



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:14 PM UTC

PDB ID : 7A0K / pdb_00007a0k
Title : Crystal structure of the entire ectodomain from the *Physcomitrella patens* receptor kinase CR4
Authors : Hothorn, M.; Okuda, S.
Deposited on : 2020-08-09
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

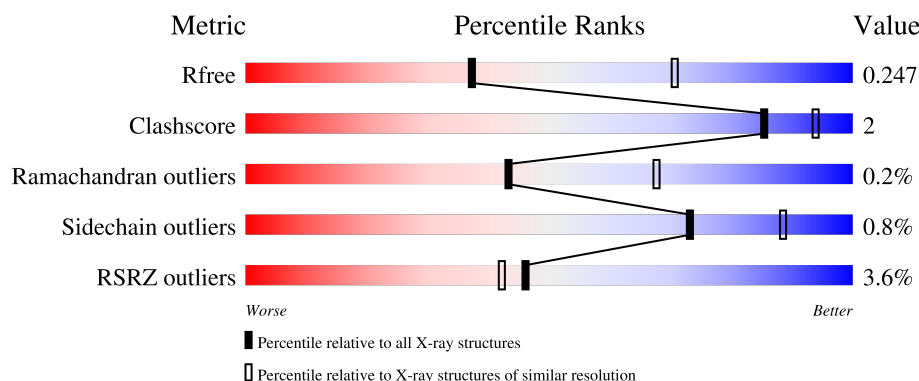
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	383	0% 91% 5% .
1	B	383	2% 89% 6% 5%
1	C	383	3% 91% . 5%
1	D	383	4% 90% 5% .
1	E	383	4% 91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	383	 3% 88% 7% 5%
1	G	383	 4% 91% 5%
1	H	383	 6% 89% 5% 7%
2	I	2	 100%
2	K	2	 50% 50%
2	M	2	 50% 50%
2	O	2	 50% 50%
2	Q	2	 50% 50%
2	S	2	 100%
2	T	2	 50% 50%
2	U	2	 100%
3	J	2	 100%
3	N	2	 100%
3	P	2	 50% 50%
3	R	2	 100%
4	L	3	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21072 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 Predicted protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2610	1639	434	505	32			
1	B	363	Total	C	N	O	S	0	0	0
			2582	1618	431	501	32			
1	C	363	Total	C	N	O	S	0	0	0
			2559	1604	429	494	32			
1	D	367	Total	C	N	O	S	0	0	0
			2576	1616	433	495	32			
1	E	367	Total	C	N	O	S	0	0	0
			2570	1611	429	498	32			
1	F	363	Total	C	N	O	S	0	0	0
			2542	1595	422	493	32			
1	G	364	Total	C	N	O	S	0	0	0
			2540	1589	423	496	32			
1	H	358	Total	C	N	O	S	0	0	0
			2435	1525	410	469	31			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	LEU	-	expression tag	UNP A9RKG8
A	407	GLU	-	expression tag	UNP A9RKG8
A	408	ASN	-	expression tag	UNP A9RKG8
A	409	LEU	-	expression tag	UNP A9RKG8
A	410	TYR	-	expression tag	UNP A9RKG8
A	411	PHE	-	expression tag	UNP A9RKG8
A	412	GLN	-	expression tag	UNP A9RKG8
B	406	LEU	-	expression tag	UNP A9RKG8
B	407	GLU	-	expression tag	UNP A9RKG8
B	408	ASN	-	expression tag	UNP A9RKG8
B	409	LEU	-	expression tag	UNP A9RKG8
B	410	TYR	-	expression tag	UNP A9RKG8
B	411	PHE	-	expression tag	UNP A9RKG8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	412	GLN	-	expression tag	UNP A9RKG8
C	406	LEU	-	expression tag	UNP A9RKG8
C	407	GLU	-	expression tag	UNP A9RKG8
C	408	ASN	-	expression tag	UNP A9RKG8
C	409	LEU	-	expression tag	UNP A9RKG8
C	410	TYR	-	expression tag	UNP A9RKG8
C	411	PHE	-	expression tag	UNP A9RKG8
C	412	GLN	-	expression tag	UNP A9RKG8
D	406	LEU	-	expression tag	UNP A9RKG8
D	407	GLU	-	expression tag	UNP A9RKG8
D	408	ASN	-	expression tag	UNP A9RKG8
D	409	LEU	-	expression tag	UNP A9RKG8
D	410	TYR	-	expression tag	UNP A9RKG8
D	411	PHE	-	expression tag	UNP A9RKG8
D	412	GLN	-	expression tag	UNP A9RKG8
E	406	LEU	-	expression tag	UNP A9RKG8
E	407	GLU	-	expression tag	UNP A9RKG8
E	408	ASN	-	expression tag	UNP A9RKG8
E	409	LEU	-	expression tag	UNP A9RKG8
E	410	TYR	-	expression tag	UNP A9RKG8
E	411	PHE	-	expression tag	UNP A9RKG8
E	412	GLN	-	expression tag	UNP A9RKG8
F	406	LEU	-	expression tag	UNP A9RKG8
F	407	GLU	-	expression tag	UNP A9RKG8
F	408	ASN	-	expression tag	UNP A9RKG8
F	409	LEU	-	expression tag	UNP A9RKG8
F	410	TYR	-	expression tag	UNP A9RKG8
F	411	PHE	-	expression tag	UNP A9RKG8
F	412	GLN	-	expression tag	UNP A9RKG8
G	406	LEU	-	expression tag	UNP A9RKG8
G	407	GLU	-	expression tag	UNP A9RKG8
G	408	ASN	-	expression tag	UNP A9RKG8
G	409	LEU	-	expression tag	UNP A9RKG8
G	410	TYR	-	expression tag	UNP A9RKG8
G	411	PHE	-	expression tag	UNP A9RKG8
G	412	GLN	-	expression tag	UNP A9RKG8
H	406	LEU	-	expression tag	UNP A9RKG8
H	407	GLU	-	expression tag	UNP A9RKG8
H	408	ASN	-	expression tag	UNP A9RKG8
H	409	LEU	-	expression tag	UNP A9RKG8
H	410	TYR	-	expression tag	UNP A9RKG8
H	411	PHE	-	expression tag	UNP A9RKG8

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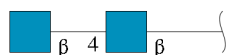
Chain	Residue	Modelled	Actual	Comment	Reference
H	412	GLN	-	expression tag	UNP A9RKG8

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	M	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	O	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	S	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	T	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	U	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



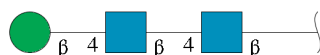
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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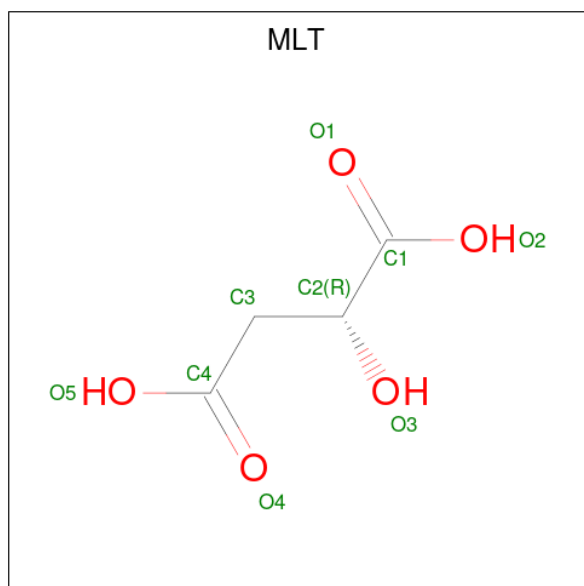
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



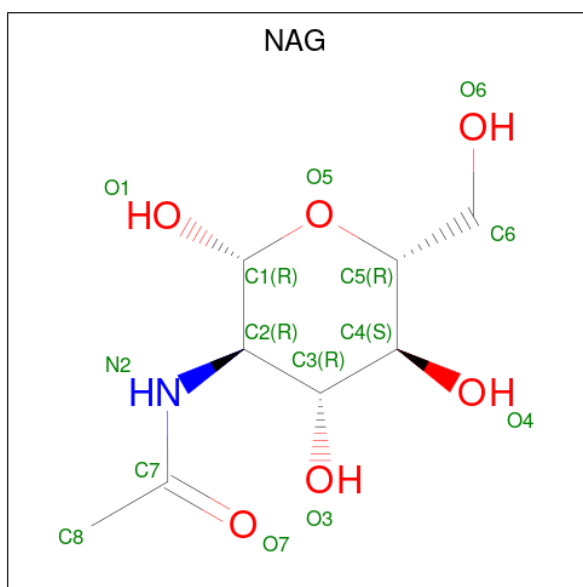
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is D-MALATE (CCD ID: MLT) (formula: C₄H₆O₅).



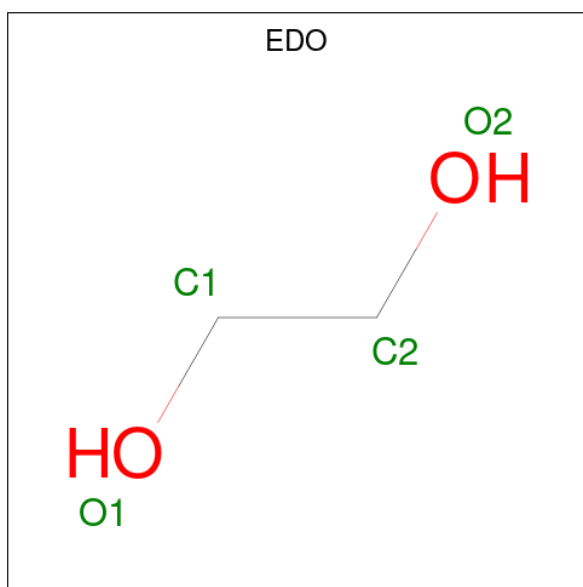
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	32	Total O 32 32	0	0
8	B	42	Total O 42 42	0	0
8	C	10	Total O 10 10	0	0
8	D	9	Total O 9 9	0	0

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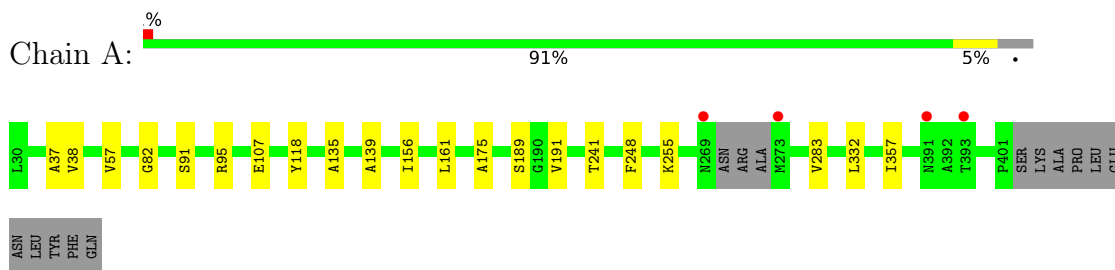
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	14	Total 14	O 14	0	0
8	F	4	Total 4	O 4	0	0
8	G	14	Total 14	O 14	0	0
8	H	9	Total 9	O 9	0	0

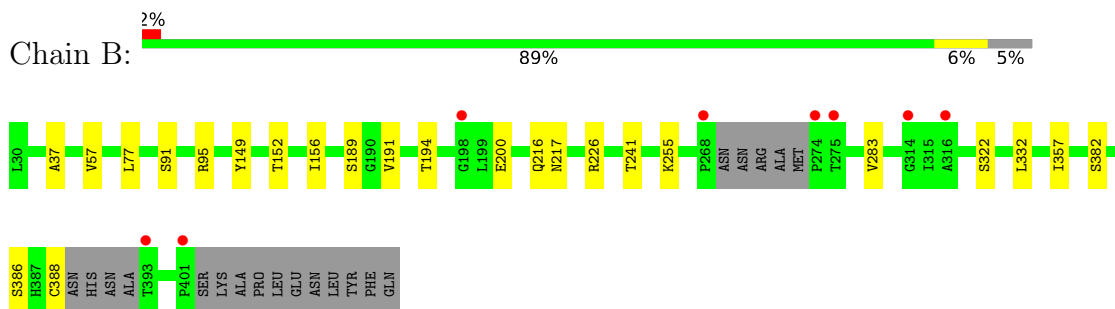
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

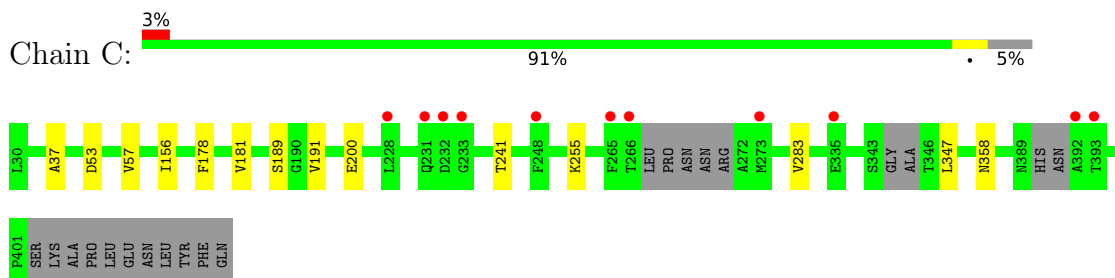
- Molecule 1: Predicted protein



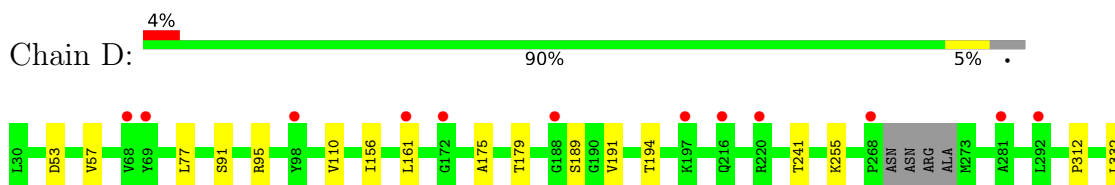
- Molecule 1: Predicted protein

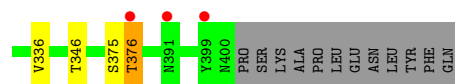


- Molecule 1: Predicted protein

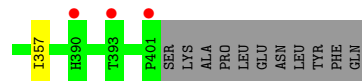
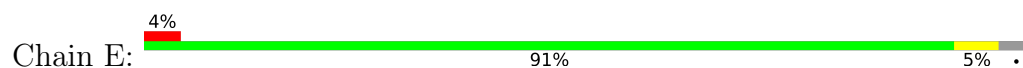


- Molecule 1: Predicted protein

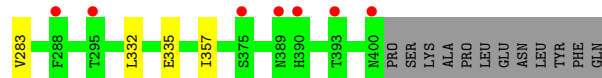
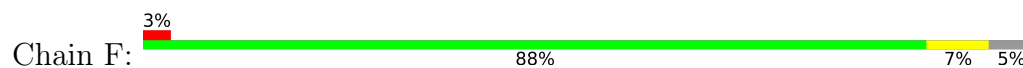




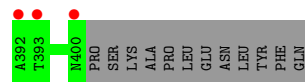
- Molecule 1: Predicted protein



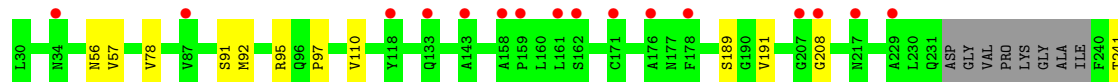
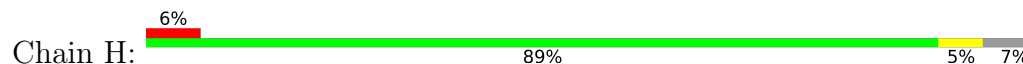
- Molecule 1: Predicted protein



- Molecule 1: Predicted protein



- Molecule 1: Predicted protein



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





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

Chain K:



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

Chain M:



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

Chain O:



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

Chain Q:



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

Chain S:



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

Chain T:



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

Chain U:



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

Chain J:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.58Å 183.96Å 98.17Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	45.87 – 2.70 45.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.87-2.70) 90.3 (45.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.216 , 0.246 0.218 , 0.247	Depositor DCC
R_{free} test set	4283 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21072	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: EDO, BMA, MLT, NAG, FUC

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	0.10	0/2678	0.33	0/3662
1	B	0.16	0/2649	0.40	0/3620
1	C	0.13	0/2624	0.36	0/3588
1	D	0.12	0/2642	0.34	0/3616
1	E	0.13	0/2636	0.37	0/3608
1	F	0.11	0/2608	0.33	0/3569
1	G	0.14	0/2605	0.35	0/3566
1	H	0.11	0/2498	0.33	0/3427
All	All	0.13	0/20940	0.35	0/28656

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	2610	0	2431	15	0
1	B	2582	0	2408	15	0
1	C	2559	0	2358	6	0
1	D	2576	0	2385	13	0
1	E	2570	0	2371	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2542	0	2330	21	0
1	G	2540	0	2318	9	0
1	H	2435	0	2145	11	0
2	I	24	0	22	0	0
2	K	24	0	22	0	0
2	M	24	0	22	0	0
2	O	24	0	22	1	0
2	Q	24	0	22	0	0
2	S	24	0	22	0	0
2	T	24	0	22	0	0
2	U	24	0	22	0	0
3	J	28	0	25	0	0
3	N	28	0	25	0	0
3	P	28	0	25	1	0
3	R	28	0	25	0	0
4	L	39	0	34	0	0
5	A	9	0	4	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	1	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
6	G	28	0	26	1	0
6	H	28	0	26	0	0
7	A	12	0	18	4	0
7	B	12	0	18	0	0
7	C	4	0	6	0	0
7	G	4	0	6	0	0
8	A	32	0	0	0	0
8	B	42	0	0	0	0
8	C	10	0	0	0	0
8	D	9	0	0	0	0
8	E	14	0	0	0	0
8	F	4	0	0	1	0
8	G	14	0	0	0	0
8	H	9	0	0	0	0
All	All	21072	0	19238	88	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 2.

The worst 5 of 88 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:F:200:GLU:OE2	1:F:216:GLN:NE2	2.24	0.70
1:A:135:ALA:HB1	1:B:382:SER:HB2	1.75	0.69
1:B:226:ARG:HG2	2:O:2:FUC:H62	1.81	0.62
1:F:332:LEU:HB2	1:F:357:ILE:CD1	2.29	0.62
1:F:241:THR:HG23	1:F:255:LYS:HA	1.85	0.59

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/383 (95%)	350 (96%)	14 (4%)	1 (0%)	36	60
1	B	357/383 (93%)	348 (98%)	8 (2%)	1 (0%)	36	60
1	C	355/383 (93%)	338 (95%)	16 (4%)	1 (0%)	36	60
1	D	363/383 (95%)	352 (97%)	10 (3%)	1 (0%)	36	60
1	E	363/383 (95%)	346 (95%)	17 (5%)	0	100	100
1	F	359/383 (94%)	345 (96%)	13 (4%)	1 (0%)	36	60
1	G	360/383 (94%)	344 (96%)	15 (4%)	1 (0%)	36	60
1	H	352/383 (92%)	339 (96%)	13 (4%)	0	100	100
All	All	2874/3064 (94%)	2762 (96%)	106 (4%)	6 (0%)	43	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ILE
1	B	156	ILE
1	C	156	ILE
1	D	156	ILE
1	F	156	ILE

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	278/301 (92%)	277 (100%)	1 (0%)	84	93
1	B	278/301 (92%)	276 (99%)	2 (1%)	76	90
1	C	269/301 (89%)	266 (99%)	3 (1%)	65	85
1	D	270/301 (90%)	267 (99%)	3 (1%)	65	85
1	E	270/301 (90%)	265 (98%)	5 (2%)	50	77
1	F	265/301 (88%)	263 (99%)	2 (1%)	73	88
1	G	265/301 (88%)	264 (100%)	1 (0%)	84	93
1	H	237/301 (79%)	236 (100%)	1 (0%)	84	93
All	All	2132/2408 (88%)	2114 (99%)	18 (1%)	73	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	57	VAL
1	H	57	VAL
1	G	194	THR
1	D	376	THR
1	E	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	157	ASN
1	F	219	GLN
1	H	56	ASN
1	F	157	ASN
1	F	231	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 ⓘ

27 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	$\# Z > 2$
2	NAG	I	1	2,1	14,14,15	0.51	0	17,19,21	0.42	0
2	FUC	I	2	2	10,10,11	0.64	0	14,14,16	0.70	0
3	NAG	J	1	3,1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.39	0
2	NAG	K	1	2,1	14,14,15	0.55	0	17,19,21	0.46	0
2	FUC	K	2	2	10,10,11	0.86	1 (10%)	14,14,16	0.91	1 (7%)
4	NAG	L	1	4,1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	L	2	4	14,14,15	0.20	0	17,19,21	0.47	0
4	BMA	L	3	4	11,11,12	0.78	0	15,15,17	0.79	0
2	NAG	M	1	2,1	14,14,15	0.60	1 (7%)	17,19,21	0.47	0
2	FUC	M	2	2	10,10,11	0.80	0	14,14,16	0.79	0
3	NAG	N	1	3,1	14,14,15	0.22	0	17,19,21	0.37	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	O	1	2,1	14,14,15	0.37	0	17,19,21	0.46	0
2	FUC	O	2	2	10,10,11	0.77	0	14,14,16	0.69	0
3	NAG	P	1	3,1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	P	2	3	14,14,15	0.27	0	17,19,21	0.61	0
2	NAG	Q	1	2,1	14,14,15	0.63	1 (7%)	17,19,21	0.48	0
2	FUC	Q	2	2	10,10,11	0.66	0	14,14,16	0.75	0
3	NAG	R	1	3,1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	R	2	3	14,14,15	0.24	0	17,19,21	0.52	0
2	NAG	S	1	2,1	14,14,15	0.65	1 (7%)	17,19,21	0.50	0
2	FUC	S	2	2	10,10,11	1.82	1 (10%)	14,14,16	2.06	5 (35%)
2	NAG	T	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	0.50	0
2	FUC	T	2	2	10,10,11	0.66	0	14,14,16	0.88	0
2	NAG	U	1	2,1	14,14,15	0.38	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	U	2	2	10,10,11	0.61	0	14,14,16	0.74	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
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	3/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	S	2	2	-	-	0/1/1/1
2	NAG	T	1	2,1	-	3/6/23/26	0/1/1/1
2	FUC	T	2	2	-	-	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	U	2	2	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	2	FUC	O5-C5	4.35	1.52	1.43
2	T	1	NAG	C1-C2	2.47	1.55	1.52
2	Q	1	NAG	C1-C2	2.13	1.55	1.52
2	K	2	FUC	C1-C2	2.13	1.57	1.52
2	S	1	NAG	C1-C2	2.06	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	2	FUC	C1-O5-C5	3.71	121.71	112.97
2	S	2	FUC	O5-C5-C4	3.55	115.95	109.55
2	S	2	FUC	O3-C3-C4	-2.88	103.58	110.38
2	S	2	FUC	C6-C5-C4	-2.83	107.91	113.08
2	S	2	FUC	C2-C3-C4	-2.33	106.77	110.86

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

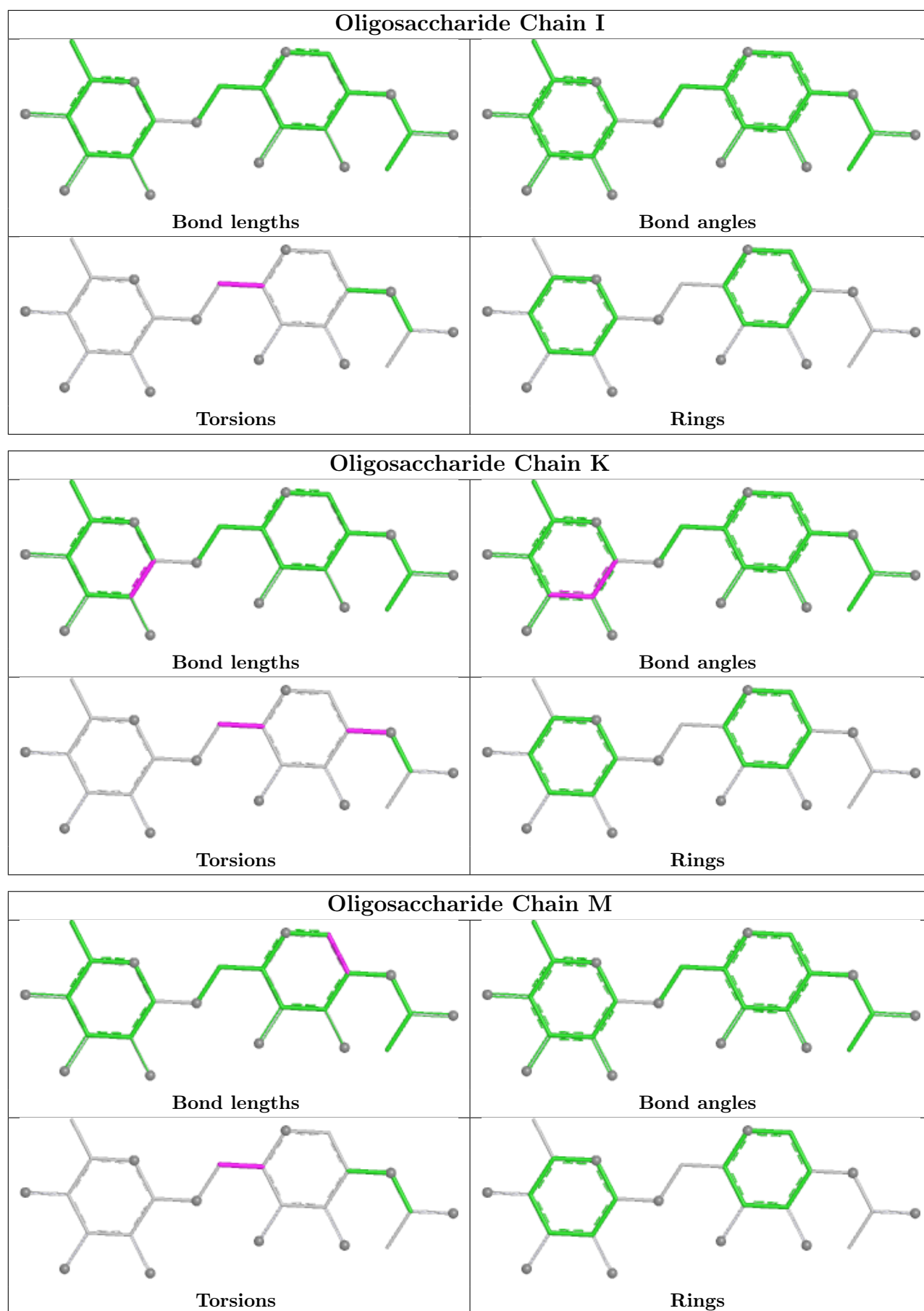
Mol	Chain	Res	Type	Atoms
2	M	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6

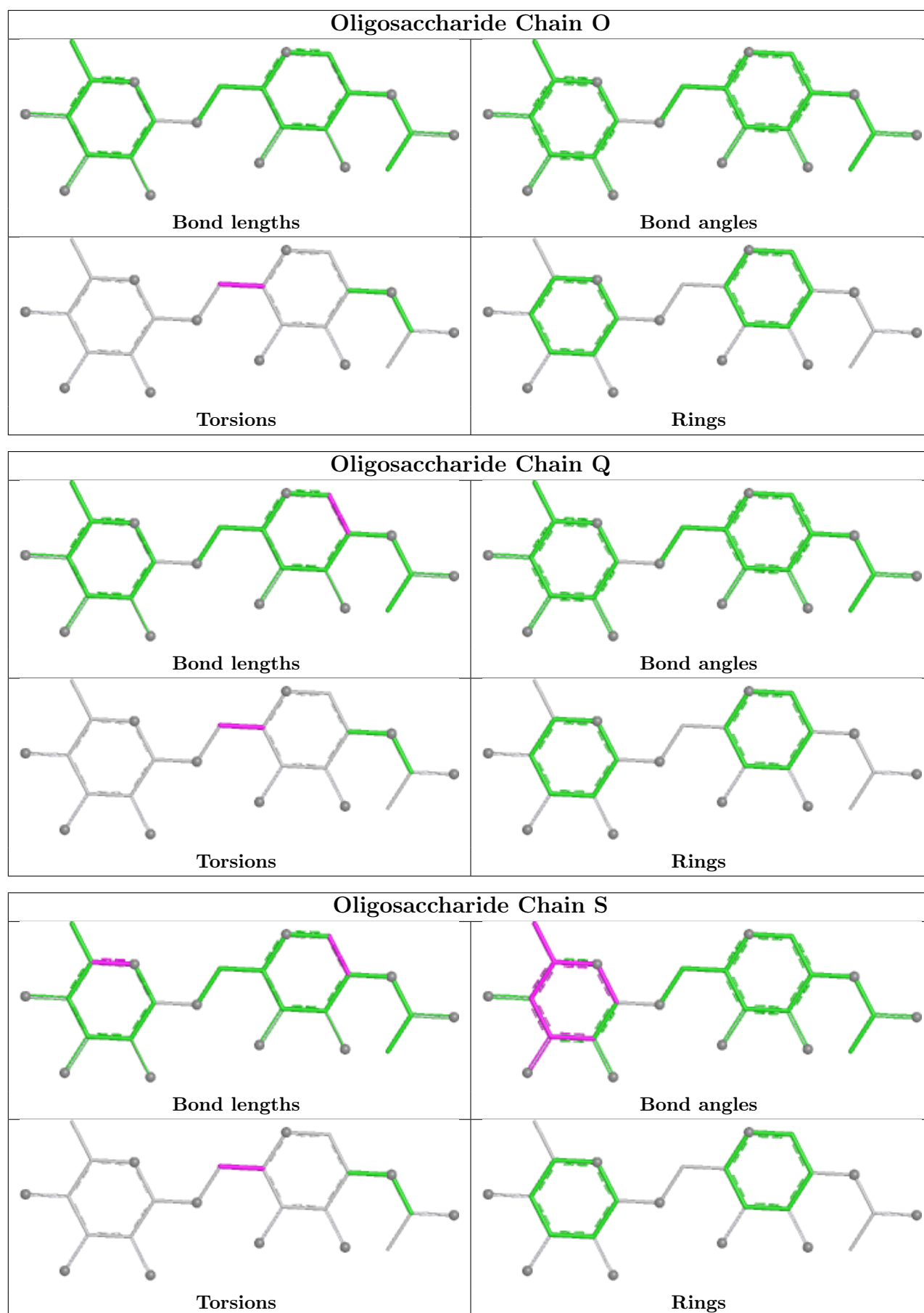
There are no ring outliers.

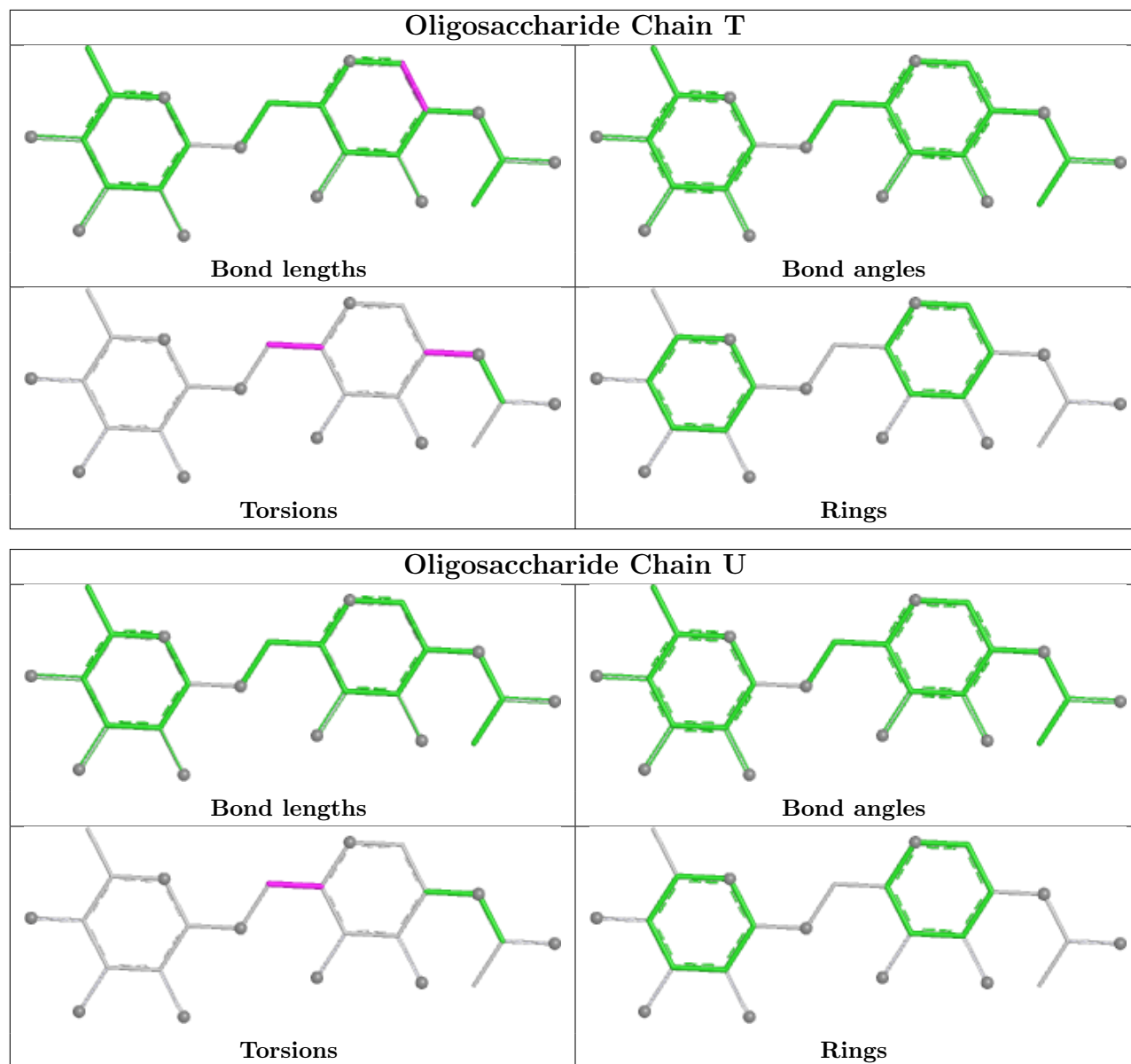
2 monomers are involved in 2 short contacts:

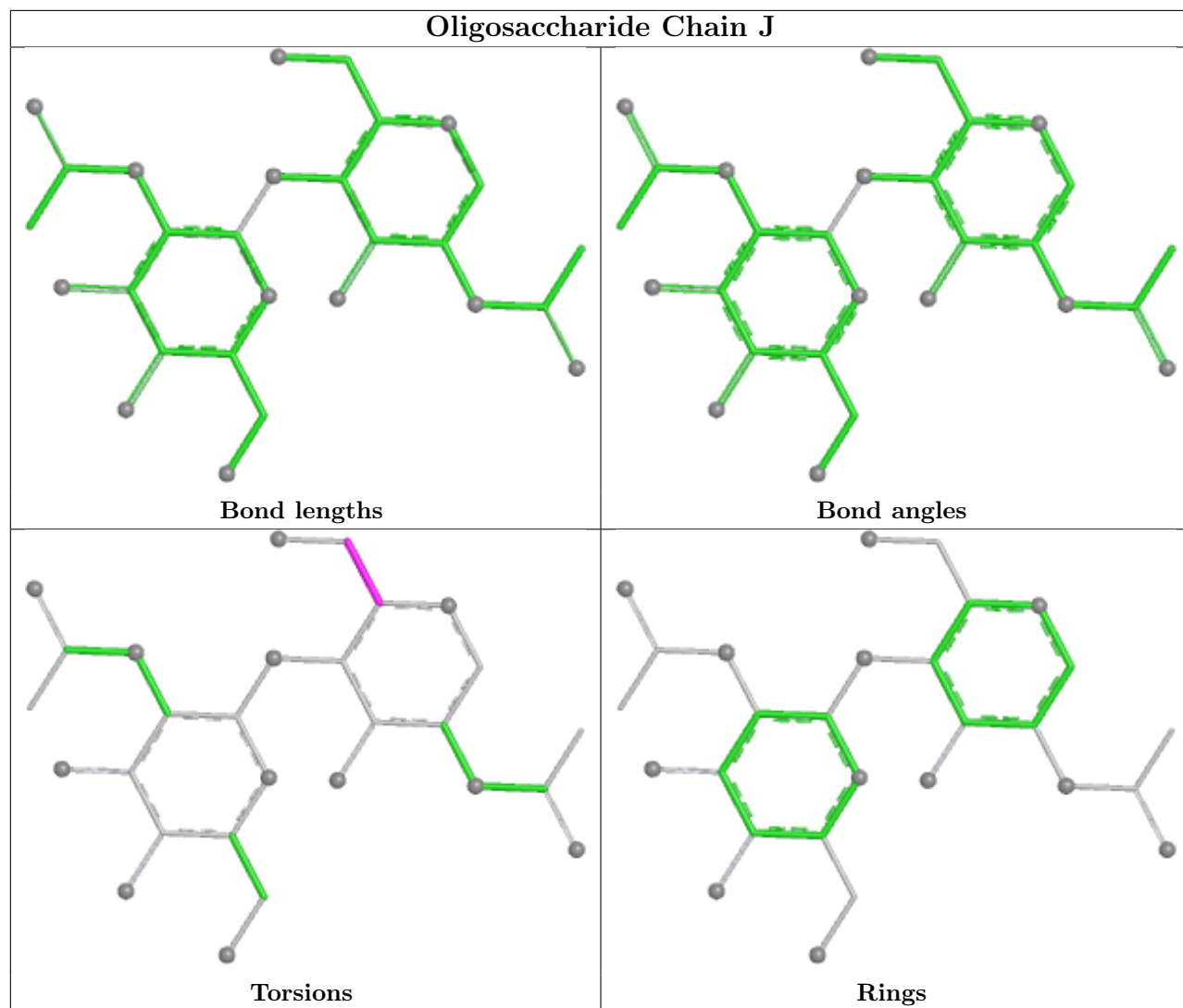
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
2	O	2	FUC	1	0

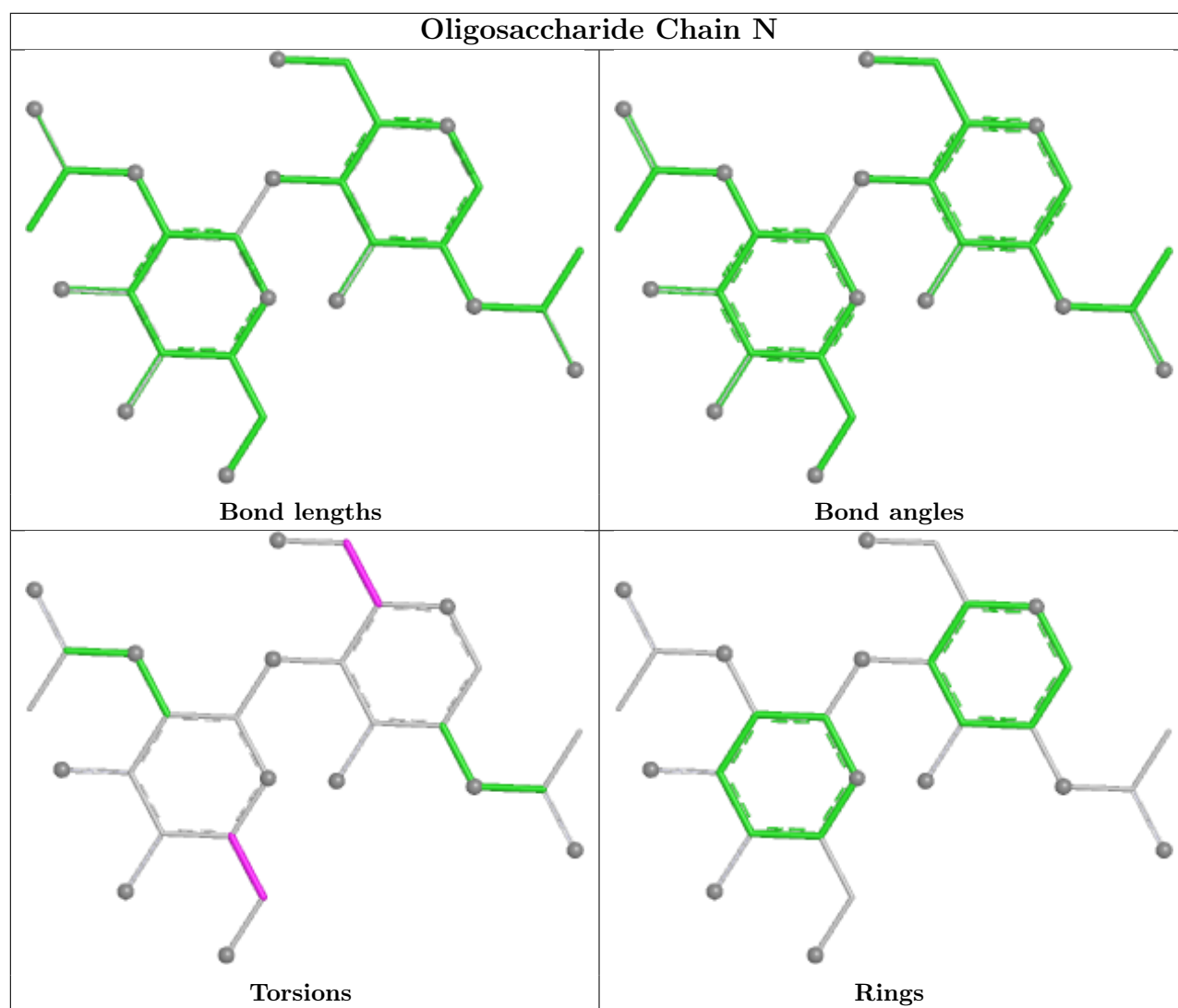
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

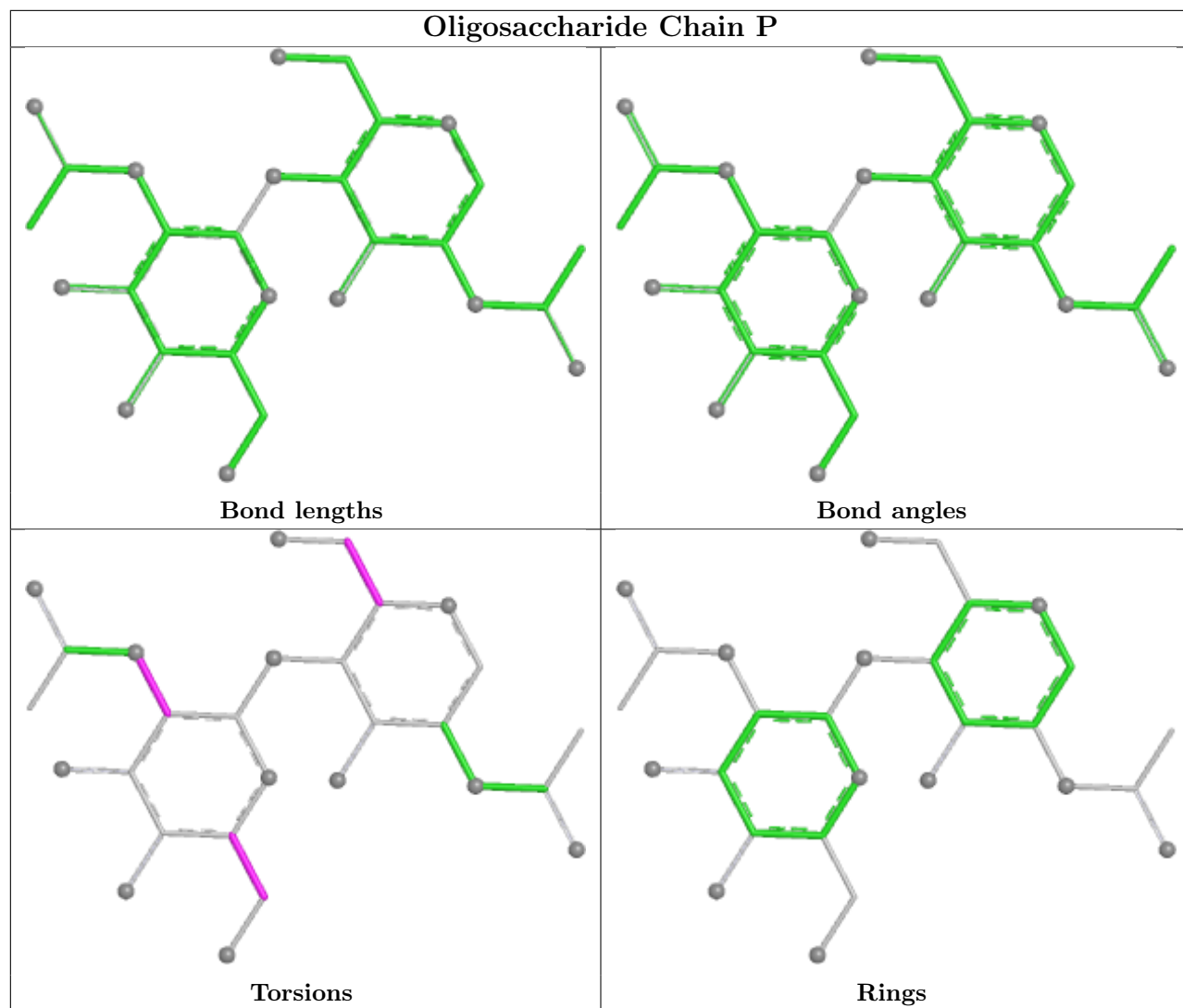


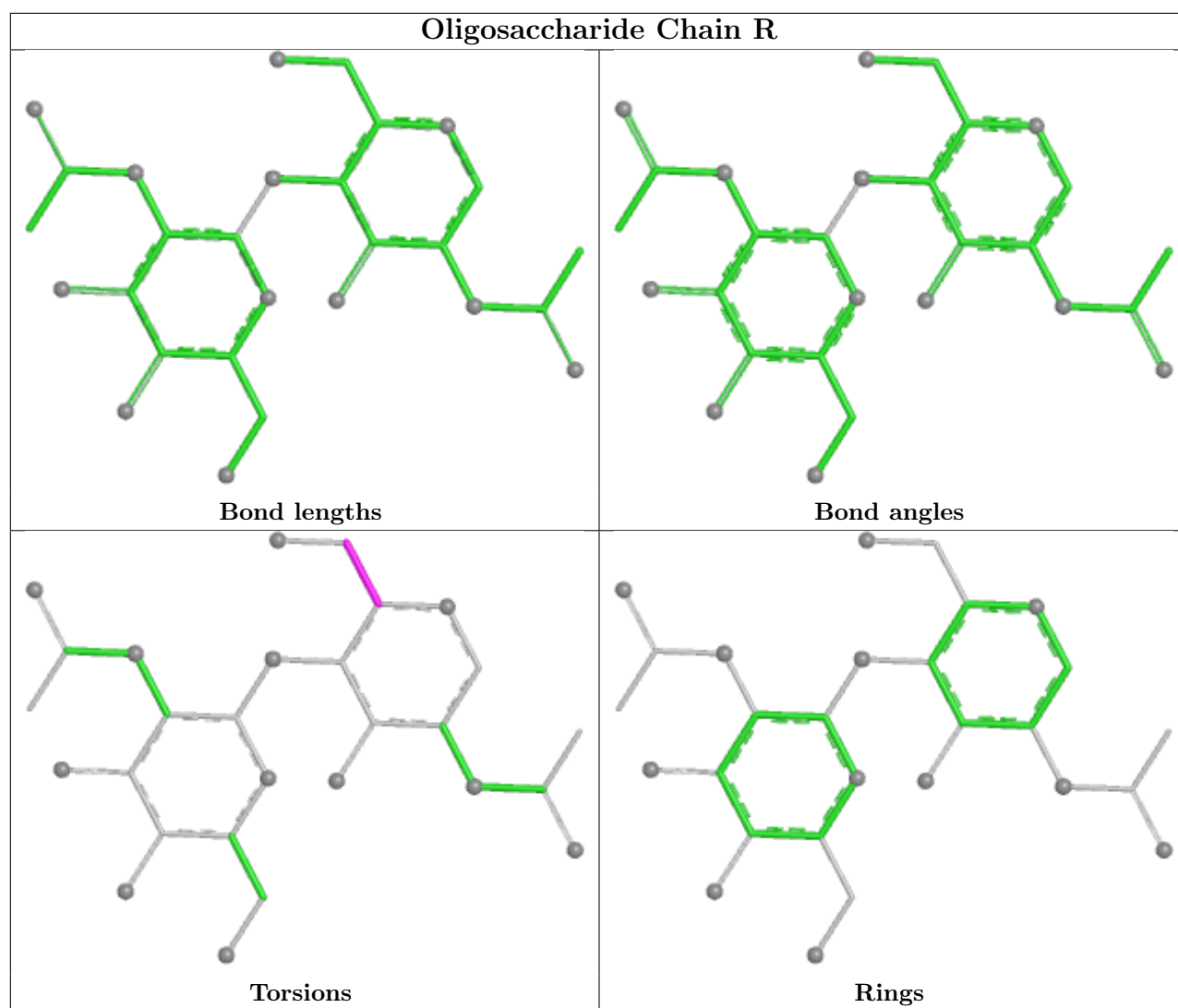


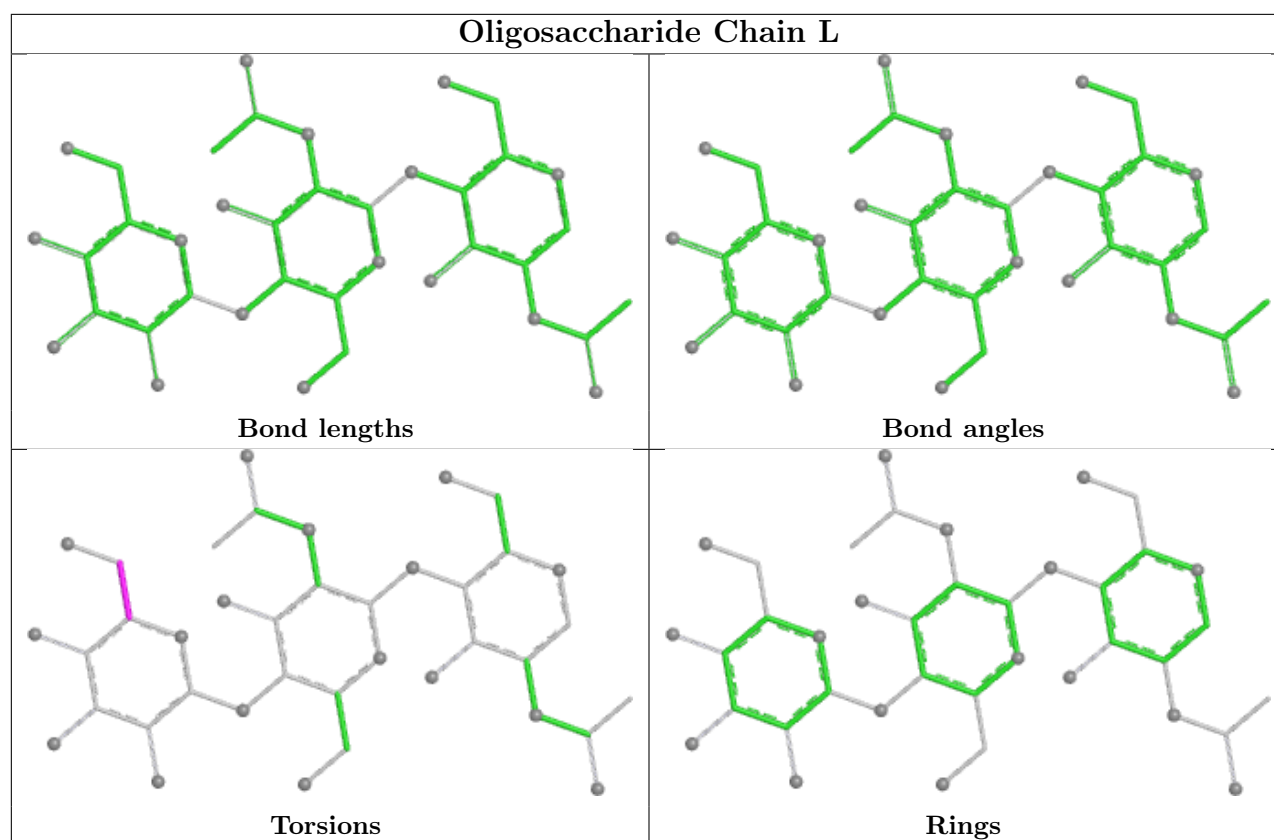












5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
6	NAG	E	501	1	14,14,15	0.30	0	17,19,21	0.47	0
6	NAG	H	502	1	14,14,15	0.28	0	17,19,21	0.43	0
7	EDO	A	504	-	3,3,3	0.37	0	2,2,2	0.15	0
5	MLT	A	501	-	8,8,8	1.10	0	10,10,10	1.64	2 (20%)
7	EDO	G	503	-	3,3,3	0.41	0	2,2,2	0.37	0
6	NAG	G	501	1	14,14,15	0.29	0	17,19,21	0.48	0
6	NAG	G	502	1	14,14,15	0.58	0	17,19,21	0.51	0
7	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.44	0
6	NAG	A	502	1	14,14,15	0.60	1 (7%)	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	501	-	3,3,3	0.43	0	2,2,2	0.35	0
6	NAG	B	503	1	14,14,15	0.50	0	17,19,21	0.48	0
7	EDO	A	503	-	3,3,3	0.42	0	2,2,2	0.27	0
7	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.32	0
6	NAG	C	501	1	14,14,15	0.36	0	17,19,21	0.45	0
7	EDO	C	502	-	3,3,3	0.41	0	2,2,2	0.42	0
6	NAG	D	501	1	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
7	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.37	0
6	NAG	F	501	1	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
6	NAG	H	501	1	14,14,15	0.29	0	17,19,21	0.46	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
6	NAG	E	501	1	-	0/6/23/26	0/1/1/1
6	NAG	H	502	1	-	0/6/23/26	0/1/1/1
7	EDO	A	504	-	-	0/1/1/1	-
5	MLT	A	501	-	-	2/8/8/8	-
7	EDO	G	503	-	-	0/1/1/1	-
6	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	NAG	G	502	1	-	0/6/23/26	0/1/1/1
7	EDO	B	502	-	-	1/1/1/1	-
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1
7	EDO	B	501	-	-	0/1/1/1	-
6	NAG	B	503	1	-	0/6/23/26	0/1/1/1
7	EDO	A	503	-	-	0/1/1/1	-
7	EDO	B	504	-	-	0/1/1/1	-
6	NAG	C	501	1	-	1/6/23/26	0/1/1/1
7	EDO	C	502	-	-	1/1/1/1	-
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
7	EDO	A	505	-	-	0/1/1/1	-
6	NAG	F	501	1	-	0/6/23/26	0/1/1/1
6	NAG	H	501	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	502	NAG	C1-C2	2.05	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	MLT	O2-C1-C2	3.54	120.22	112.74
6	F	501	NAG	C1-O5-C5	2.56	115.61	112.19
6	D	501	NAG	C1-O5-C5	2.46	115.49	112.19
5	A	501	MLT	O5-C4-C3	2.09	120.49	114.00

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	NAG	O5-C5-C6-O6
6	A	502	NAG	C4-C5-C6-O6
6	C	501	NAG	O5-C5-C6-O6
6	H	501	NAG	O5-C5-C6-O6
5	A	501	MLT	O1-C1-C2-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	EDO	2	0
6	G	502	NAG	1	0
7	A	503	EDO	2	0
6	C	501	NAG	1	0
6	F	501	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	A	369/383 (96%)	0.07	4 (1%)	78 76	41, 63, 114, 172	0
1	B	363/383 (94%)	0.07	8 (2%)	62 59	40, 61, 110, 158	0
1	C	363/383 (94%)	0.28	11 (3%)	52 49	48, 83, 143, 172	0
1	D	367/383 (95%)	0.42	15 (4%)	41 37	56, 94, 140, 199	0
1	E	367/383 (95%)	0.43	15 (4%)	41 37	60, 93, 147, 197	0
1	F	363/383 (94%)	0.47	12 (3%)	49 45	59, 92, 143, 198	0
1	G	364/383 (95%)	0.40	16 (4%)	39 35	62, 94, 135, 204	0
1	H	358/383 (93%)	0.73	24 (6%)	24 21	62, 109, 164, 188	0
All	All	2914/3064 (95%)	0.36	105 (3%)	46 42	40, 87, 145, 204	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	PHE	4.2
1	B	314	GLY	4.0
1	C	266	THR	3.9
1	H	268	PRO	3.7
1	A	269	ASN	3.6

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,

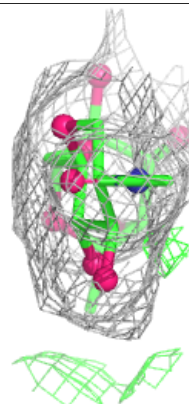
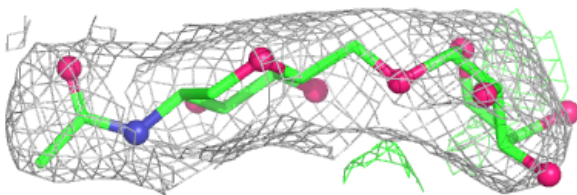
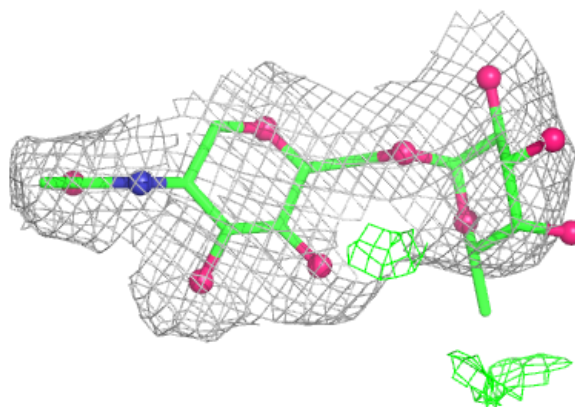
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	L	3	11/12	0.40	0.11	120,125,132,134	0
3	NAG	P	2	14/15	0.47	0.11	130,138,139,140	0
3	NAG	N	2	14/15	0.62	0.11	114,125,128,128	0
2	FUC	U	2	10/11	0.63	0.16	104,108,112,116	0
3	NAG	R	2	14/15	0.66	0.10	118,126,131,131	0
2	FUC	M	2	10/11	0.71	0.16	110,112,114,118	0
2	FUC	I	2	10/11	0.72	0.13	99,110,113,115	0
2	FUC	K	2	10/11	0.74	0.13	87,94,96,99	0
3	NAG	J	2	14/15	0.74	0.11	105,112,117,121	0
2	FUC	Q	2	10/11	0.74	0.12	106,108,108,109	0
3	NAG	P	1	14/15	0.79	0.10	84,103,108,120	0
4	NAG	L	2	14/15	0.81	0.10	97,112,116,121	0
2	FUC	S	2	10/11	0.82	0.11	108,119,123,127	0
3	NAG	R	1	14/15	0.83	0.09	69,89,102,107	0
2	FUC	O	2	10/11	0.84	0.11	87,94,99,100	0
2	FUC	T	2	10/11	0.86	0.10	98,102,105,107	0
3	NAG	N	1	14/15	0.87	0.08	79,93,100,106	0
2	NAG	S	1	14/15	0.89	0.09	64,74,91,100	0
2	NAG	O	1	14/15	0.90	0.10	57,74,85,92	0
2	NAG	M	1	14/15	0.91	0.09	61,66,89,100	0
2	NAG	Q	1	14/15	0.91	0.09	63,78,88,98	0
2	NAG	T	1	14/15	0.92	0.08	72,81,88,95	0
2	NAG	U	1	14/15	0.92	0.10	63,78,94,97	0
3	NAG	J	1	14/15	0.93	0.08	63,74,90,95	0
4	NAG	L	1	14/15	0.93	0.08	52,64,75,86	0
2	NAG	K	1	14/15	0.94	0.08	53,62,72,74	0
2	NAG	I	1	14/15	0.95	0.07	48,57,72,83	0

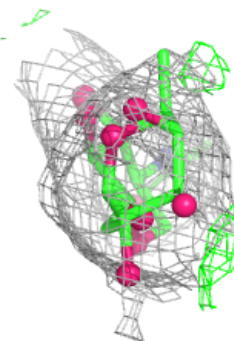
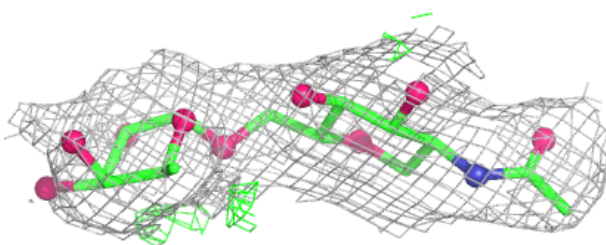
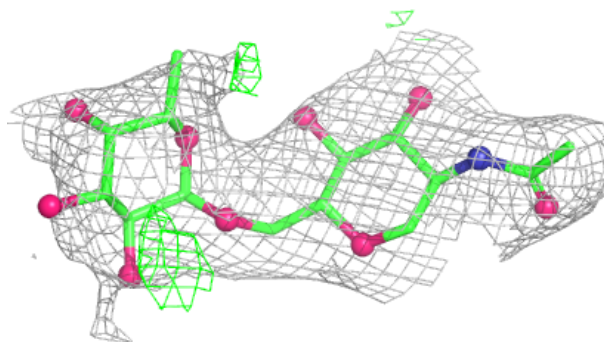
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

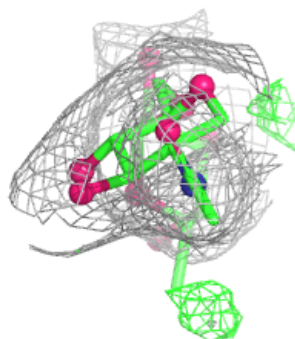
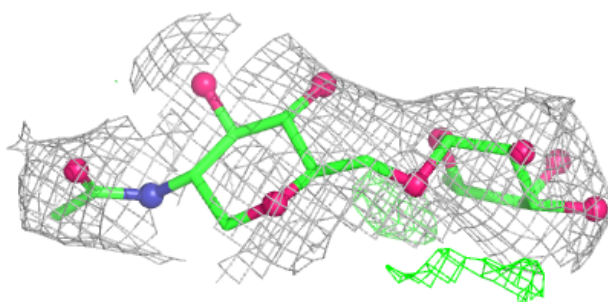
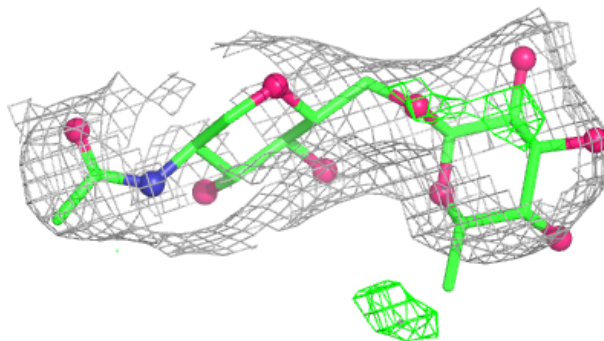
**Electron density around Chain K:**

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

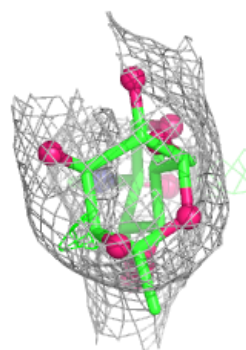
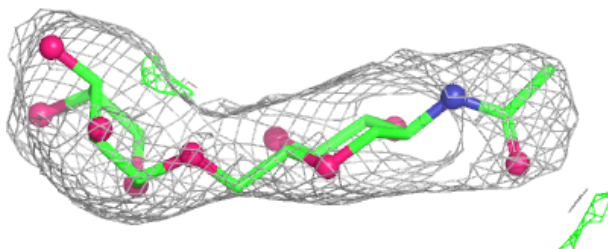
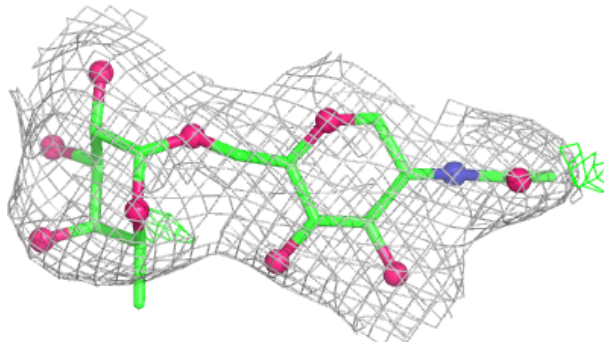


Electron density around Chain M:

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

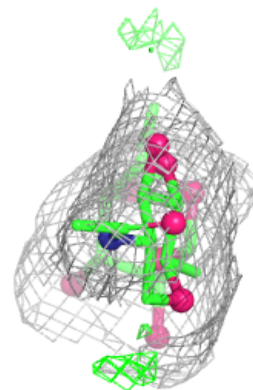
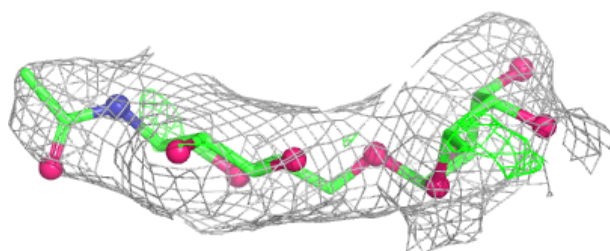
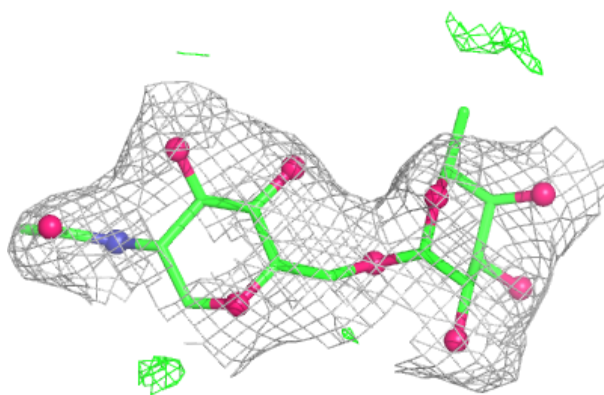
**Electron density around Chain O:**

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

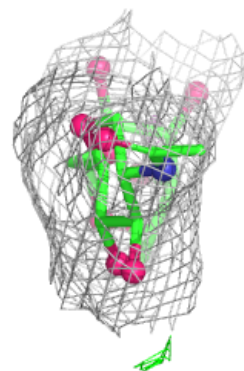
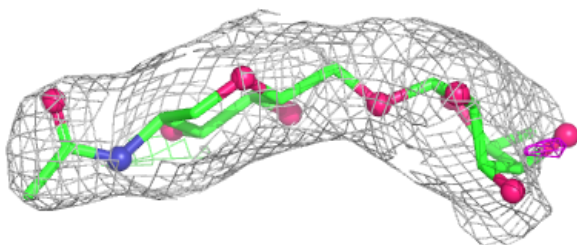
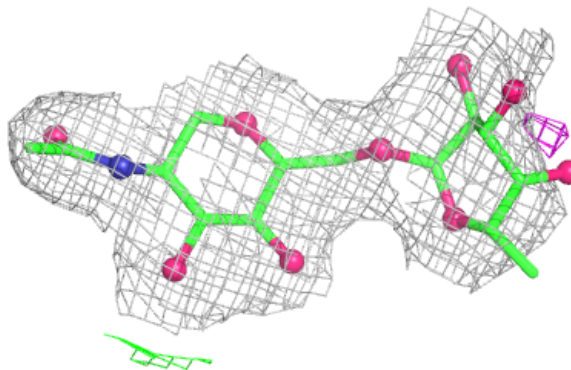


Electron density around Chain Q:

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

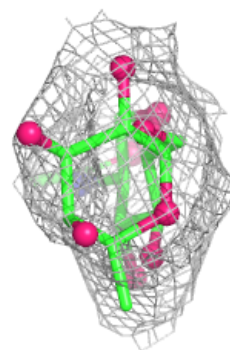
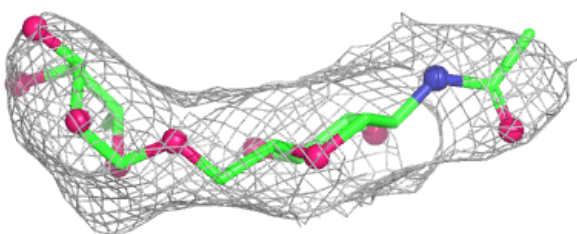
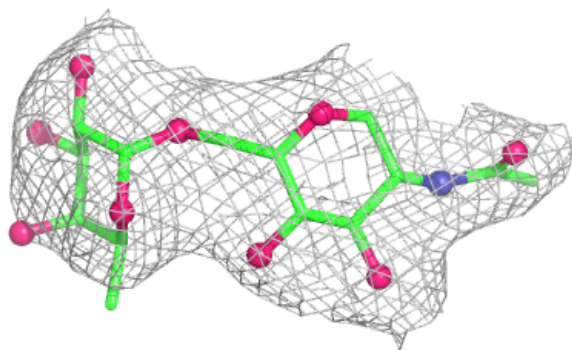
**Electron density around Chain S:**

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

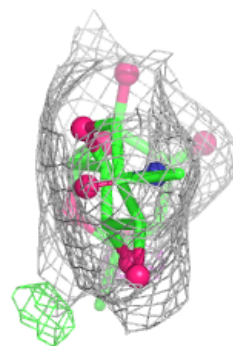
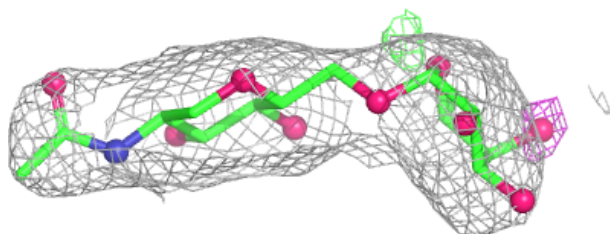
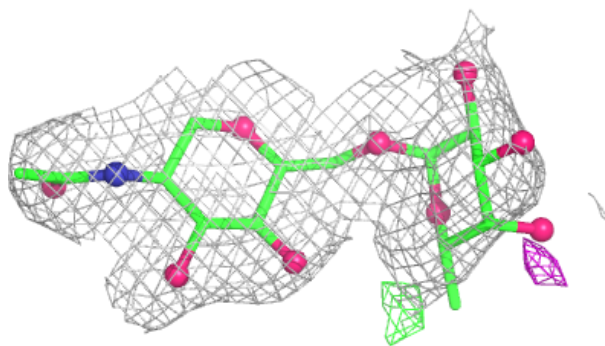


Electron density around Chain T:

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

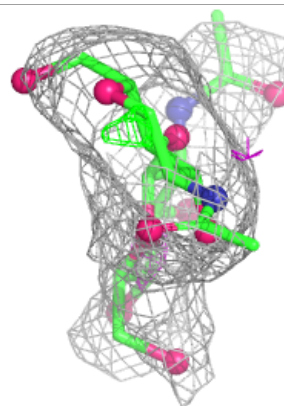
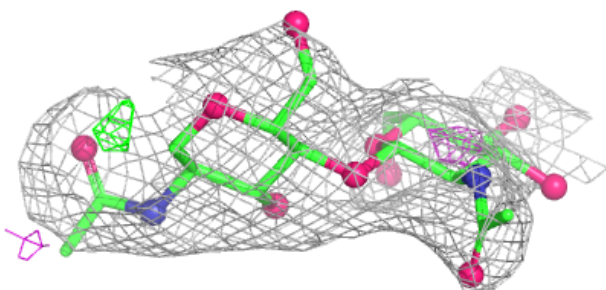
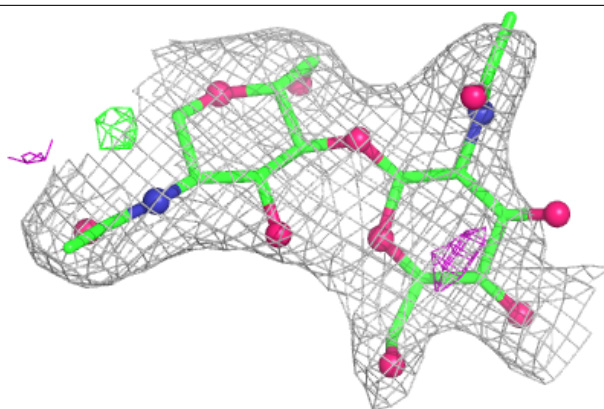
**Electron density around Chain U:**

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

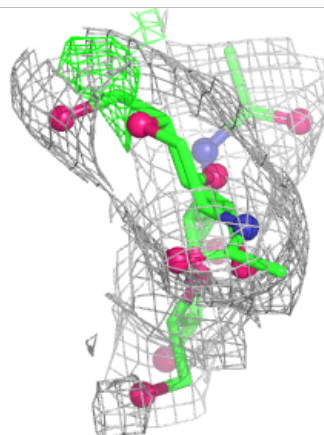
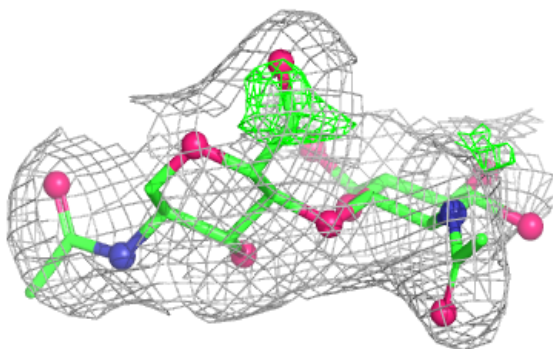
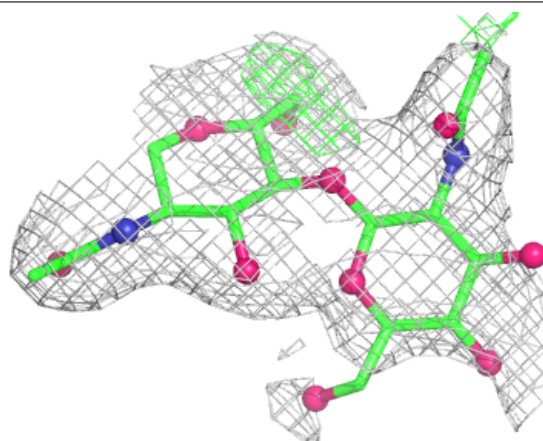


Electron density around Chain J:

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

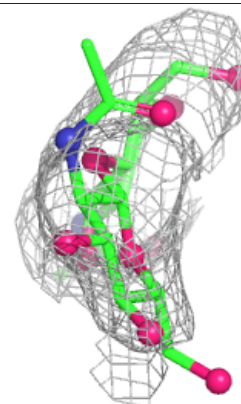
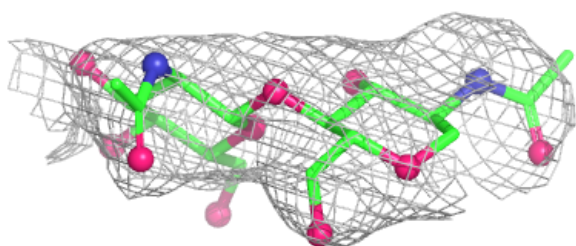
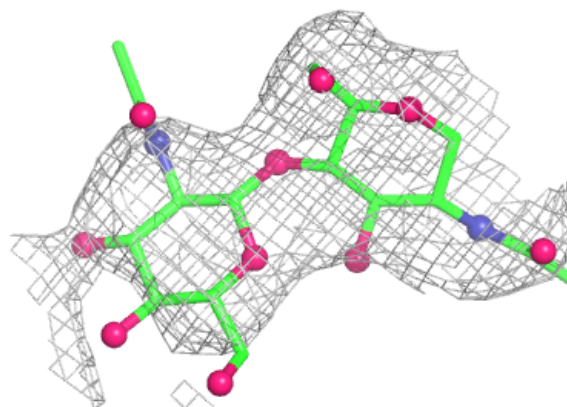
**Electron density around Chain N:**

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

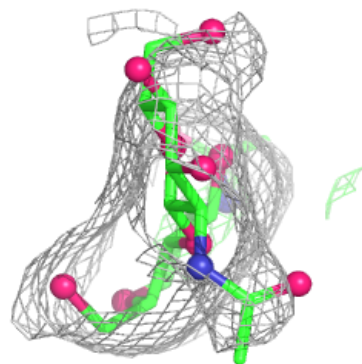
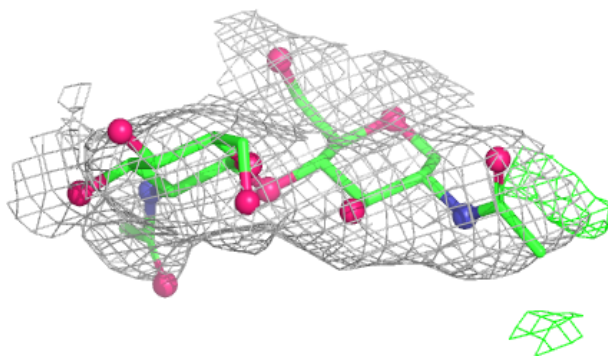
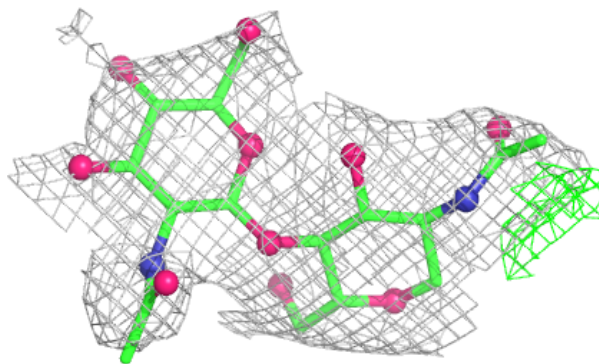


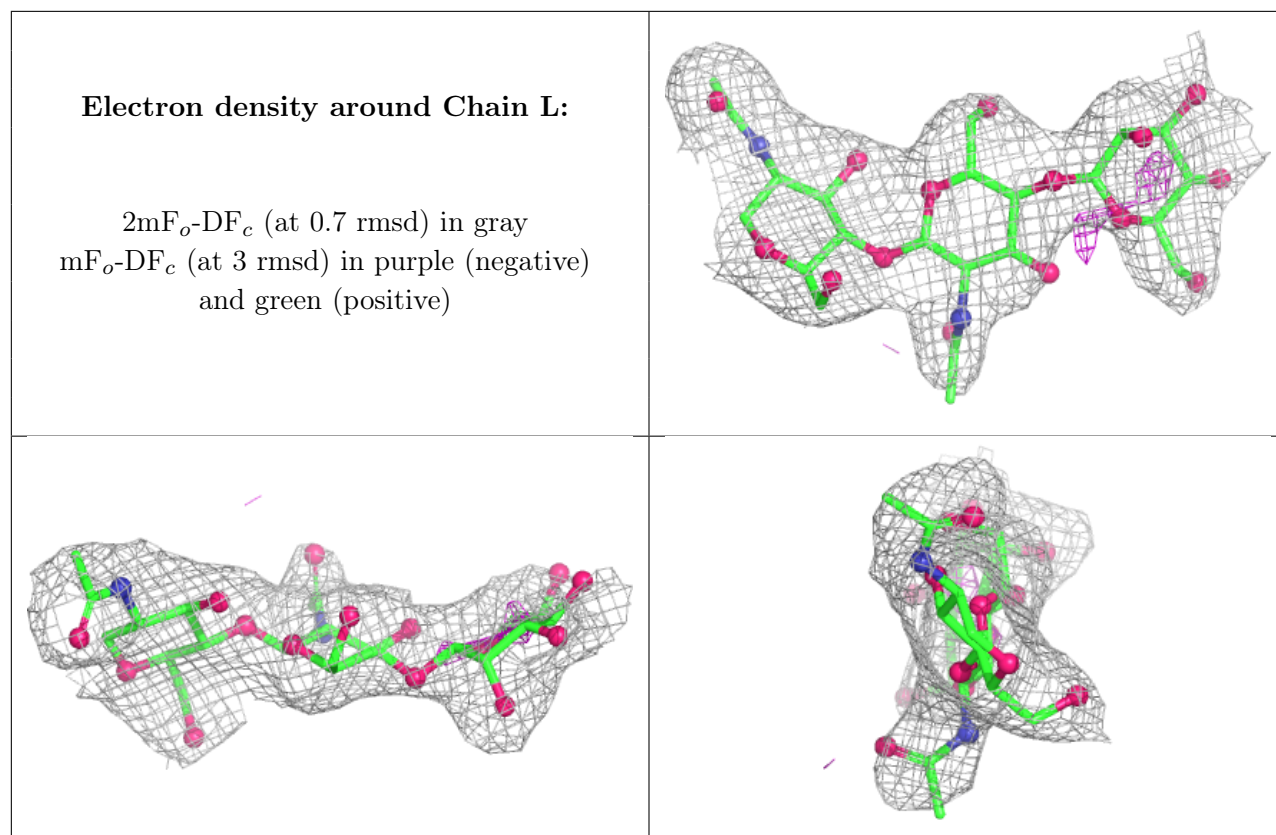
Electron density around Chain P:

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

**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)





6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
6	NAG	E	501	14/15	0.54	0.12	96,107,115,115	0
6	NAG	D	501	14/15	0.62	0.13	103,114,123,125	0
6	NAG	H	502	14/15	0.62	0.13	95,114,119,120	0
6	NAG	A	502	14/15	0.65	0.12	76,91,103,108	0
6	NAG	C	501	14/15	0.68	0.12	92,108,118,121	0
7	EDO	B	504	4/4	0.68	0.31	77,79,79,82	0
6	NAG	H	501	14/15	0.70	0.12	90,96,114,122	0
6	NAG	F	501	14/15	0.72	0.11	94,100,129,134	0
6	NAG	B	503	14/15	0.72	0.11	91,105,118,122	0
6	NAG	G	502	14/15	0.73	0.11	101,115,119,121	0
7	EDO	B	501	4/4	0.81	0.19	71,72,76,77	0
7	EDO	A	504	4/4	0.81	0.28	88,90,90,90	0
7	EDO	A	505	4/4	0.82	0.12	92,92,94,97	0
5	MLT	A	501	9/9	0.83	0.15	96,106,114,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	503	4/4	0.86	0.32	120,121,123,127	0
7	EDO	G	503	4/4	0.86	0.11	70,72,78,86	0
6	NAG	G	501	14/15	0.90	0.07	65,82,88,94	0
7	EDO	C	502	4/4	0.93	0.14	71,74,74,78	0
7	EDO	B	502	4/4	0.94	0.10	52,53,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.