



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 08:05 AM BST

PDB ID : 6RUR
Title : Structure of the SCIN stabilized C3bBb convertase bound to properdin
Authors : Pedersen, D.V.; Gadeberg, T.A.F.; Andersen, G.R.
Deposited on : 2019-05-29
Resolution : 6.00 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

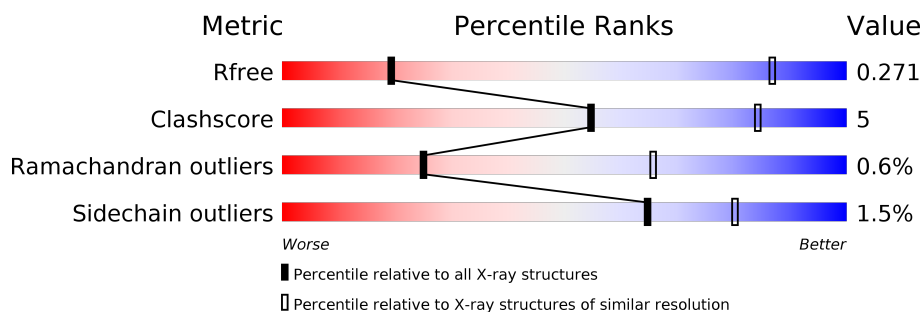
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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.

















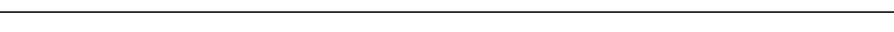



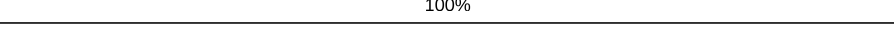
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	U	234	
1	X	234	
2	V	215	
2	Y	215	
3	A	645	
3	G	645	
4	B	915	

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Mol	Chain	Length	Quality of chain
4	H	915	 84% 16%
5	J	505	 91% 9%
5	L	505	 85% 14%
6	N	85	 84% 14% ..
6	Q	85	 84% 15% .
7	C	2	 50% 50%
7	D	2	 50% 50%
7	F	2	 50% 50%
7	I	2	 50% 50%
8	E	3	 33% 33% 33%
8	K	3	 33% 33% 33%
9	M	2	 100%
9	O	2	 100%
9	P	2	 100%
9	R	2	 50% 50%
9	S	2	 50% 50%
9	T	2	 50% 50%
9	W	2	 100%
9	Z	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	FUC	E	3	X	-	-	-
8	FUC	K	3	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 39456 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	106	Total	C	N	O	S	0	0	0
			806	495	144	154	13			
1	X	106	Total	C	N	O	S	0	0	0
			806	495	144	154	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	256	GLU	-	expression tag	UNP P27918
U	257	ASN	-	expression tag	UNP P27918
U	258	LEU	-	expression tag	UNP P27918
U	259	TYR	-	expression tag	UNP P27918
U	260	PHE	-	expression tag	UNP P27918
U	261	GLN	-	expression tag	UNP P27918
X	256	GLU	-	expression tag	UNP P27918
X	257	ASN	-	expression tag	UNP P27918
X	258	LEU	-	expression tag	UNP P27918
X	259	TYR	-	expression tag	UNP P27918
X	260	PHE	-	expression tag	UNP P27918
X	261	GLN	-	expression tag	UNP P27918

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	210	Total	C	N	O	S	0	0	0
			1622	1004	308	288	22			
2	Y	210	Total	C	N	O	S	0	0	0
			1622	1004	308	288	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	255	GLY	-	expression tag	UNP P27918
Y	255	GLY	-	expression tag	UNP P27918

- Molecule 3 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			
3	G	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			

- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			
4	H	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			

- Molecule 5 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			
5	L	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			

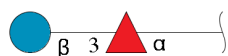
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	254	GLY	ASP	conflict	UNP P00751
J	674	ALA	SER	conflict	UNP P00751
L	254	GLY	ASP	conflict	UNP P00751
L	674	ALA	SER	conflict	UNP P00751

- Molecule 6 is a protein called Inhibitor.

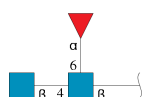
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			
6	Q	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			

- Molecule 7 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	C	2	Total	C	O	0	0	0
			21	12	9			
7	D	2	Total	C	O	0	0	0
			21	12	9			
7	F	2	Total	C	O	0	0	0
			21	12	9			
7	I	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
8	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



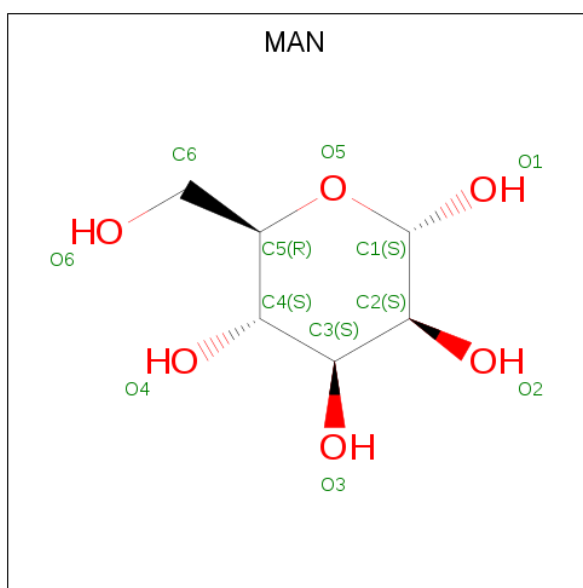
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	U	1	Total	C	O	0	0
			11	6	5		
10	U	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	V	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		
10	V	1	Total	C	O	0	0
			11	6	5		
10	X	1	Total	C	O	0	0
			11	6	5		
10	X	1	Total	C	O	0	0
			11	6	5		
10	Y	1	Total	C	O	0	0
			11	6	5		
10	Y	1	Total	C	O	0	0
			11	6	5		
10	Y	1	Total	C	O	0	0
			11	6	5		
10	Y	1	Total	C	O	0	0
			11	6	5		
10	Y	1	Total	C	O	0	0
			11	6	5		

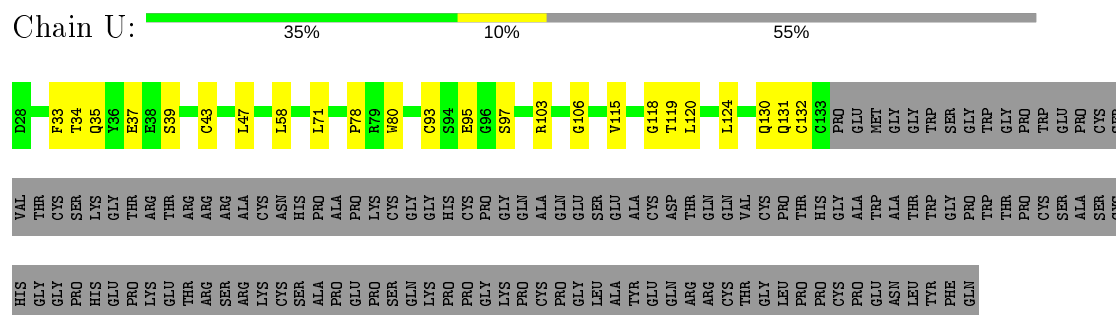
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	1	Total	Mg	0	0
			1	1		
11	B	1	Total	Mg	0	0
			1	1		

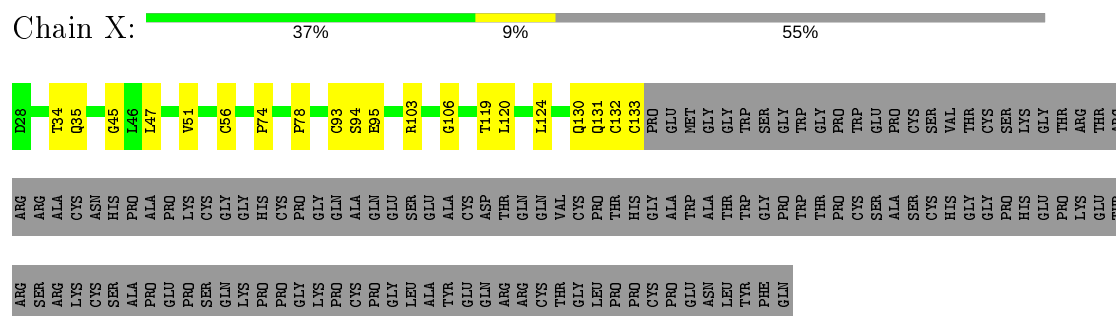
3 Residue-property plots

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. 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. 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.

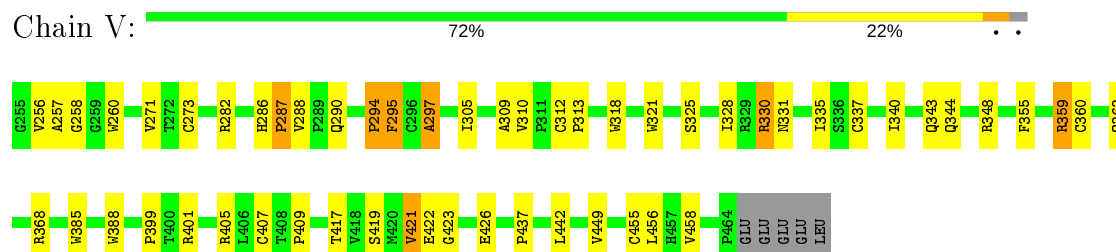
- Molecule 1: Properdin



- Molecule 1: Properdin

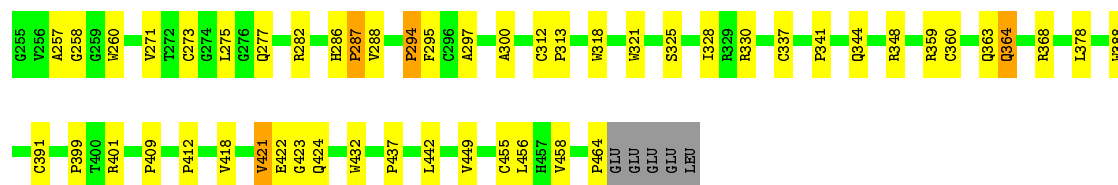


- Molecule 2: Properdin

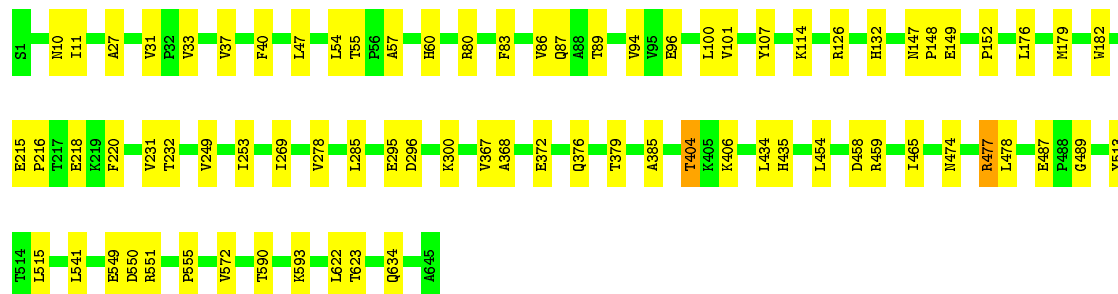
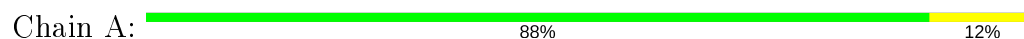


- Molecule 2: Properdin

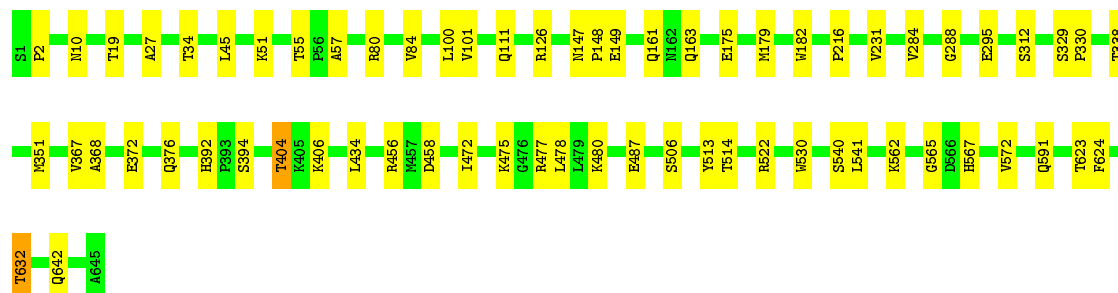


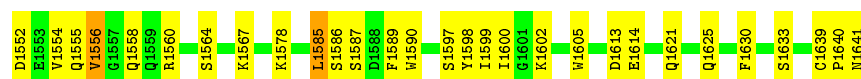


• Molecule 3: Complement C3



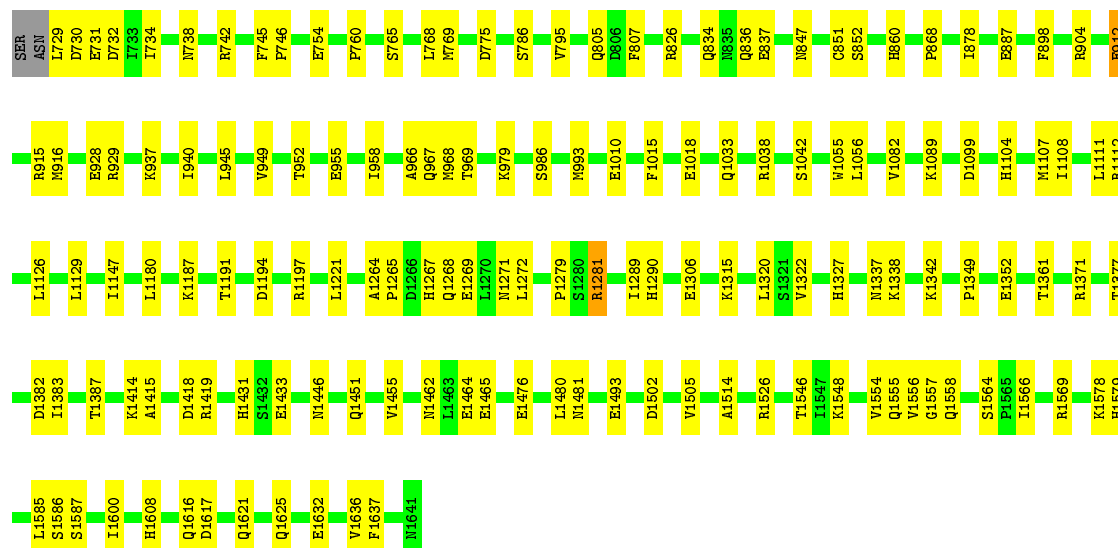
• Molecule 3: Complement C3





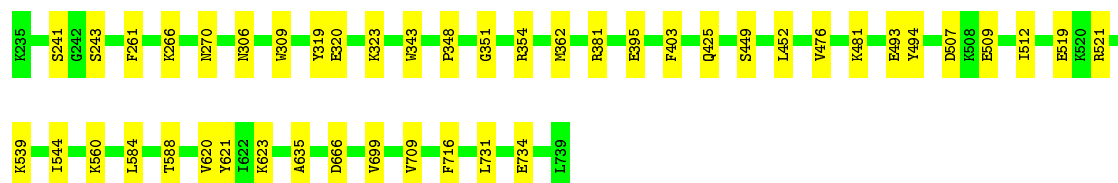
• Molecule 4: Complement C3

Chain H: 84% 16%



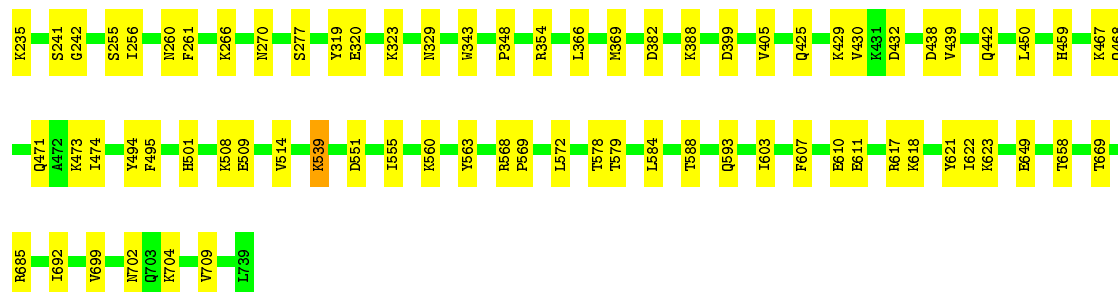
• Molecule 5: Complement factor B

Chain J: 91% 9%



• Molecule 5: Complement factor B

Chain L: 85% 14%

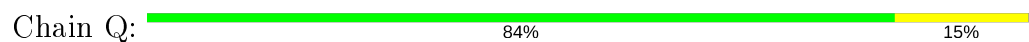


• Molecule 6: Inhibitor

Chain N: 84% 14%



- Molecule 6: Inhibitor



- Molecule 7: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 7: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 7: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 7: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	634.87Å 121.98Å 264.42Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	48.76 – 6.00 48.76 – 6.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.76-6.00) 98.8 (48.76-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.234 , 0.272 0.233 , 0.271	Depositor DCC
R_{free} test set	1174 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	301.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 302.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.048 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	39456	wwPDB-VP
Average B, all atoms (Å ²)	397.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: FUC, MG, BGC, 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	U	0.24	0/825	0.43	0/1117
1	X	0.24	0/825	0.44	0/1117
2	V	0.23	0/1676	0.43	0/2283
2	Y	0.23	0/1675	0.43	0/2279
3	A	0.25	0/5127	0.46	0/6966
3	G	0.24	0/5127	0.45	0/6966
4	B	0.24	0/7439	0.44	0/10073
4	H	0.24	0/7439	0.43	0/10073
5	J	0.24	0/4095	0.41	0/5542
5	L	0.24	0/4095	0.41	0/5542
6	N	0.23	0/691	0.35	0/923
6	Q	0.23	0/691	0.35	0/923
All	All	0.24	0/39705	0.43	0/53804

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	U	806	0	747	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	806	0	747	14	0
2	V	1622	0	1538	33	0
2	Y	1622	0	1538	29	0
3	A	5025	0	5084	51	0
3	G	5025	0	5084	40	0
4	B	7293	0	7217	94	0
4	H	7293	0	7217	79	0
5	J	4007	0	3994	27	0
5	L	4007	0	3994	45	0
6	N	683	0	697	12	0
6	Q	683	0	697	10	0
7	C	21	0	19	0	0
7	D	21	0	19	0	0
7	F	21	0	19	2	0
7	I	21	0	19	0	0
8	E	38	0	34	3	0
8	K	38	0	34	2	0
9	M	28	0	25	0	0
9	O	28	0	25	0	0
9	P	28	0	25	0	0
9	R	28	0	25	0	0
9	S	28	0	25	2	0
9	T	28	0	25	0	0
9	W	28	0	25	4	0
9	Z	28	0	25	1	0
10	U	22	0	20	0	0
10	V	77	0	70	0	0
10	X	22	0	20	0	0
10	Y	77	0	70	1	0
11	B	1	0	0	0	0
11	H	1	0	0	0	0
All	All	39456	0	39078	410	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 5.

The worst 5 of 410 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)
5:L:539:LYS:NZ	5:L:649:GLU:OE1	2.09	0.85
5:J:241:SER:O	5:J:354:ARG:NH2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:331:ASN:HB2	4:B:1640:PRO:HG2	1.62	0.80
3:A:83:PHE:HD2	3:A:100:LEU:HA	1.47	0.78
5:L:242:GLY:HA2	5:L:354:ARG:HH22	1.51	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	104/234 (44%)	95 (91%)	9 (9%)	0	100	100
1	X	104/234 (44%)	96 (92%)	8 (8%)	0	100	100
2	V	208/215 (97%)	188 (90%)	14 (7%)	6 (3%)	4	29
2	Y	206/215 (96%)	187 (91%)	13 (6%)	6 (3%)	4	29
3	A	643/645 (100%)	622 (97%)	20 (3%)	1 (0%)	47	81
3	G	643/645 (100%)	618 (96%)	22 (3%)	3 (0%)	29	69
4	B	911/915 (100%)	867 (95%)	37 (4%)	7 (1%)	19	60
4	H	911/915 (100%)	867 (95%)	39 (4%)	5 (0%)	29	69
5	J	503/505 (100%)	484 (96%)	19 (4%)	0	100	100
5	L	503/505 (100%)	480 (95%)	23 (5%)	0	100	100
6	N	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
6	Q	82/85 (96%)	80 (98%)	0	2 (2%)	6	33
All	All	4900/5198 (94%)	4665 (95%)	205 (4%)	30 (1%)	25	66

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	294	PRO
2	Y	294	PRO

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Mol	Chain	Res	Type
4	B	1261	GLN
4	B	1262	LYS
4	B	1358	ALA

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	U	89/193 (46%)	86 (97%)	3 (3%)	37	60
1	X	89/193 (46%)	86 (97%)	3 (3%)	37	60
2	V	179/184 (97%)	171 (96%)	8 (4%)	27	52
2	Y	179/184 (97%)	173 (97%)	6 (3%)	37	60
3	A	567/567 (100%)	562 (99%)	5 (1%)	78	88
3	G	567/567 (100%)	563 (99%)	4 (1%)	84	90
4	B	808/810 (100%)	793 (98%)	15 (2%)	57	75
4	H	808/810 (100%)	789 (98%)	19 (2%)	49	69
5	J	444/444 (100%)	444 (100%)	0	100	100
5	L	444/444 (100%)	443 (100%)	1 (0%)	93	96
6	N	76/77 (99%)	75 (99%)	1 (1%)	69	82
6	Q	76/77 (99%)	75 (99%)	1 (1%)	69	82
All	All	4326/4550 (95%)	4260 (98%)	66 (2%)	65	80

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	967	GLN
4	B	1515	CYS
4	H	1433	GLU
4	B	1267	HIS
4	B	1431	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	10	ASN
3	A	60	HIS
4	B	1305	ASN
4	H	738	ASN
6	Q	49	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 ⓘ

30 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	$\# Z > 2$
7	FUC	C	1	1,7	10,10,11	0.87	0	14,14,16	0.93	0
7	BGC	C	2	7	11,11,12	1.74	2 (18%)	15,15,17	1.09	1 (6%)
7	FUC	D	1	2,7	10,10,11	0.69	0	14,14,16	0.89	0
7	BGC	D	2	7	11,11,12	1.76	3 (27%)	15,15,17	0.82	0
8	NAG	E	1	8,2	14,14,15	0.23	0	17,19,21	0.52	0
8	NAG	E	2	8	14,14,15	0.64	1 (7%)	17,19,21	1.26	1 (5%)
8	FUC	E	3	8	10,10,11	0.73	0	14,14,16	0.87	0
7	FUC	F	1	1,7	10,10,11	0.82	0	14,14,16	0.97	0
7	BGC	F	2	7	11,11,12	1.74	2 (18%)	15,15,17	1.06	1 (6%)
7	FUC	I	1	2,7	10,10,11	0.75	0	14,14,16	0.89	0
7	BGC	I	2	7	11,11,12	1.78	3 (27%)	15,15,17	1.02	2 (13%)
8	NAG	K	1	8,2	14,14,15	0.26	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	K	2	8	14,14,15	0.64	1 (7%)	17,19,21	1.26	1 (5%)
8	FUC	K	3	8	10,10,11	0.68	0	14,14,16	0.87	0
9	NAG	M	1	9,3	14,14,15	0.30	0	17,19,21	0.42	0
9	NAG	M	2	9	14,14,15	0.38	0	17,19,21	0.40	0
9	NAG	O	1	9,4	14,14,15	0.33	0	17,19,21	0.53	0
9	NAG	O	2	9	14,14,15	0.22	0	17,19,21	0.46	0
9	NAG	P	1	9,3	14,14,15	0.25	0	17,19,21	0.53	0
9	NAG	P	2	9	14,14,15	0.28	0	17,19,21	0.41	0
9	NAG	R	1	9,4	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
9	NAG	R	2	9	14,14,15	0.41	0	17,19,21	0.56	0
9	NAG	S	1	9,5	14,14,15	0.27	0	17,19,21	0.53	0
9	NAG	S	2	9	14,14,15	0.57	0	17,19,21	1.29	1 (5%)
9	NAG	T	1	9,5	14,14,15	0.90	1 (7%)	17,19,21	0.96	1 (5%)
9	NAG	T	2	9	14,14,15	0.27	0	17,19,21	0.41	0
9	NAG	W	1	9,5	14,14,15	0.83	2 (14%)	17,19,21	1.67	3 (17%)
9	NAG	W	2	9	14,14,15	0.70	1 (7%)	17,19,21	1.30	2 (11%)
9	NAG	Z	1	9,5	14,14,15	0.94	2 (14%)	17,19,21	0.97	1 (5%)
9	NAG	Z	2	9	14,14,15	0.20	0	17,19,21	0.41	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	FUC	C	1	1,7	-	-	0/1/1/1
7	BGC	C	2	7	-	0/2/19/22	0/1/1/1
7	FUC	D	1	2,7	-	-	0/1/1/1
7	BGC	D	2	7	-	1/2/19/22	0/1/1/1
8	NAG	E	1	8,2	-	3/6/23/26	0/1/1/1
8	NAG	E	2	8	-	5/6/23/26	0/1/1/1
8	FUC	E	3	8	1/1/4/5	-	0/1/1/1
7	FUC	F	1	1,7	-	-	0/1/1/1
7	BGC	F	2	7	-	0/2/19/22	0/1/1/1
7	FUC	I	1	2,7	-	-	0/1/1/1
7	BGC	I	2	7	-	2/2/19/22	0/1/1/1
8	NAG	K	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	5/6/23/26	0/1/1/1
8	FUC	K	3	8	1/1/4/5	-	0/1/1/1
9	NAG	M	1	9,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	NAG	O	1	9,4	-	1/6/23/26	0/1/1/1
9	NAG	O	2	9	-	4/6/23/26	0/1/1/1
9	NAG	P	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	P	2	9	-	2/6/23/26	0/1/1/1
9	NAG	R	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	NAG	S	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	S	2	9	-	4/6/23/26	0/1/1/1
9	NAG	T	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	T	2	9	-	4/6/23/26	0/1/1/1
9	NAG	W	1	9,5	-	3/6/23/26	0/1/1/1
9	NAG	W	2	9	-	5/6/23/26	0/1/1/1
9	NAG	Z	1	9,5	-	4/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	4/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	2	BGC	O5-C1	4.61	1.51	1.43
7	C	2	BGC	O5-C1	4.56	1.51	1.43
7	D	2	BGC	O5-C1	4.44	1.50	1.43
7	I	2	BGC	O5-C1	4.32	1.50	1.43
7	I	2	BGC	C2-C3	-2.84	1.48	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	1	NAG	C1-O5-C5	5.44	119.56	112.19
9	W	2	NAG	C2-N2-C7	4.44	129.22	122.90
8	E	2	NAG	C2-N2-C7	4.29	129.01	122.90
8	K	2	NAG	C2-N2-C7	4.27	128.98	122.90
9	S	2	NAG	C2-N2-C7	4.26	128.97	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	E	3	FUC	C1
8	K	3	FUC	C1

5 of 64 torsion outliers are listed below:

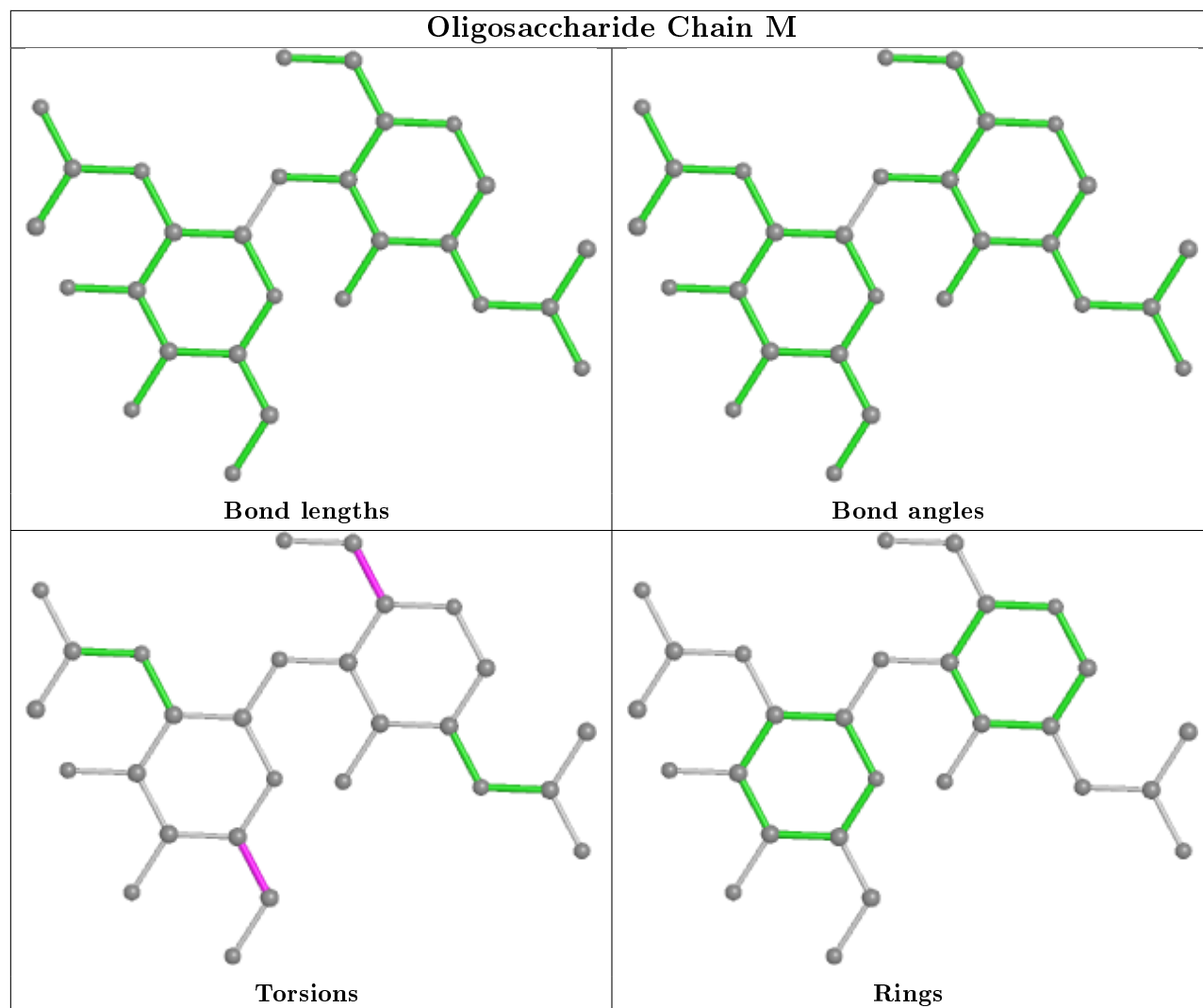
Mol	Chain	Res	Type	Atoms
9	W	2	NAG	O5-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6

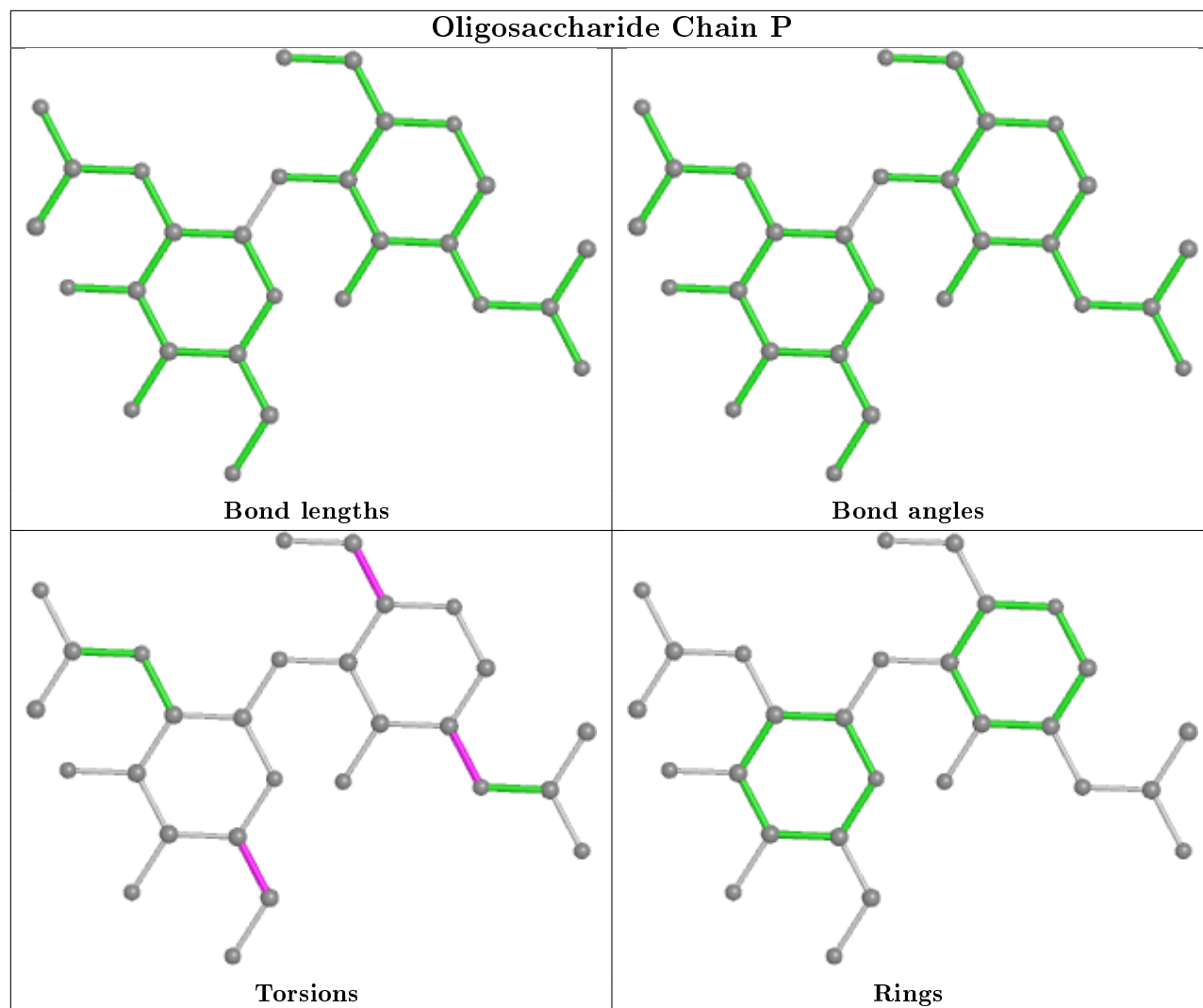
There are no ring outliers.

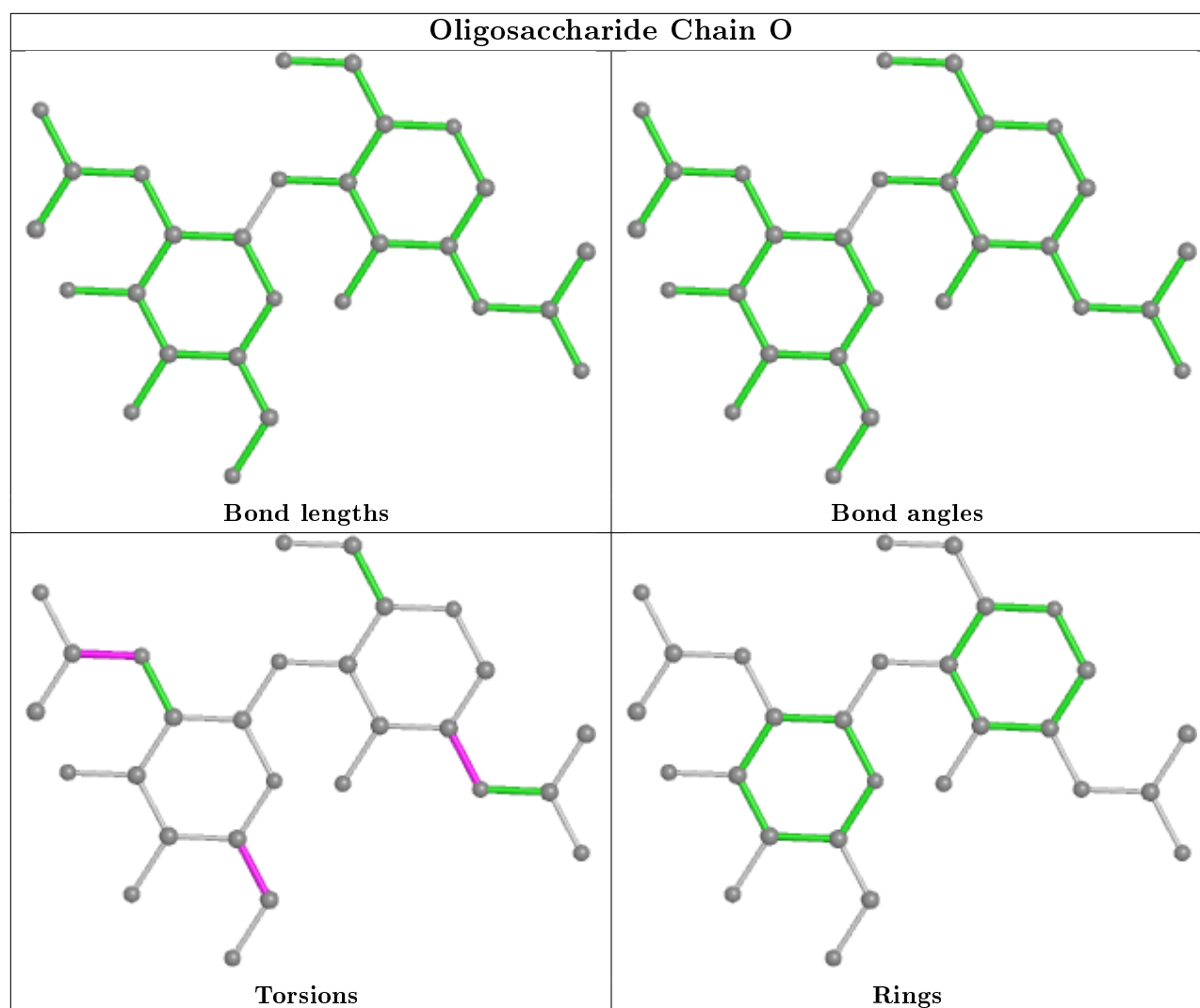
11 monomers are involved in 14 short contacts:

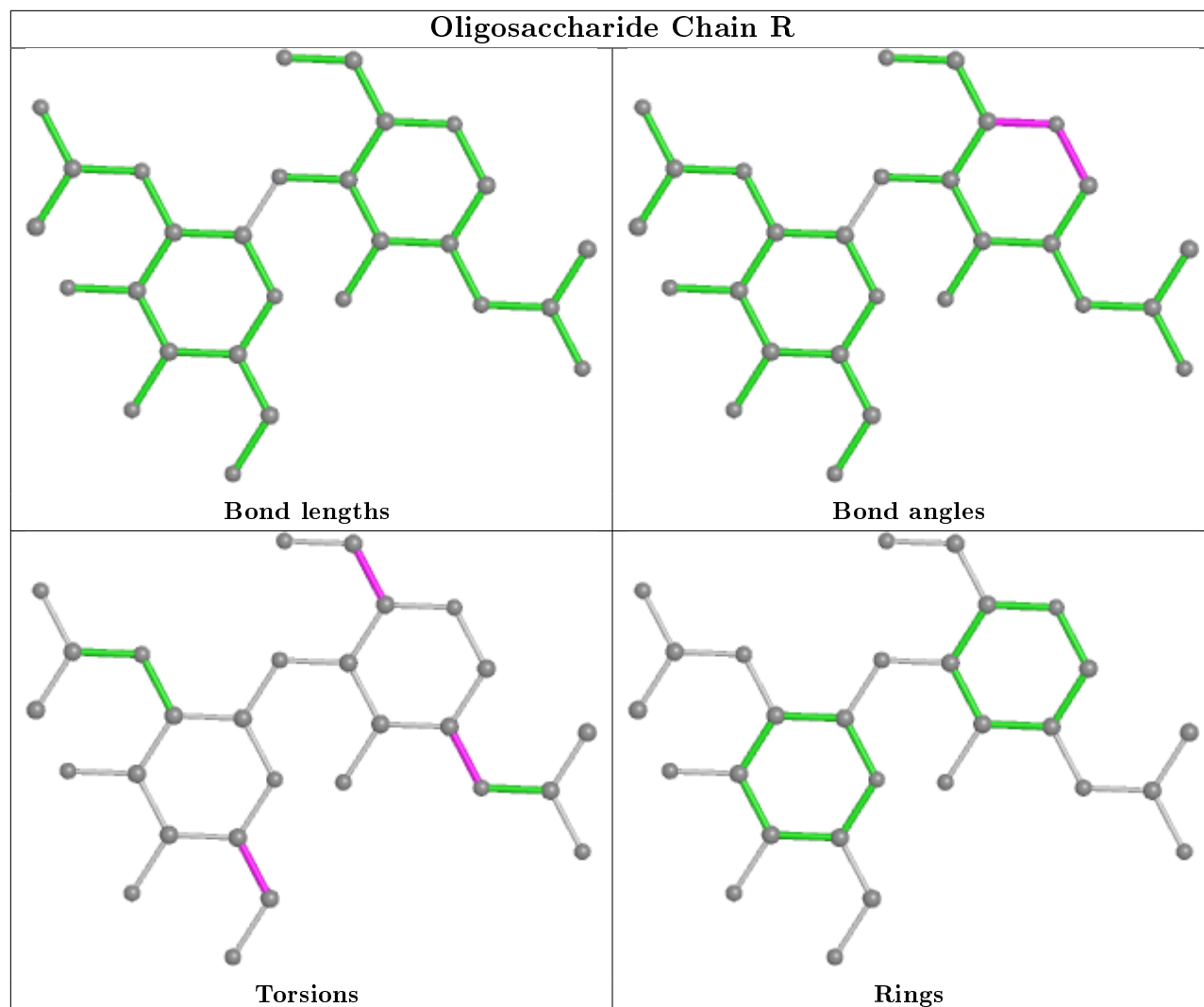
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1	NAG	1	0
7	F	2	BGC	2	0
8	K	2	NAG	2	0
9	S	2	NAG	2	0
9	W	2	NAG	1	0
9	W	1	NAG	3	0
8	E	1	NAG	2	0
9	Z	1	NAG	1	0
7	F	1	FUC	1	0
9	S	1	NAG	1	0
8	E	2	NAG	3	0

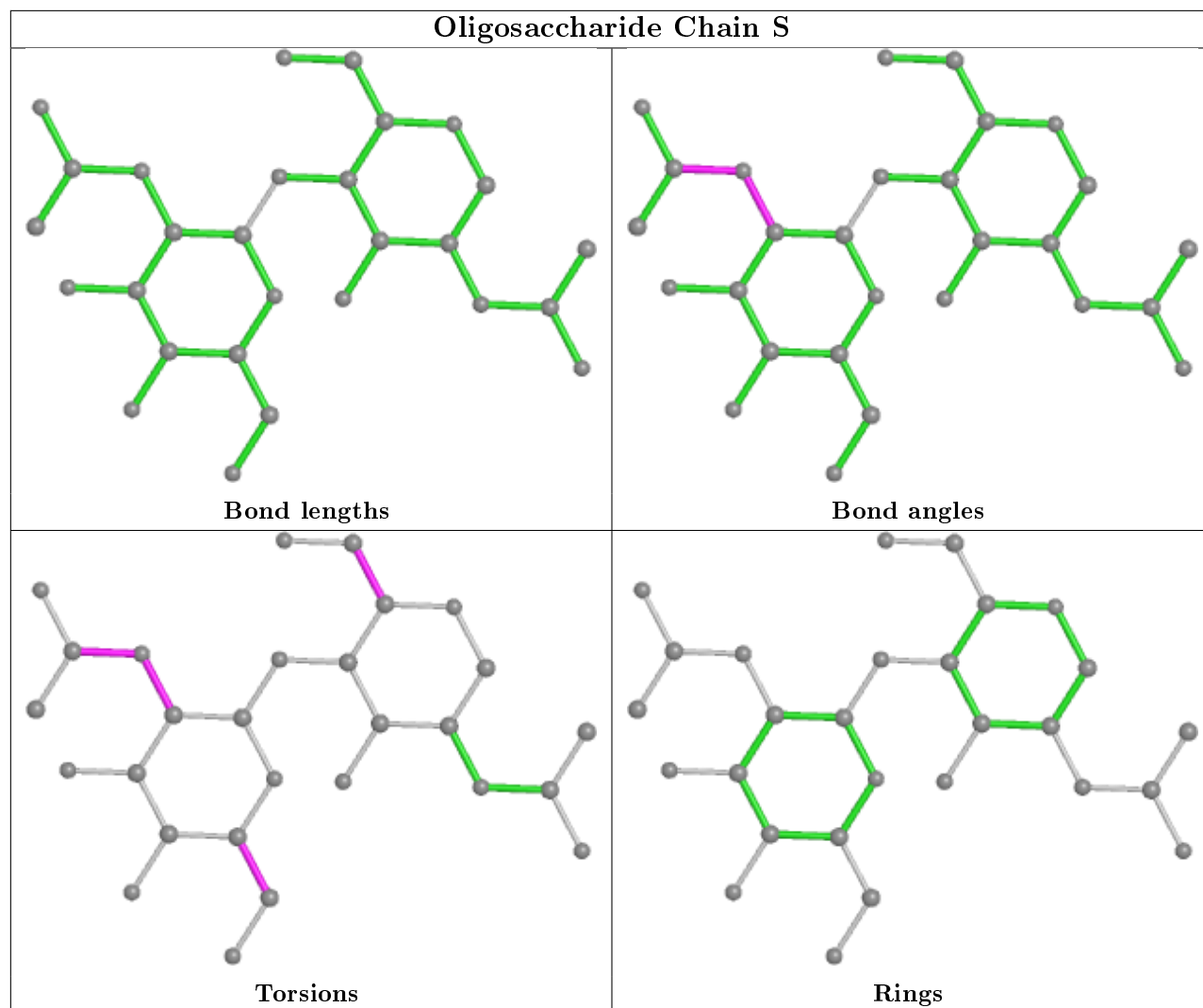
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

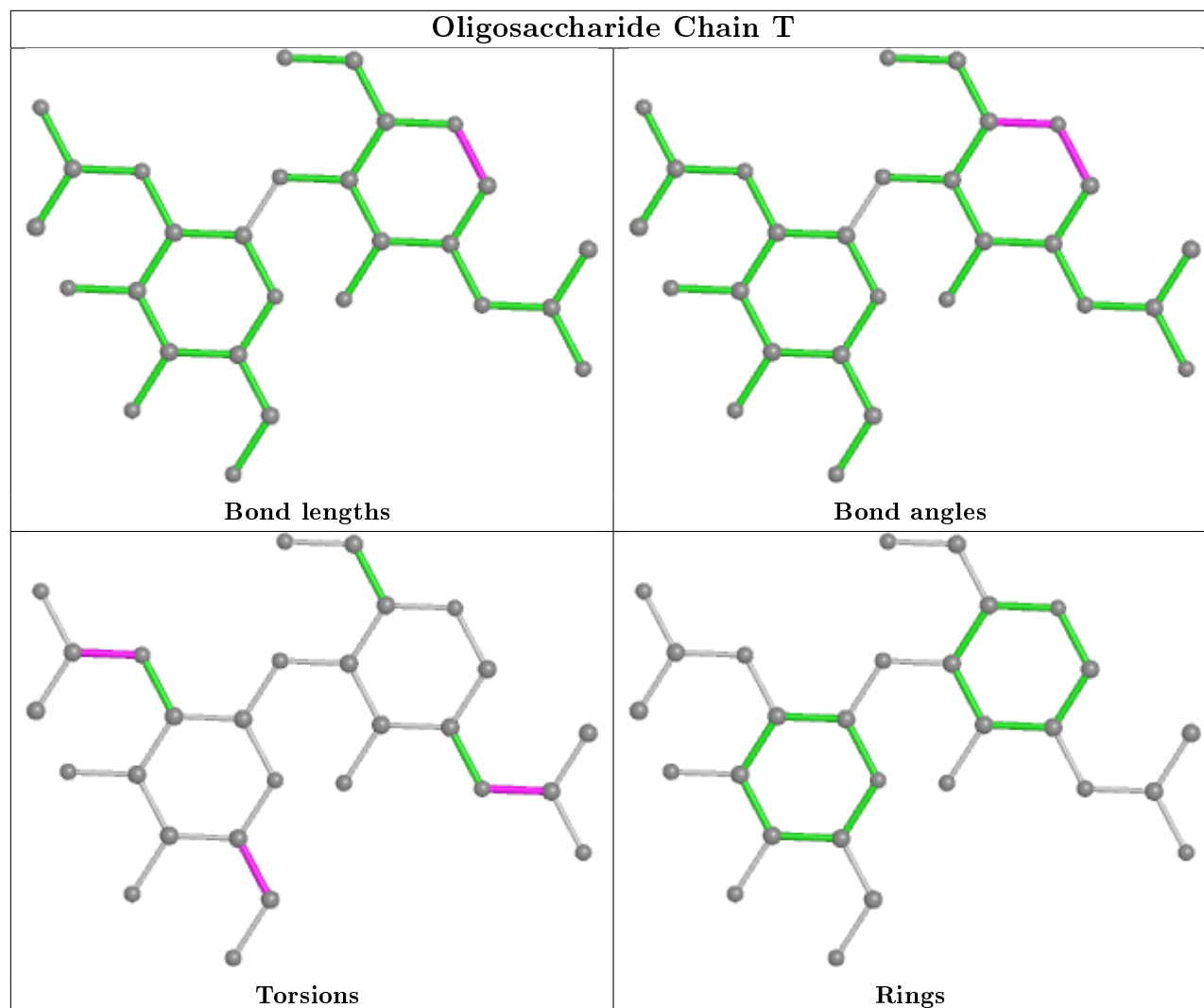


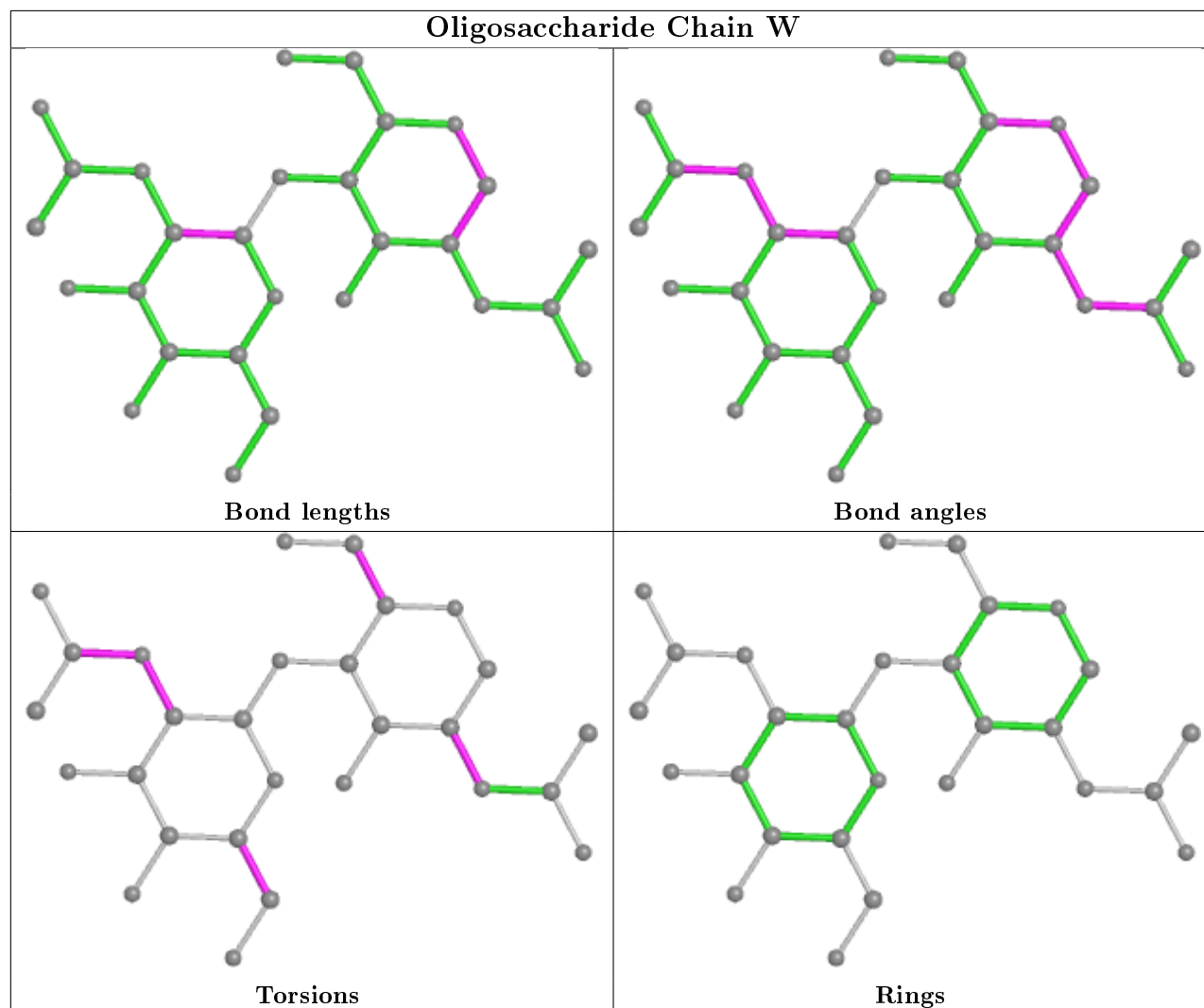


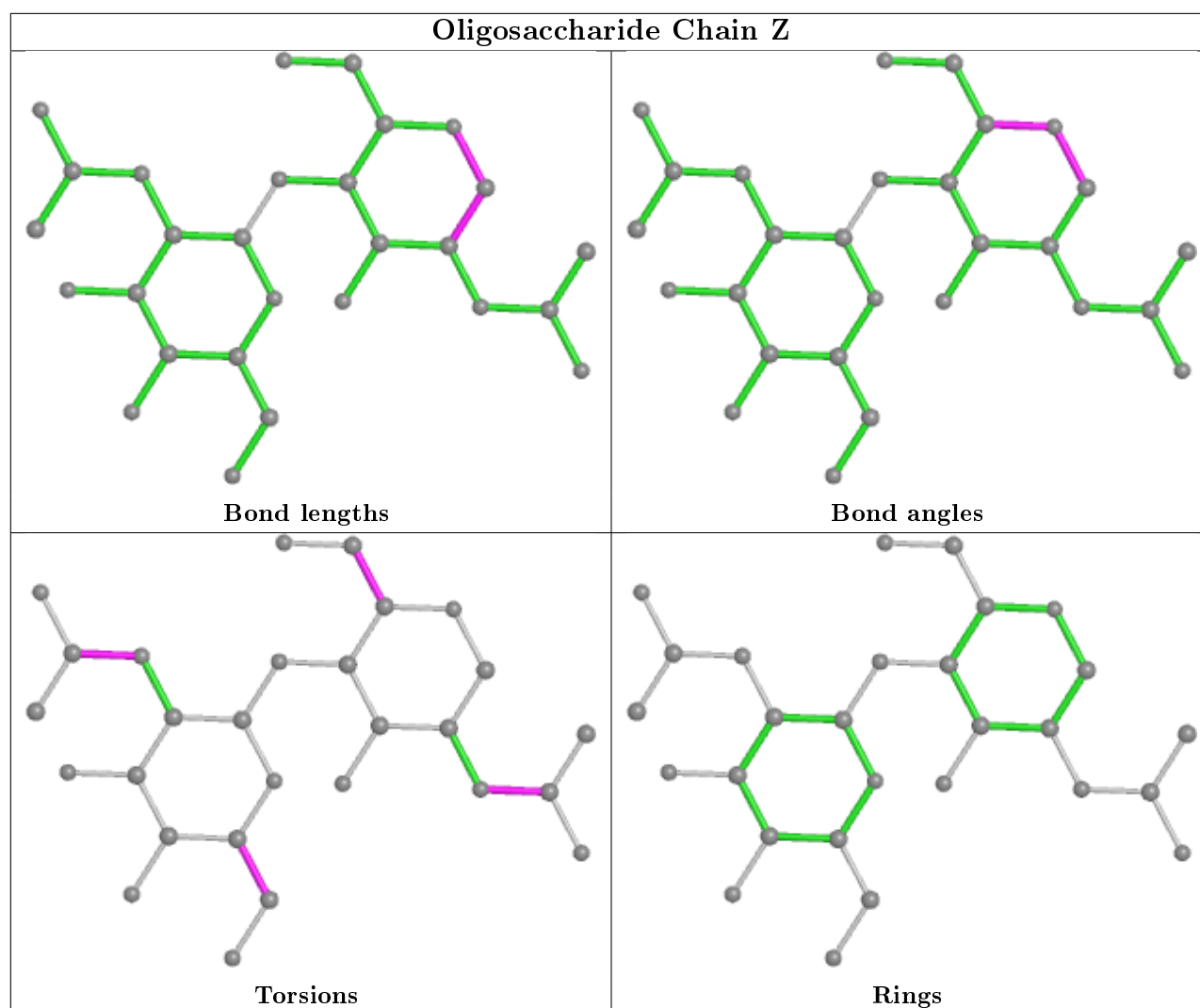












5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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	$\# Z > 2$
10	MAN	Y	511	2	11,11,12	0.82	0	15,15,17	1.60	3 (20%)
10	MAN	Y	509	2	11,11,12	0.78	0	15,15,17	1.59	3 (20%)
10	MAN	Y	503	2	11,11,12	0.80	0	15,15,17	1.62	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	V	505	2	11,11,12	0.82	0	15,15,17	1.59	3 (20%)
10	MAN	Y	510	2	11,11,12	0.80	0	15,15,17	1.59	3 (20%)
10	MAN	V	509	2	11,11,12	0.79	0	15,15,17	1.62	3 (20%)
10	MAN	V	504	2	11,11,12	0.80	0	15,15,17	1.66	3 (20%)
10	MAN	V	512	2	11,11,12	0.77	0	15,15,17	1.57	3 (20%)
10	MAN	V	503	2	11,11,12	0.78	0	15,15,17	1.63	3 (20%)
10	MAN	X	301	1	11,11,12	0.77	0	15,15,17	1.56	3 (20%)
10	MAN	V	510	2	11,11,12	0.76	0	15,15,17	1.65	3 (20%)
10	MAN	U	301	1	11,11,12	0.74	0	15,15,17	1.63	3 (20%)
10	MAN	Y	512	2	11,11,12	0.78	0	15,15,17	1.56	3 (20%)
10	MAN	Y	504	2	11,11,12	0.81	0	15,15,17	1.61	3 (20%)
10	MAN	V	511	2	11,11,12	0.80	0	15,15,17	1.63	3 (20%)
10	MAN	U	302	1	11,11,12	0.76	0	15,15,17	1.62	3 (20%)
10	MAN	X	302	1	11,11,12	0.78	0	15,15,17	1.61	3 (20%)
10	MAN	Y	505	2	11,11,12	0.77	0	15,15,17	1.62	3 (20%)

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
10	MAN	Y	511	2	-	0/2/19/22	0/1/1/1
10	MAN	Y	509	2	-	0/2/19/22	0/1/1/1
10	MAN	Y	503	2	-	0/2/19/22	0/1/1/1
10	MAN	V	505	2	-	1/2/19/22	0/1/1/1
10	MAN	Y	510	2	-	0/2/19/22	0/1/1/1
10	MAN	V	509	2	-	0/2/19/22	0/1/1/1
10	MAN	V	504	2	-	0/2/19/22	0/1/1/1
10	MAN	V	512	2	-	0/2/19/22	0/1/1/1
10	MAN	V	503	2	-	0/2/19/22	0/1/1/1
10	MAN	X	301	1	-	0/2/19/22	0/1/1/1
10	MAN	V	510	2	-	0/2/19/22	0/1/1/1
10	MAN	U	301	1	-	0/2/19/22	0/1/1/1
10	MAN	Y	512	2	-	0/2/19/22	0/1/1/1
10	MAN	Y	504	2	-	0/2/19/22	0/1/1/1
10	MAN	V	511	2	-	0/2/19/22	0/1/1/1
10	MAN	U	302	1	-	0/2/19/22	0/1/1/1
10	MAN	X	302	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	Y	505	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	504	MAN	C1-O5-C5	4.65	118.49	112.19
10	V	510	MAN	C1-O5-C5	4.63	118.47	112.19
10	V	503	MAN	C1-O5-C5	4.56	118.37	112.19
10	U	302	MAN	C1-O5-C5	4.54	118.35	112.19
10	V	509	MAN	C1-O5-C5	4.53	118.33	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	V	505	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Y	504	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	312:CYS	C	313:PRO	N	3.24

6 Fit of model and data [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

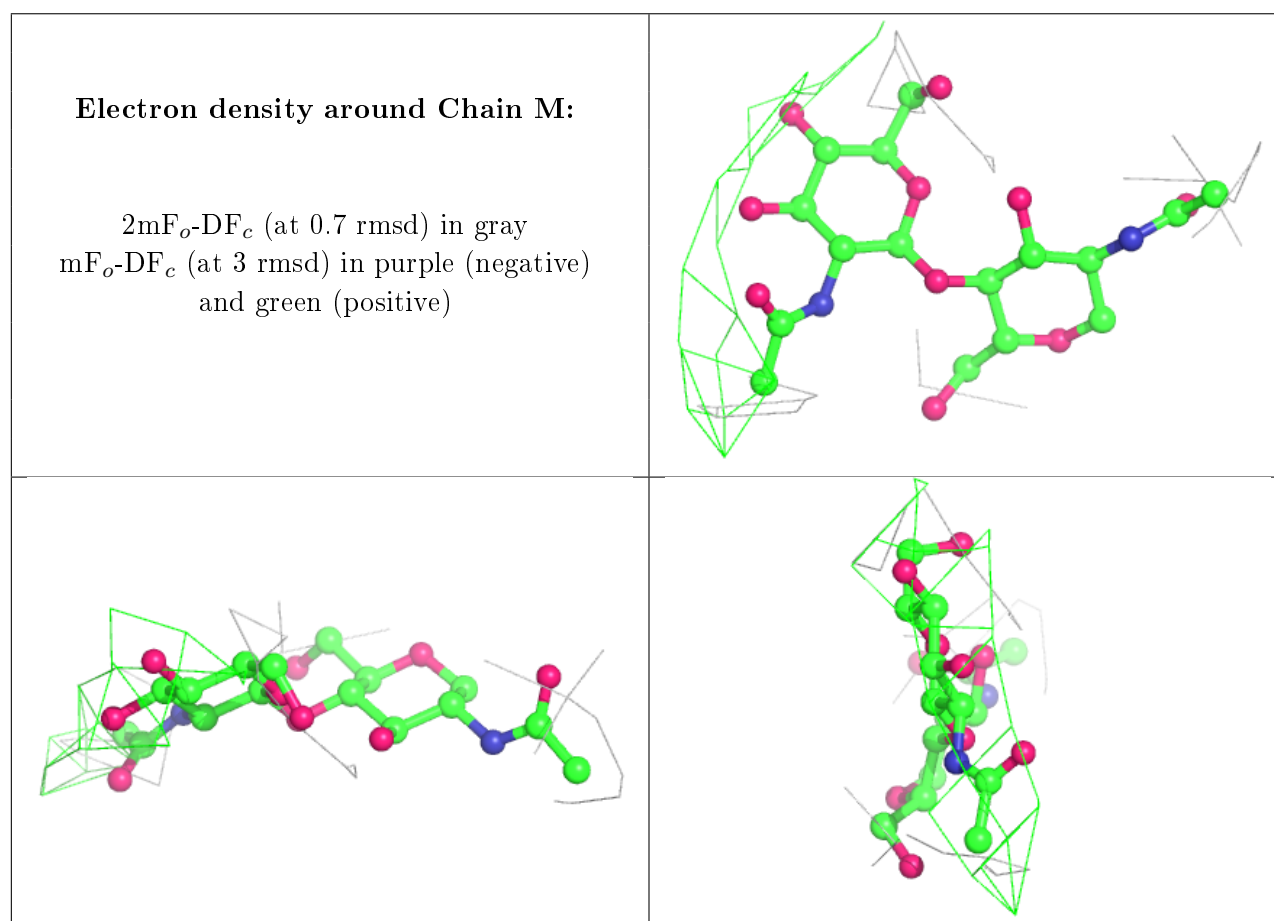
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

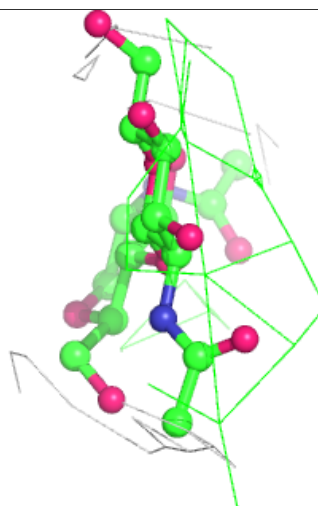
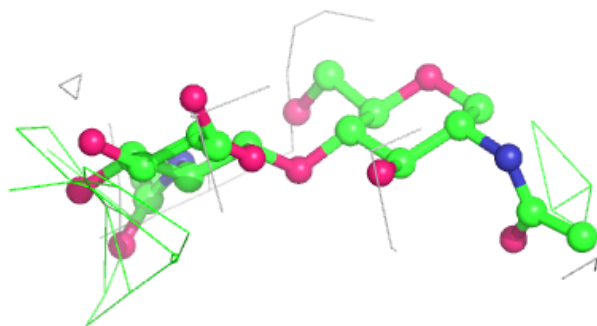
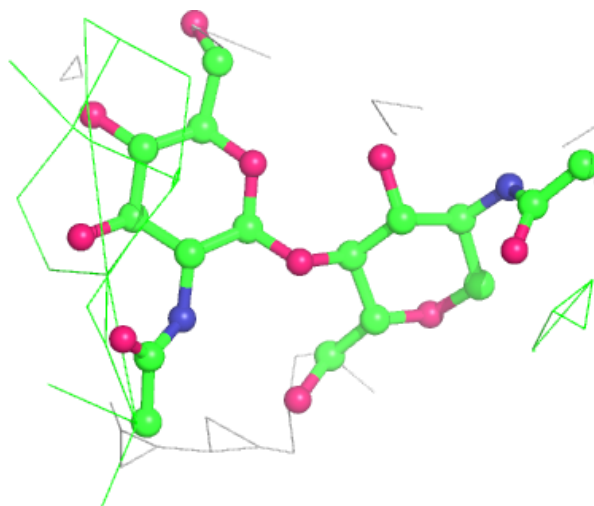
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



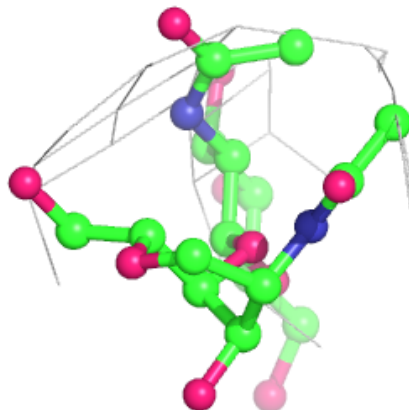
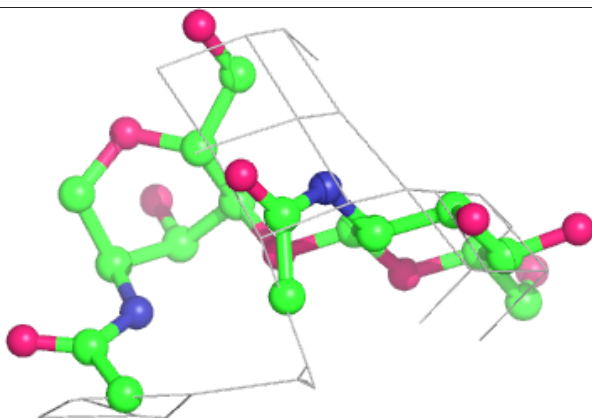
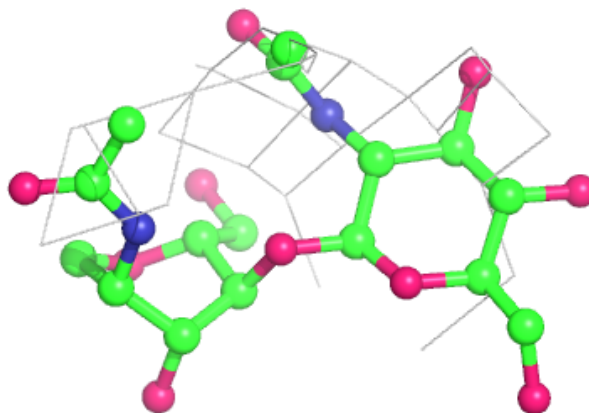
Electron density around Chain P:

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



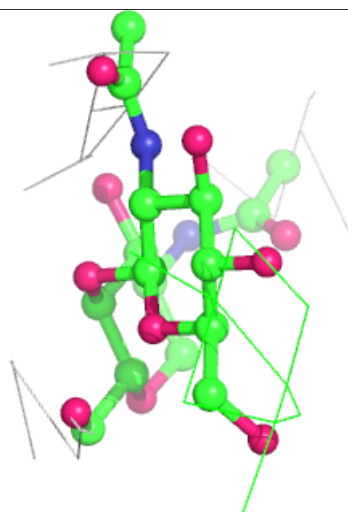
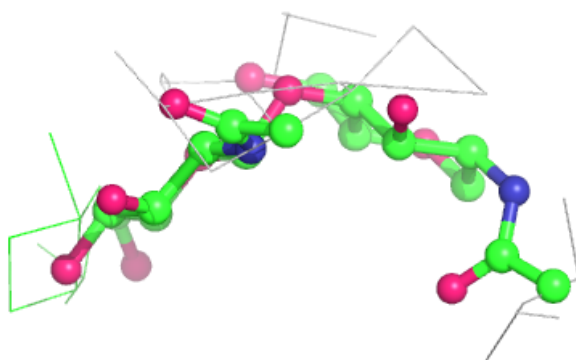
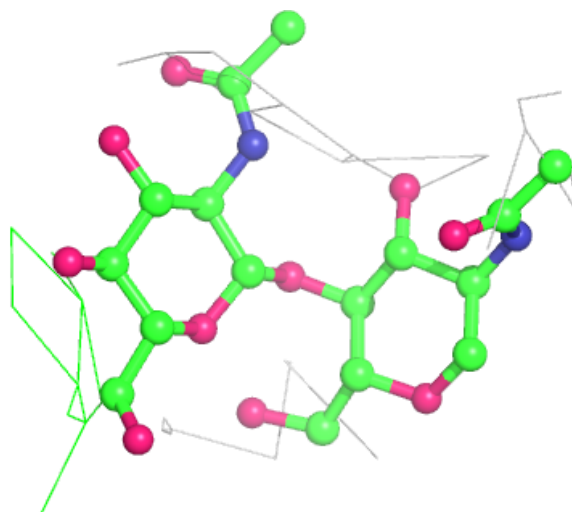
Electron density around Chain O:

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



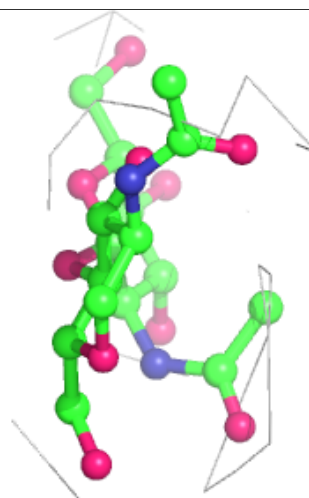
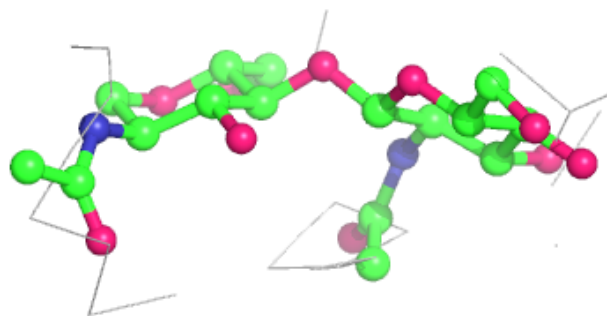
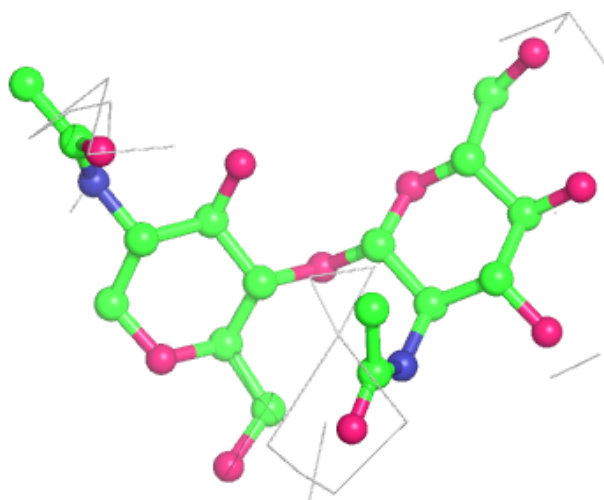
Electron density around Chain R:

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



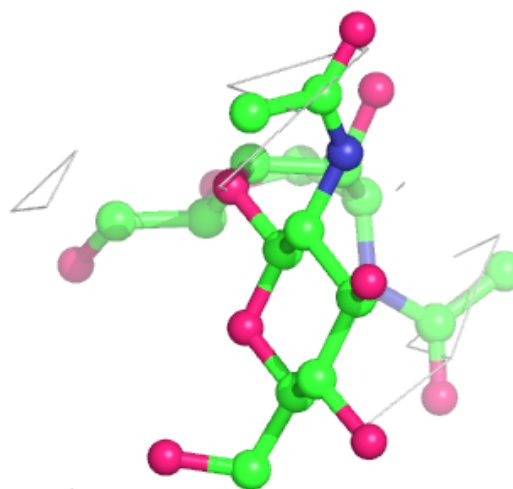
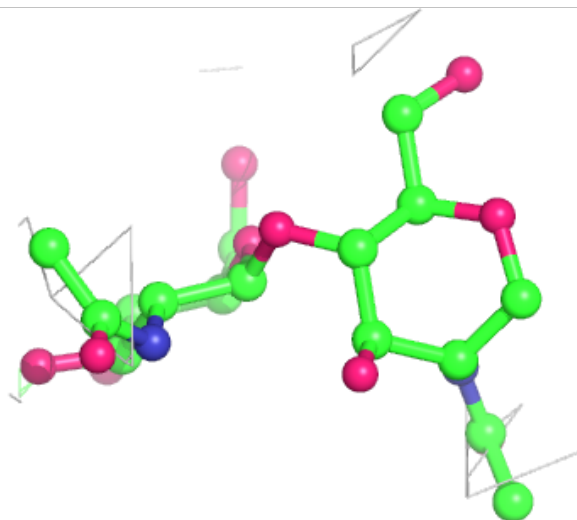
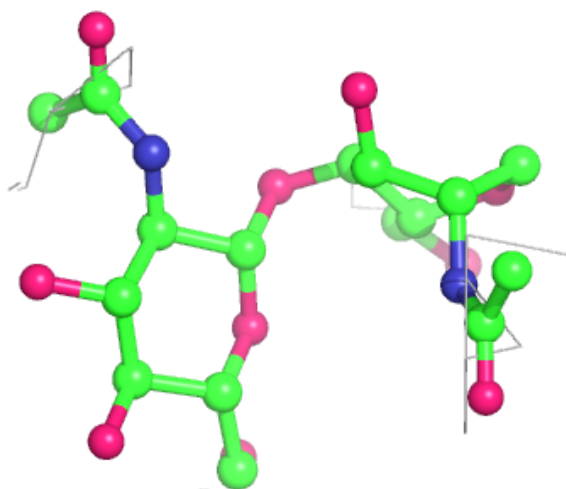
Electron density around Chain S:

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



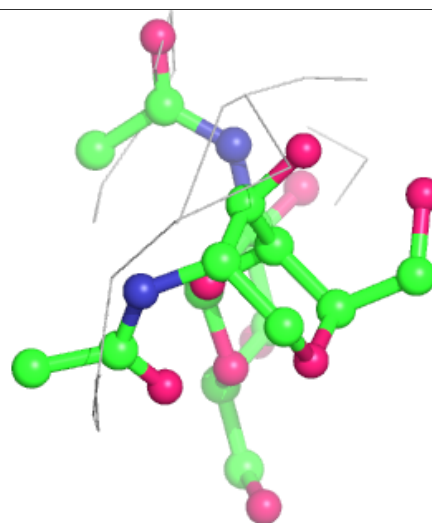
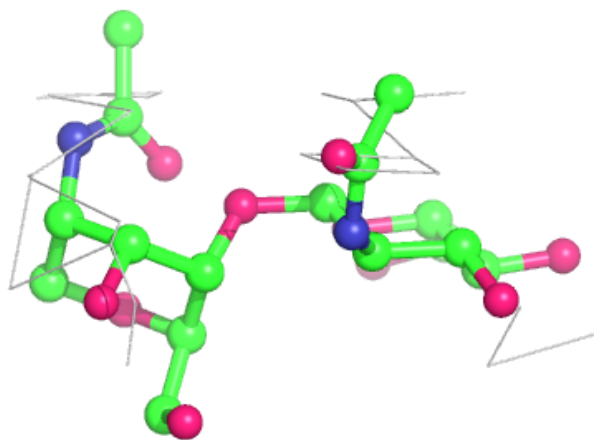
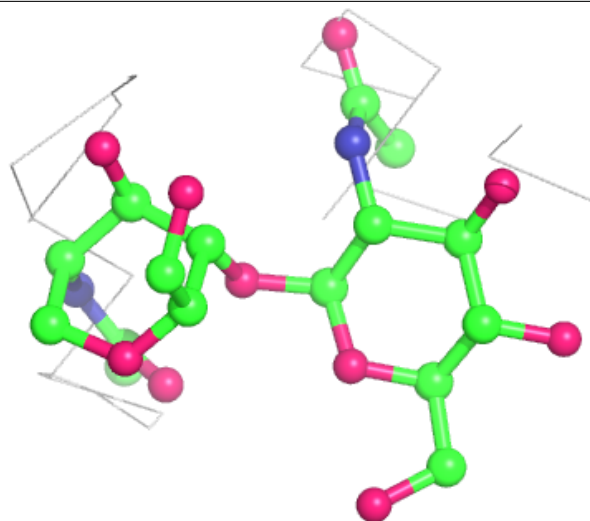
Electron density around Chain T:

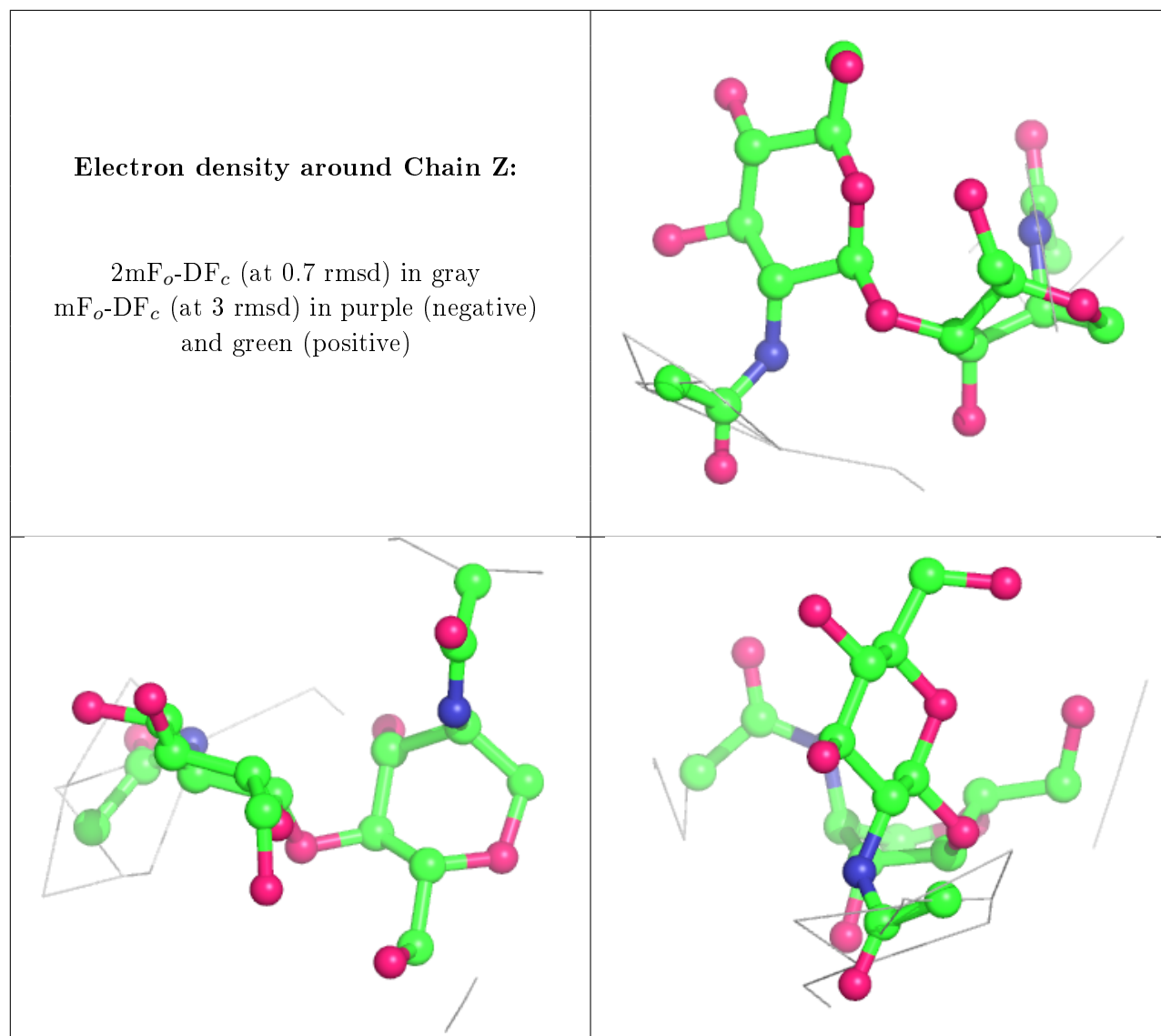
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

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





6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.