	132/239 (55%)	0.76	25 (18%) 1 1	224, 272, 298, 313	0
7	R	112/216 (51%)	0.12	2 (1%) 68 60	202, 216, 232, 236	0
8	S	168/272 (61%)	0.31	16 (9%) 8 8	179, 248, 270, 274	0
All	All	1310/2022 (64%)	0.20	69 (5%) 26 23	152, 208, 287, 313	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	K	19	SER	7.1
8	S	9	PRO	6.3
6	K	18	LEU	5.7
6	K	13	GLU	5.1
6	K	20	LEU	4.9

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

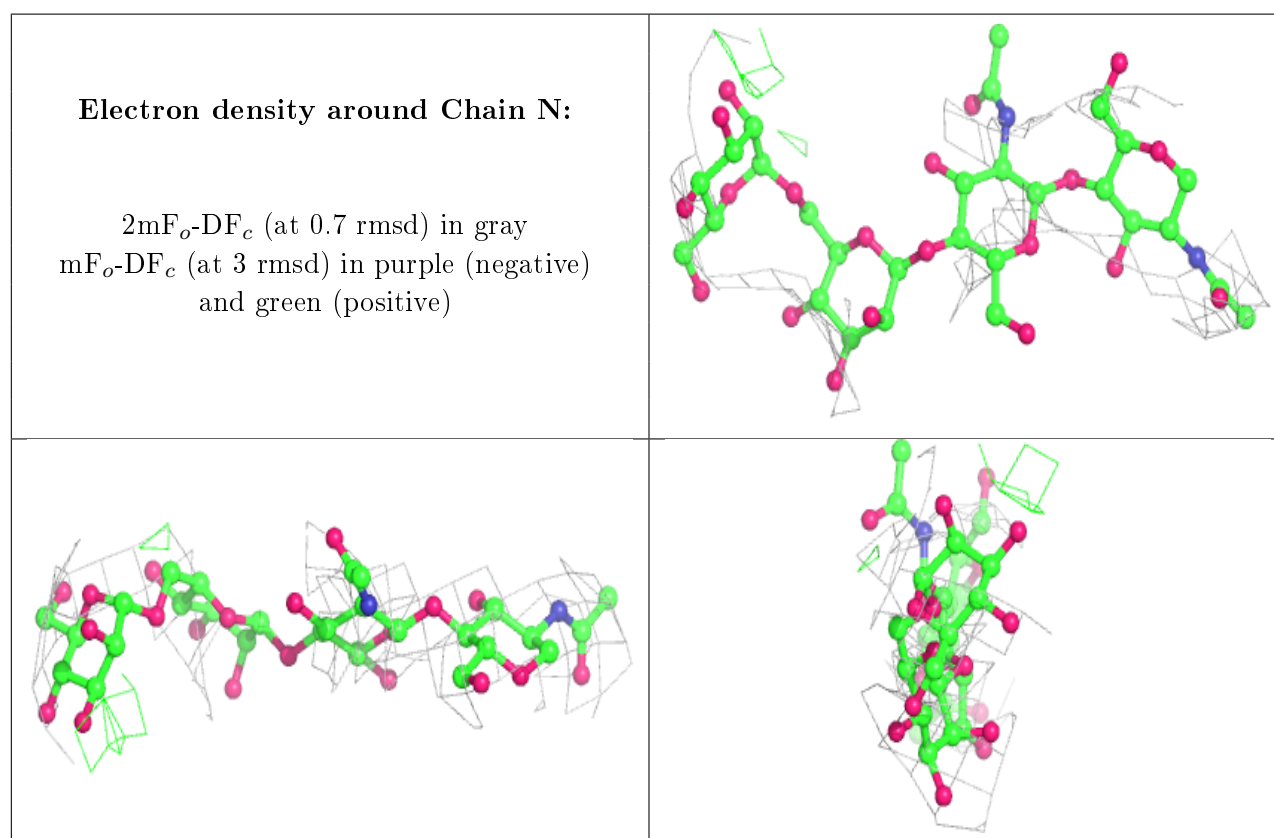
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	MAN	H	4	11/12	0.46	0.28	234,236,238,238	0
12	MAN	N	4	11/12	0.46	0.39	256,258,261,261	0
13	MAN	P	4	11/12	0.47	0.52	227,228,231,232	0
13	MAN	M	4	11/12	0.49	0.70	236,239,244,245	0
12	BMA	N	3	11/12	0.55	0.27	254,255,256,258	0
13	MAN	M	5	11/12	0.61	0.47	226,229,232,233	0
14	BMA	T	3	11/12	0.65	0.34	267,268,270,270	0
13	MAN	U	5	11/12	0.69	0.32	270,272,274,275	0
13	BMA	U	3	11/12	0.71	0.17	263,265,268,268	0
13	MAN	P	5	11/12	0.73	0.16	231,234,237,238	0
10	NAG	C	2	14/15	0.74	0.40	239,241,245,246	0
13	MAN	O	4	11/12	0.74	0.38	245,247,248,249	0
12	NAG	N	2	14/15	0.75	0.52	239,241,242,242	0
13	NAG	U	2	14/15	0.75	0.23	242,243,245,245	0
9	MAN	A	6	11/12	0.76	0.59	219,222,226,227	0
14	NAG	T	2	14/15	0.76	0.23	244,246,248,248	0
11	BMA	Q	3	11/12	0.76	0.21	246,247,249,250	0
11	BMA	D	3	11/12	0.78	0.26	237,239,241,241	0
13	MAN	O	5	11/12	0.78	0.28	245,245,245,245	0
14	NAG	T	1	14/15	0.78	0.26	219,220,221,221	0
13	BMA	M	3	11/12	0.78	0.34	223,226,228,230	0
12	NAG	N	1	14/15	0.79	0.31	212,213,216,216	0
11	NAG	D	2	14/15	0.79	0.32	220,224,226,227	0
9	BMA	A	3	11/12	0.79	0.23	202,206,210,211	0
10	NAG	L	2	14/15	0.79	0.47	213,215,217,218	0
12	BMA	H	3	11/12	0.81	0.29	229,230,232,232	0
11	NAG	Q	1	14/15	0.82	0.24	215,216,217,217	0
10	NAG	L	1	14/15	0.82	0.34	196,198,200,202	0
13	NAG	M	2	14/15	0.82	0.31	197,200,203,204	0
9	MAN	A	5	11/12	0.83	0.26	211,214,217,217	0
14	MAN	T	4	11/12	0.83	0.32	275,276,277,277	0
11	NAG	D	1	14/15	0.83	0.43	204,210,214,215	0
11	NAG	Q	2	14/15	0.83	0.21	231,234,236,236	0
9	NAG	A	2	14/15	0.83	0.35	186,189,191,191	0
12	NAG	H	2	14/15	0.83	0.41	208,211,216,217	0
9	MAN	A	4	11/12	0.84	0.19	213,215,219,219	0
11	NAG	E	2	14/15	0.84	0.38	221,226,230,230	0
10	NAG	C	1	14/15	0.85	0.33	225,228,233,234	0
12	NAG	H	1	14/15	0.85	0.47	198,203,208,209	0
13	NAG	O	1	14/15	0.87	0.55	221,229,234,235	0

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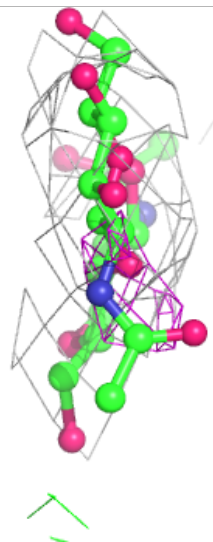
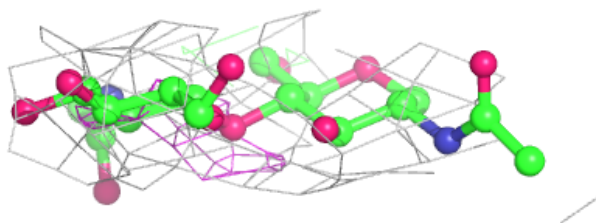
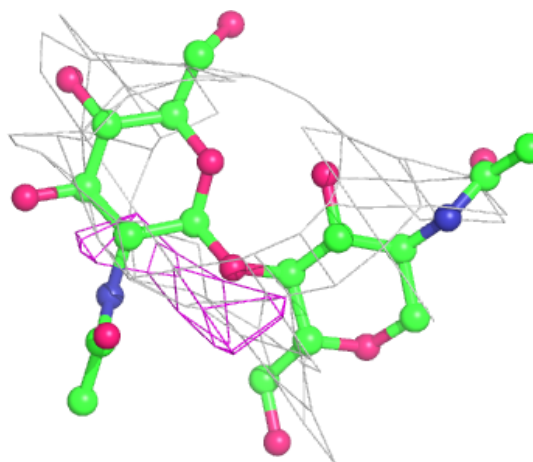
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	NAG	E	1	14/15	0.88	0.33	201,207,209,211	0
9	NAG	A	1	14/15	0.88	0.39	176,180,183,185	0
13	NAG	U	1	14/15	0.88	0.36	218,220,221,222	0
13	MAN	U	4	11/12	0.89	0.20	266,268,272,272	0
11	BMA	E	3	11/12	0.89	0.21	235,236,241,241	0
13	NAG	P	1	14/15	0.91	0.49	211,212,214,216	0
13	BMA	P	3	11/12	0.92	0.31	226,227,229,231	0
13	BMA	O	3	11/12	0.92	0.14	244,246,250,250	0
13	NAG	P	2	14/15	0.93	0.22	214,217,218,219	0
9	MAN	A	7	11/12	0.93	0.21	204,206,211,212	0
13	NAG	O	2	14/15	0.93	0.31	236,242,244,245	0
13	NAG	M	1	14/15	0.95	0.26	181,182,185,185	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.



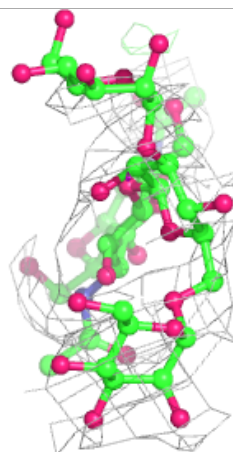
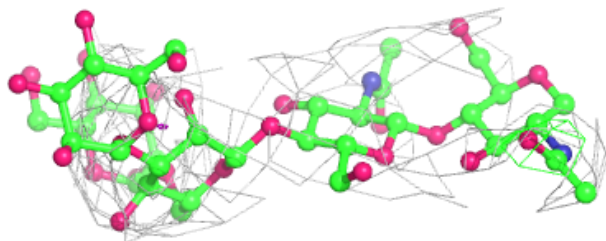
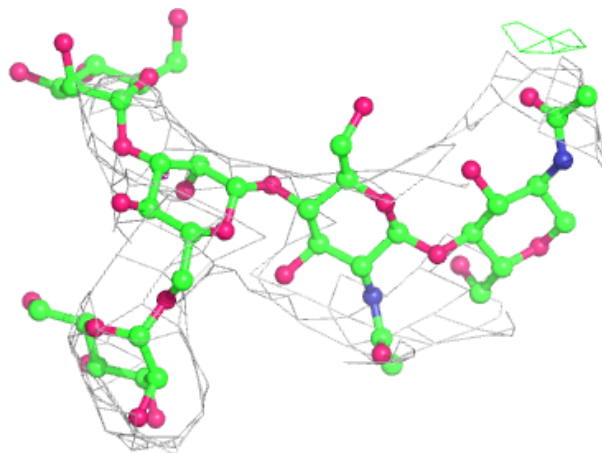
Electron density around Chain L:

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



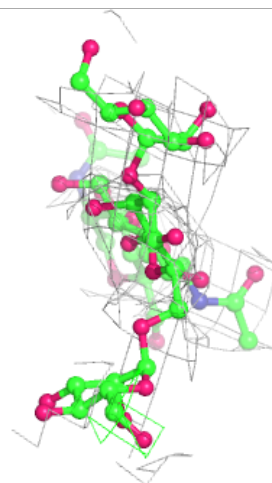
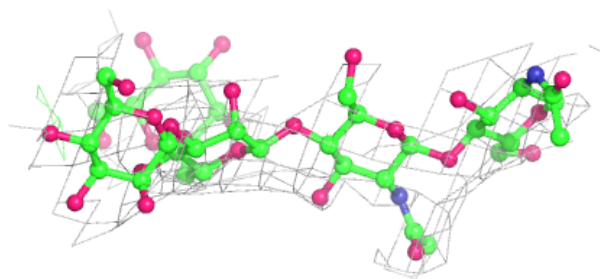
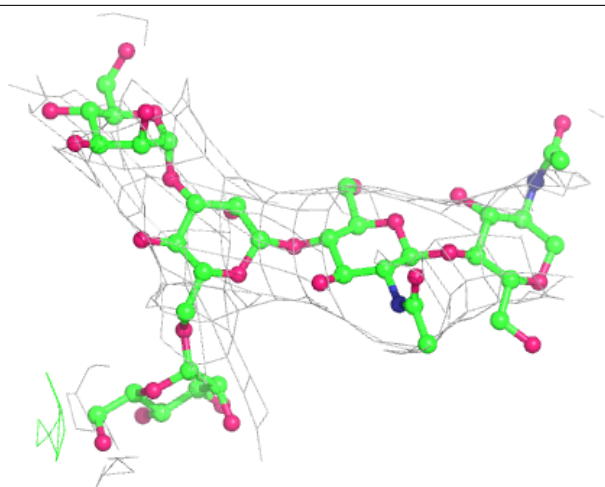
Electron density around Chain M:

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



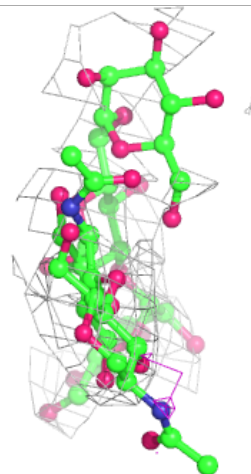
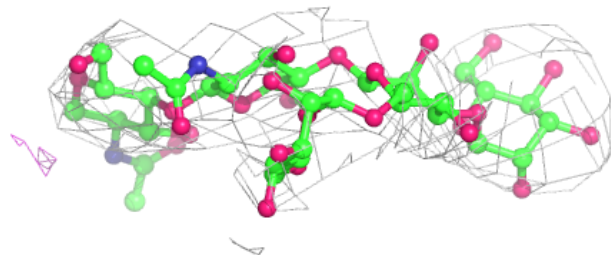
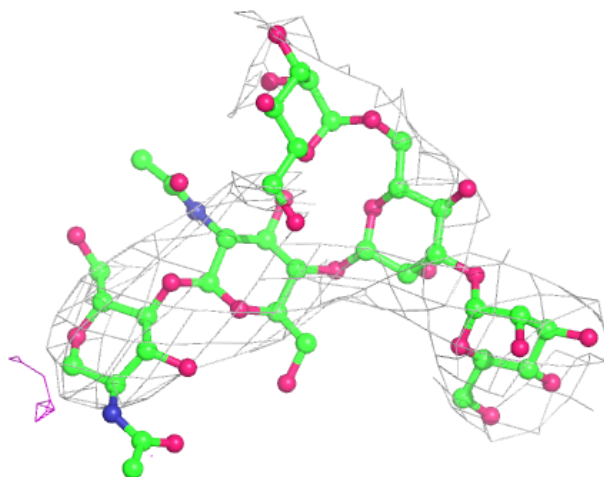
Electron density around Chain P:

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



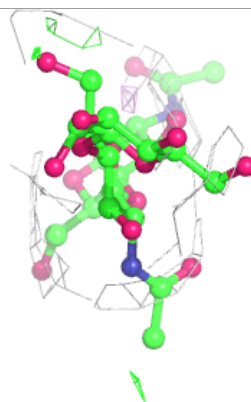
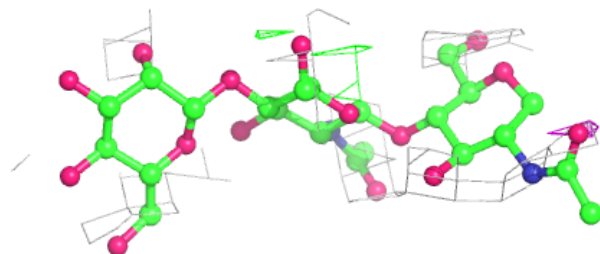
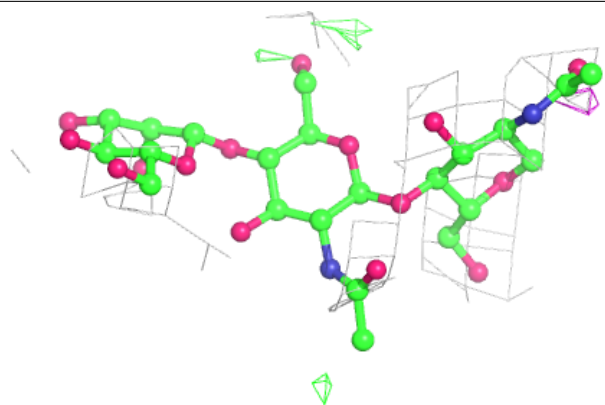
Electron density around Chain O:

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



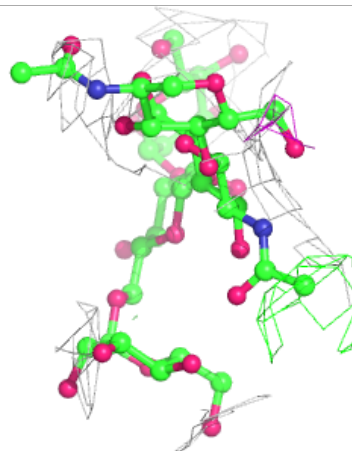
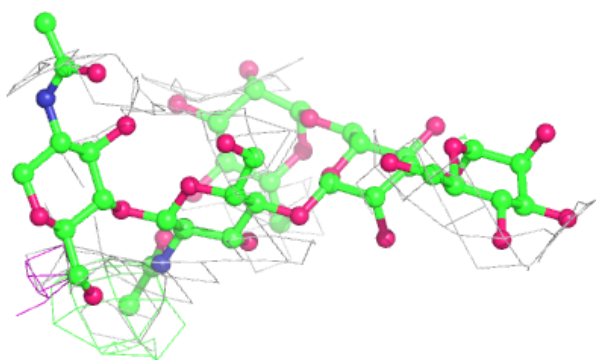
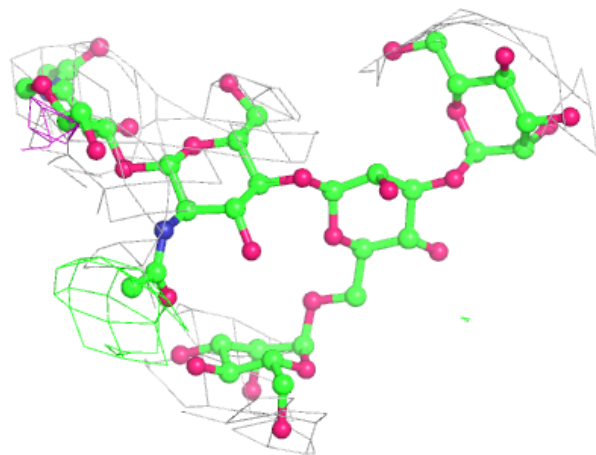
Electron density around Chain Q:

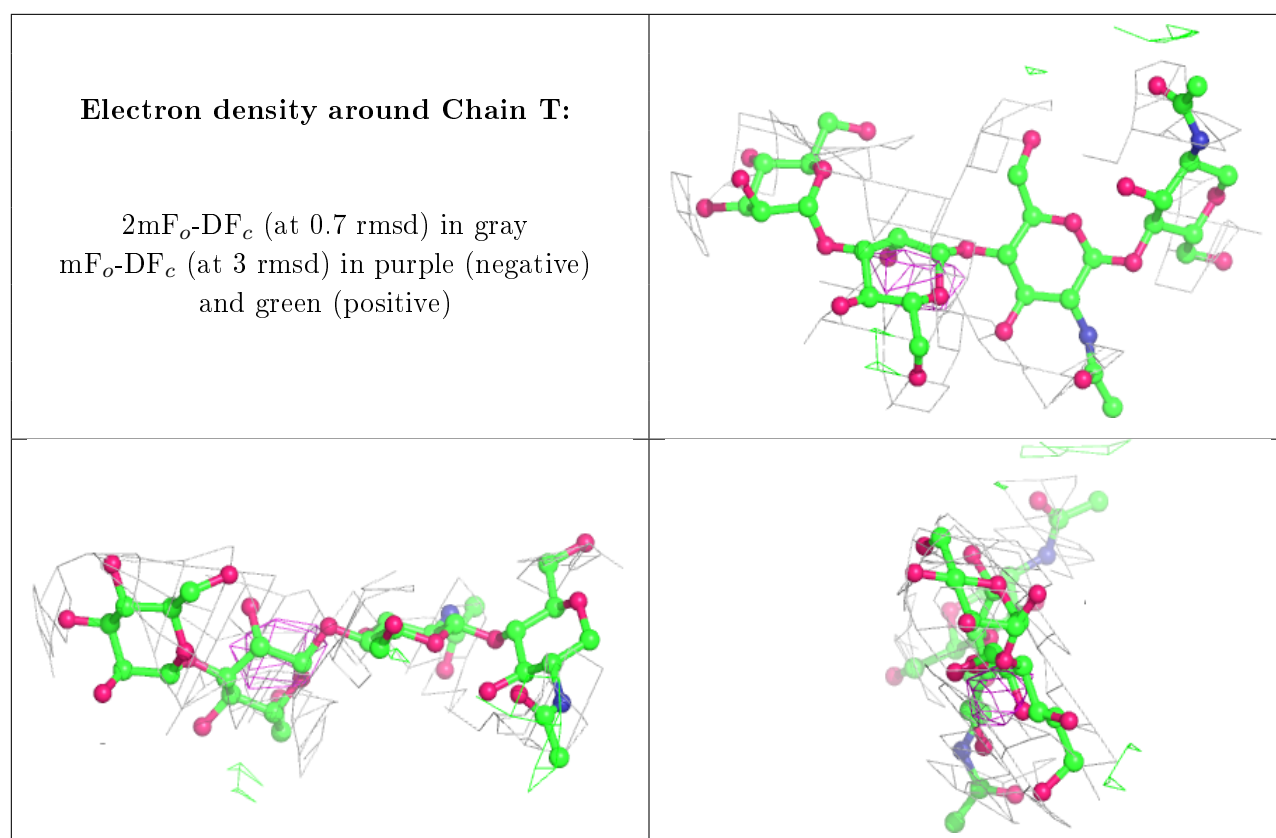
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain U:

$2mF_o-DF_c$ (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
15	NAG	B	801	14/15	0.77	0.32	185,188,190,191	0
15	NAG	B	802	14/15	0.84	0.41	202,204,206,207	0

6.5 Other polymers [i](#)

There are no such residues in this entry.