



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 28, 2022 – 12:06 PM JST

PDB ID : 7WHU
Title : Human Neutrophil Elastase in-complex with Ecotin Peptide
Authors : Shankar, S.; Jayaraman, S.
Deposited on : 2021-12-31
Resolution : 2.89 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

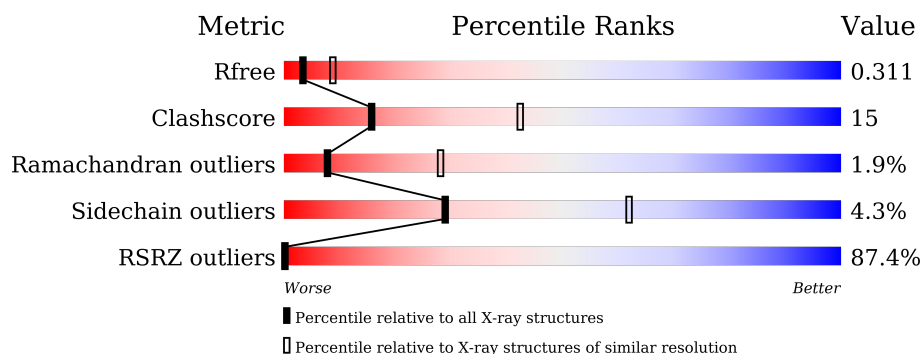
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	267	<div> <div>72%</div> <div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	267	<div> <div>66%</div> <div> <div>55%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	267	<div> <div>73%</div> <div> <div>51%</div> <div>29%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	267	<div> <div>73%</div> <div> <div>57%</div> <div>24%</div> <div>•</div> <div>18%</div> </div> </div>
2	E	8	<div> <div>88%</div> <div> <div>62%</div> <div>38%</div> </div> </div>
2	F	8	<div> <div>100%</div> <div> <div>50%</div> <div>38%</div> <div>12%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	8	
2	H	8	
3	K	3	
3	N	3	
3	O	3	
3	P	3	
4	I	2	
5	J	4	
6	L	2	
7	M	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	K	1	-	-	-	X
3	NAG	K	2	-	-	-	X
3	FUC	K	3	-	-	-	X
3	NAG	N	1	-	-	-	X
3	NAG	N	2	-	-	-	X
3	FUC	N	3	-	-	-	X
3	NAG	O	1	-	-	-	X
3	NAG	O	2	-	-	-	X
3	FUC	O	3	-	-	-	X
3	NAG	P	1	-	-	-	X
3	NAG	P	2	-	-	-	X
3	FUC	P	3	-	-	-	X
4	NAG	I	1	-	-	-	X
4	FUC	I	2	-	-	-	X
5	NAG	J	1	-	-	-	X
5	NAG	J	2	-	-	-	X
5	BMA	J	3	-	-	-	X
5	FUC	J	4	-	-	-	X
6	NAG	L	1	-	-	-	X
6	NAG	L	2	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	M	1	-	-	-	X
7	NAG	M	3	-	-	-	X
8	GOL	A	301	-	-	-	X
8	GOL	B	303	-	-	-	X
8	GOL	B	305	-	-	-	X
8	GOL	C	301	-	-	-	X
8	GOL	D	301	-	-	-	X
9	SO4	B	301	-	-	-	X
9	SO4	B	302	-	-	-	X
9	SO4	C	302	-	-	-	X
9	SO4	C	303	-	-	-	X
9	SO4	D	302	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7019 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.

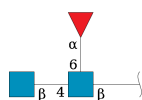
- Molecule 1 is a protein called Neutrophil elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	218	Total	C	N	O	S	0	0	0
			1597	1001	306	279	11			
1	A	218	Total	C	N	O	S	0	0	0
			1610	1012	308	279	11			
1	B	218	Total	C	N	O	S	0	0	0
			1610	1012	309	278	11			
1	C	218	Total	C	N	O	S	0	0	0
			1627	1019	316	281	11			

- Molecule 2 is a protein called Ecotin Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	S	0	0	0
			47	29	8	9	1			
2	F	8	Total	C	N	O	S	0	0	0
			51	31	8	11	1			
2	G	8	Total	C	N	O	S	0	0	0
			51	32	8	10	1			
2	H	8	Total	C	N	O	S	0	0	0
			46	27	8	10	1			

- Molecule 3 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
3	P	3	Total	C	N	O	0	0	0
			38	22	2	14			

Continued on next page...

Continued from previous page...

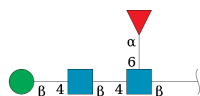
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	N	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	O	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



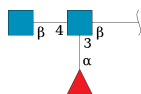
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



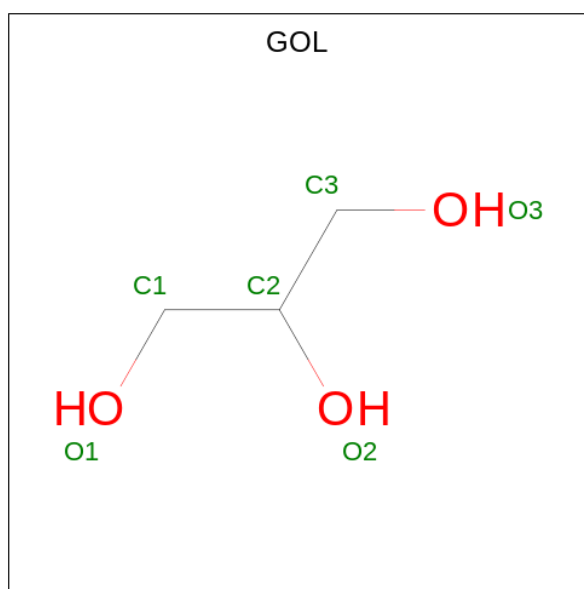
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



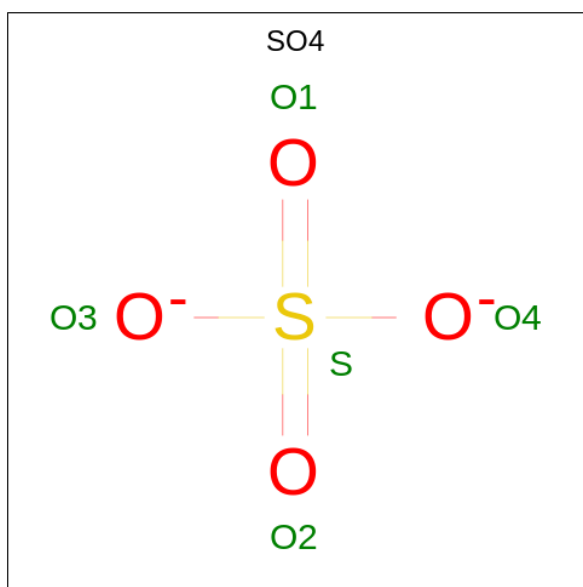
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		

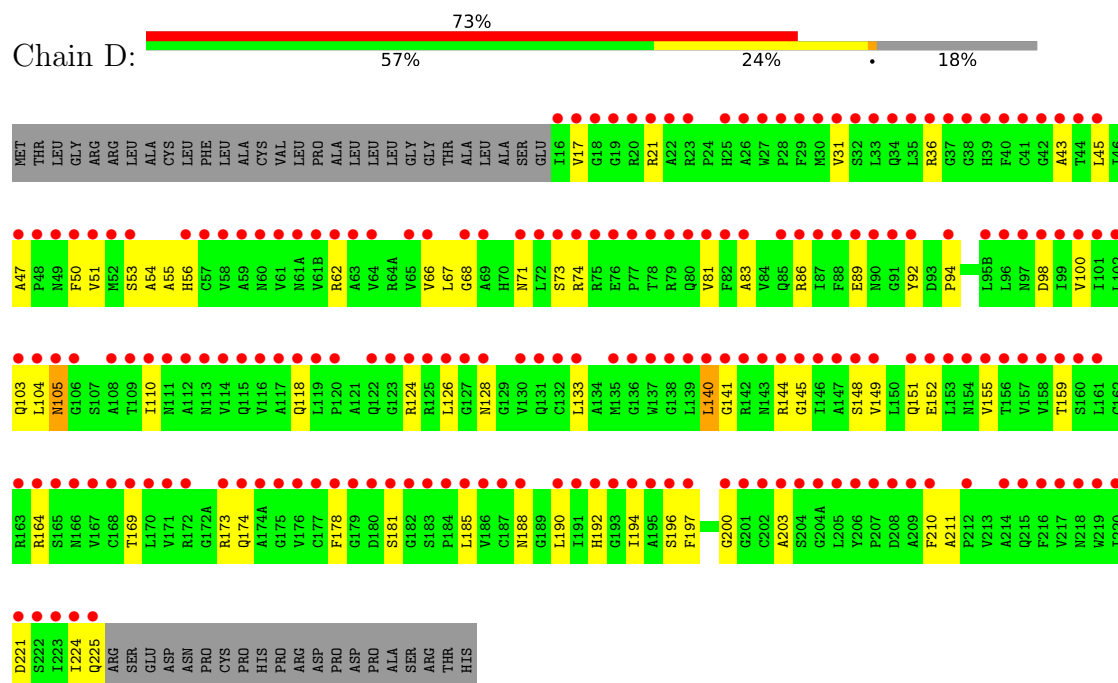
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	O	0	0
			2	2		
10	A	11	Total	O	0	0
			11	11		
10	B	11	Total	O	0	0
			11	11		
10	C	2	Total	O	0	0
			2	2		
10	F	1	Total	O	0	0
			1	1		
10	G	1	Total	O	0	0
			1	1		

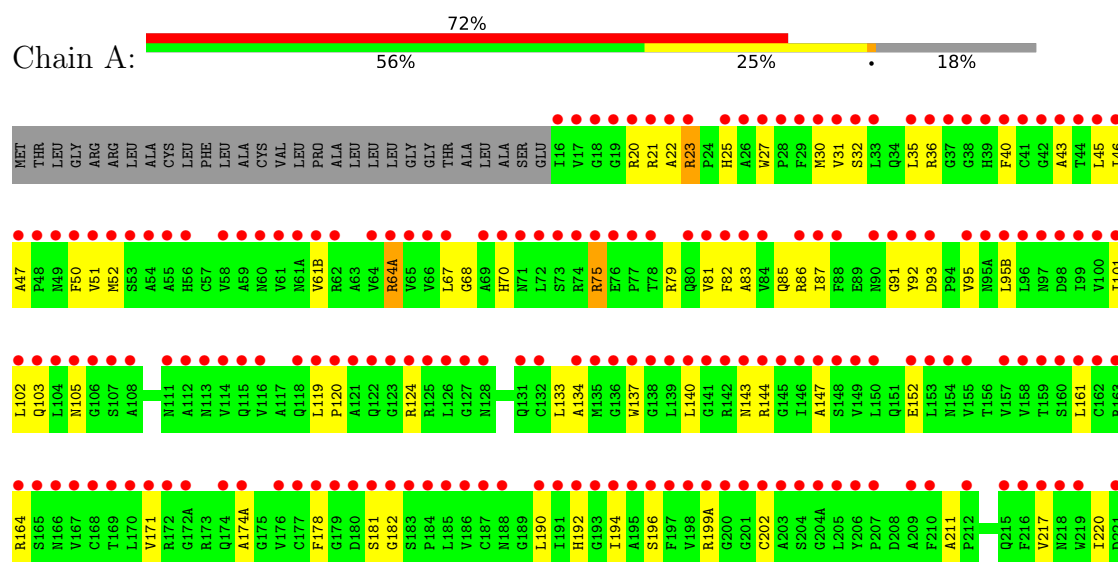
3 Residue-property plots

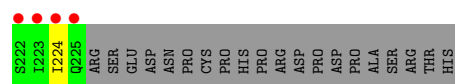
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neutrophil elastase

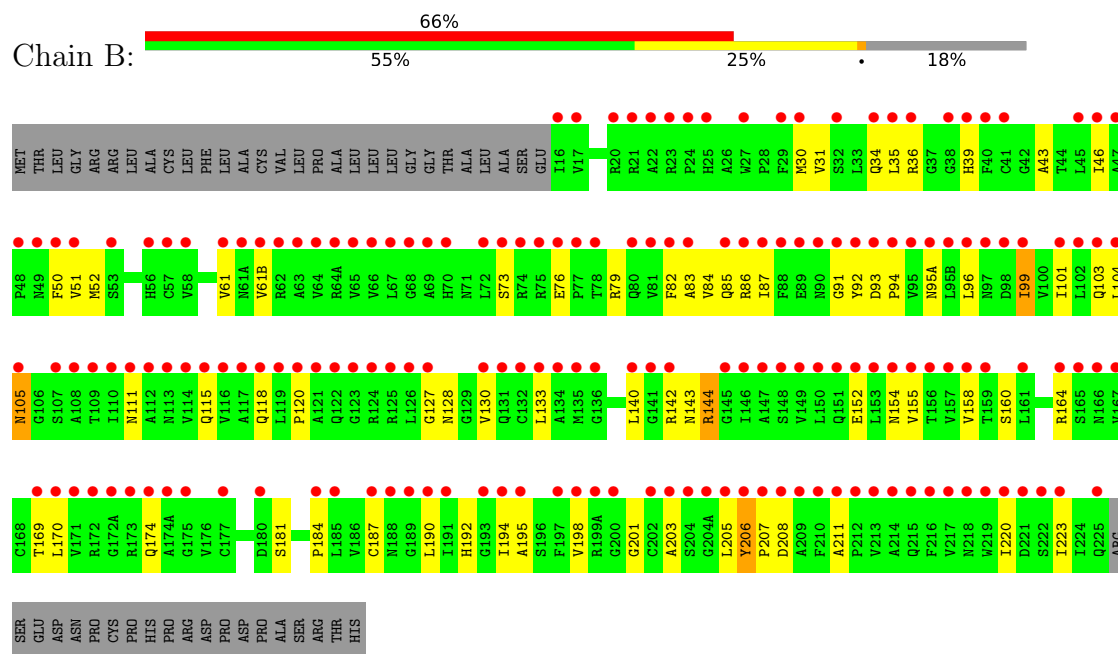


• Molecule 1: Neutrophil elastase

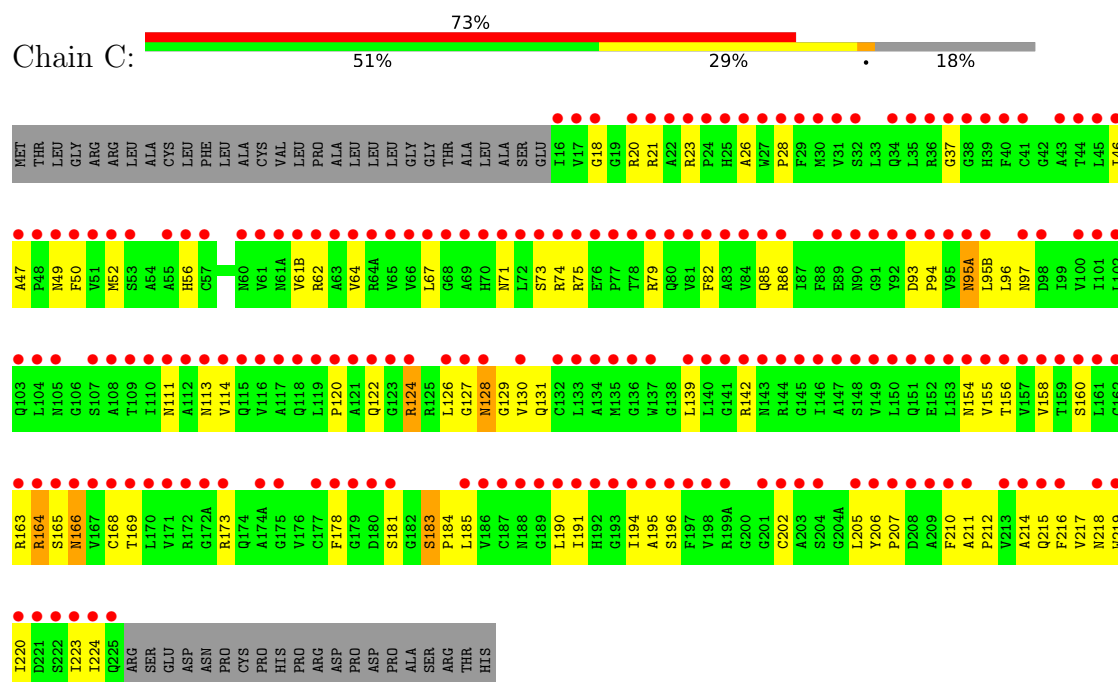




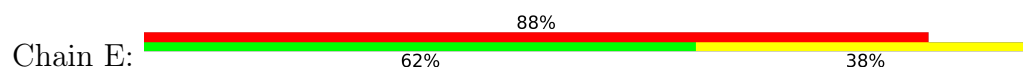
• Molecule 1: Neutrophil elastase

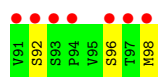


• Molecule 1: Neutrophil elastase

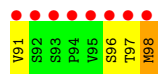


• Molecule 2: Ecotin Peptide

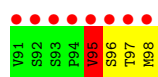




- Molecule 2: Ecotin Peptide



- Molecule 2: Ecotin Peptide



- Molecule 2: Ecotin Peptide



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




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



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



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

Chain O:  67% 33%



- Molecule 4: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%




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

Chain L:  100%



- Molecule 7: α -L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.24Å 68.91Å 130.85Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	47.45 – 2.89 47.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.45-2.89) 99.2 (47.45-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	51.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.252 , 0.306 0.253 , 0.311	Depositor DCC
R_{free} test set	2006 reflections (8.78%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7019	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6532e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FUC, BMA, NAG, GOL

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	0.47	1/1636 (0.1%)	0.80	7/2227 (0.3%)
1	B	0.34	0/1640	0.59	0/2231
1	C	0.34	0/1657	0.64	0/2252
1	D	0.35	0/1626	0.66	2/2213 (0.1%)
2	E	0.34	0/47	0.70	0/62
2	F	0.37	0/51	0.67	0/69
2	G	0.28	0/51	0.59	0/69
2	H	0.32	0/45	0.69	0/58
All	All	0.38	1/6753 (0.0%)	0.68	9/9181 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ARG	CG-CD	-7.72	1.32	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	CB-CG-CD	-10.81	83.48	111.60
1	A	23	ARG	NE-CZ-NH1	8.38	124.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	CA-CB-CG	-8.25	95.25	113.40
1	A	23	ARG	CB-CG-CD	7.75	131.74	111.60
1	A	75	ARG	NE-CZ-NH1	6.89	123.74	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	LEU	Peptide
1	D	104	LEU	Peptide
1	D	73	SER	Peptide

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	1610	0	1589	50	0
1	B	1610	0	1604	59	0
1	C	1627	0	1627	54	2
1	D	1597	0	1558	42	2
2	E	47	0	40	4	0
2	F	51	0	45	4	0
2	G	51	0	47	5	0
2	H	46	0	35	3	0
3	K	38	0	34	1	0
3	N	38	0	34	1	0
3	O	38	0	34	0	0
3	P	38	0	34	0	0
4	I	24	0	22	0	0
5	J	49	0	43	0	0
6	L	28	0	25	2	0
7	M	38	0	34	1	0
8	A	6	0	8	1	0
8	B	18	0	23	0	0
8	C	6	0	8	1	0
8	D	6	0	8	0	0
9	B	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	10	0	0	0	0
9	D	5	0	0	0	0
10	A	11	0	0	4	0
10	B	11	0	0	9	0
10	C	2	0	0	2	0
10	D	2	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	1	0
All	All	7019	0	6852	204	2

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 15.

The worst 5 of 204 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:D:178:PHE:HA	2:H:98:MET:HB3	1.59	0.85
1:A:147:ALA:O	10:A:401:HOH:O	1.96	0.82
1:D:194:ILE:HB	1:D:211:ALA:HB3	1.62	0.80
1:C:183:SER:O	10:C:401:HOH:O	2.00	0.79
1:B:61(B):VAL:HG12	1:B:84:VAL:HG21	1.63	0.79

All (2) 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)
1:D:62:ARG:NH1	1:C:94:PRO:O[1_655]	1.93	0.27
1:D:94:PRO:O	1:C:62:ARG:NH2[1_655]	2.16	0.04

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	216/267 (81%)	191 (88%)	23 (11%)	2 (1%)	17	48
1	B	216/267 (81%)	192 (89%)	19 (9%)	5 (2%)	6	23
1	C	216/267 (81%)	191 (88%)	23 (11%)	2 (1%)	17	48
1	D	216/267 (81%)	192 (89%)	21 (10%)	3 (1%)	11	36
2	E	6/8 (75%)	1 (17%)	4 (67%)	1 (17%)	0	0
2	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	G	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	H	6/8 (75%)	1 (17%)	3 (50%)	2 (33%)	0	0
All	All	888/1100 (81%)	776 (87%)	95 (11%)	17 (2%)	8	28

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	ASN
1	B	105	ASN
2	G	97	THR
2	H	95	VAL
1	B	144	ARG

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	164/212 (77%)	156 (95%)	8 (5%)	25	57
1	B	166/212 (78%)	162 (98%)	4 (2%)	49	79
1	C	169/212 (80%)	159 (94%)	10 (6%)	19	49
1	D	160/212 (76%)	156 (98%)	4 (2%)	47	78
2	E	5/8 (62%)	5 (100%)	0	100	100
2	F	6/8 (75%)	5 (83%)	1 (17%)	2	6
2	G	6/8 (75%)	5 (83%)	1 (17%)	2	6
2	H	5/8 (62%)	4 (80%)	1 (20%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	681/880 (77%)	652 (96%)	29 (4%)	29	62

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	ARG
2	G	95	VAL
1	C	82	PHE
1	C	166	ASN
1	C	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	B	128	ASN
1	C	97	ASN
1	C	128	ASN
1	C	166	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 ⓘ

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	1	1,4	14,14,15	0.49	0	17,19,21	0.63	0
4	FUC	I	2	4	10,10,11	0.69	0	14,14,16	1.21	2 (14%)
5	NAG	J	1	1,5	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	J	2	5	14,14,15	0.33	0	17,19,21	0.54	0
5	BMA	J	3	5	11,11,12	0.89	0	15,15,17	0.76	0
5	FUC	J	4	5	10,10,11	0.76	0	14,14,16	1.04	0
3	NAG	K	1	1,3	14,14,15	0.46	0	17,19,21	0.54	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.66	0
3	FUC	K	3	3	10,10,11	1.53	2 (20%)	14,14,16	1.80	3 (21%)
6	NAG	L	1	1,6	14,14,15	0.37	0	17,19,21	0.55	0
6	NAG	L	2	6	14,14,15	0.31	0	17,19,21	0.67	0
7	NAG	M	1	1,7	14,14,15	1.64	3 (21%)	17,19,21	1.32	2 (11%)
7	FUC	M	2	7	10,10,11	0.99	1 (10%)	14,14,16	1.96	4 (28%)
7	NAG	M	3	7	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	N	1	1,3	14,14,15	0.23	0	17,19,21	0.95	1 (5%)
3	NAG	N	2	3	14,14,15	0.44	0	17,19,21	0.54	0
3	FUC	N	3	3	10,10,11	1.04	1 (10%)	14,14,16	0.63	0
3	NAG	O	1	1,3	14,14,15	0.47	0	17,19,21	0.59	0
3	NAG	O	2	3	14,14,15	0.16	0	17,19,21	0.61	1 (5%)
3	FUC	O	3	3	10,10,11	0.93	0	14,14,16	0.87	0
3	NAG	P	1	3	14,14,15	0.87	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	FUC	P	3	3	10,10,11	0.71	0	14,14,16	0.87	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	I	2	4	-	-	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	FUC	J	4	5	-	-	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	M	2	7	-	-	0/1/1/1
7	NAG	M	3	7	-	3/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	FUC	N	3	3	-	-	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	FUC	O	3	3	-	-	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	FUC	P	3	3	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1	NAG	C1-C2	4.37	1.58	1.52
7	M	1	NAG	O5-C1	-3.54	1.38	1.43
3	K	3	FUC	C4-C5	3.42	1.60	1.52
3	P	1	NAG	O5-C1	-3.08	1.38	1.43
3	N	3	FUC	O5-C1	-2.51	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	2	FUC	C1-O5-C5	4.74	123.53	112.78
3	K	3	FUC	O5-C5-C4	4.41	117.43	109.52
7	M	1	NAG	C4-C3-C2	4.29	117.30	111.02
3	K	3	FUC	C3-C4-C5	3.48	115.19	109.77
7	M	2	FUC	O5-C1-C2	3.19	115.70	110.77

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	2	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

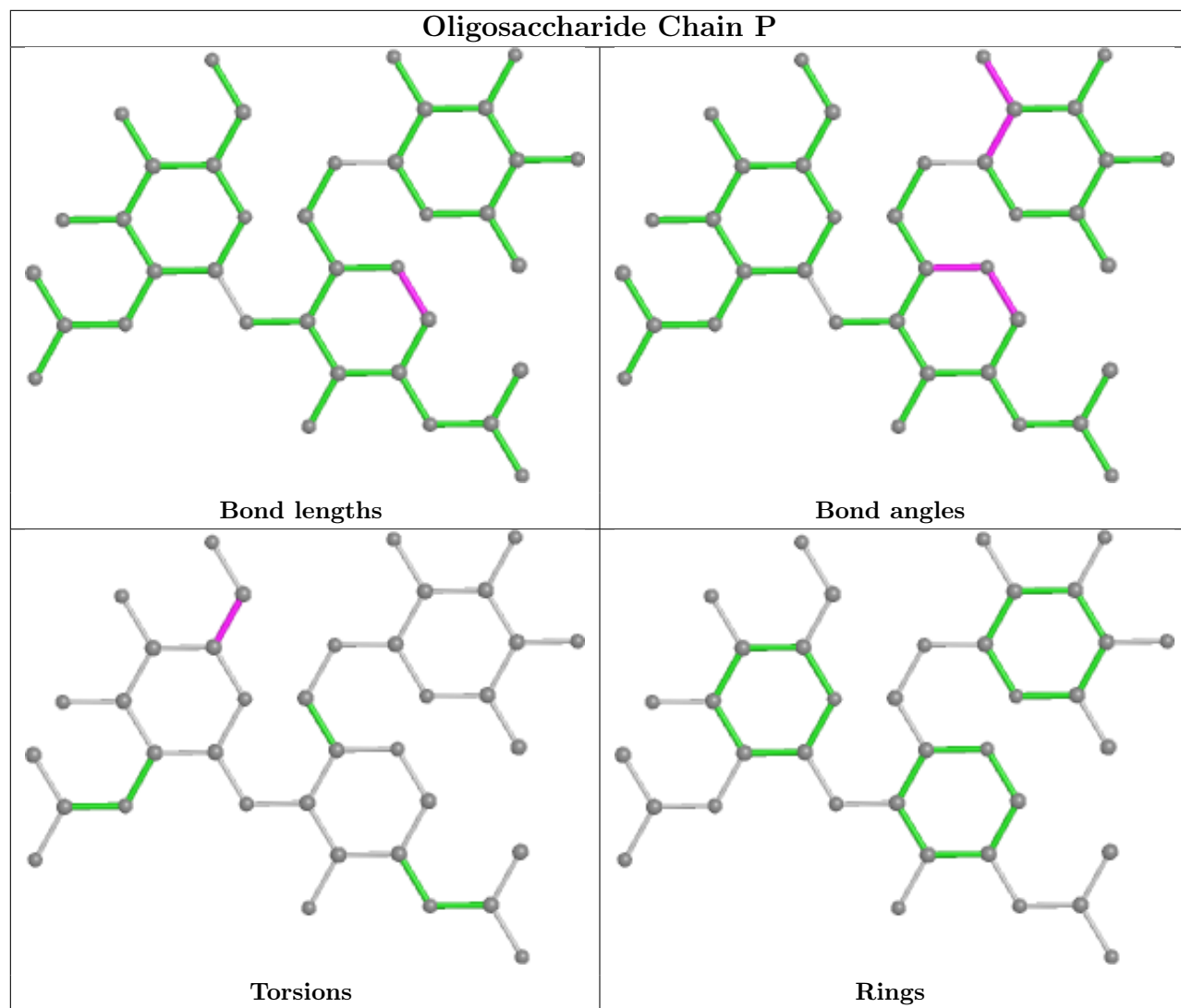
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6

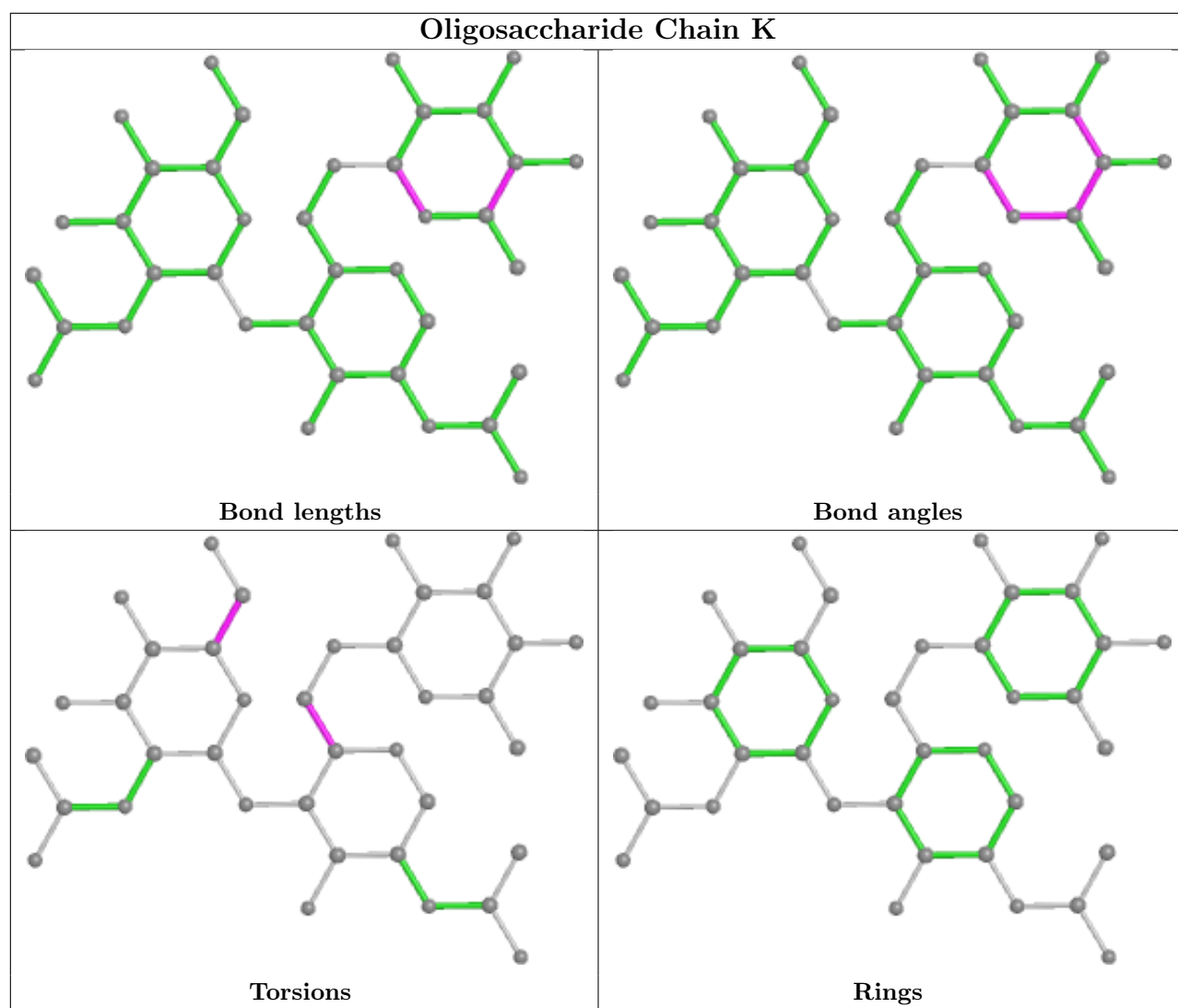
There are no ring outliers.

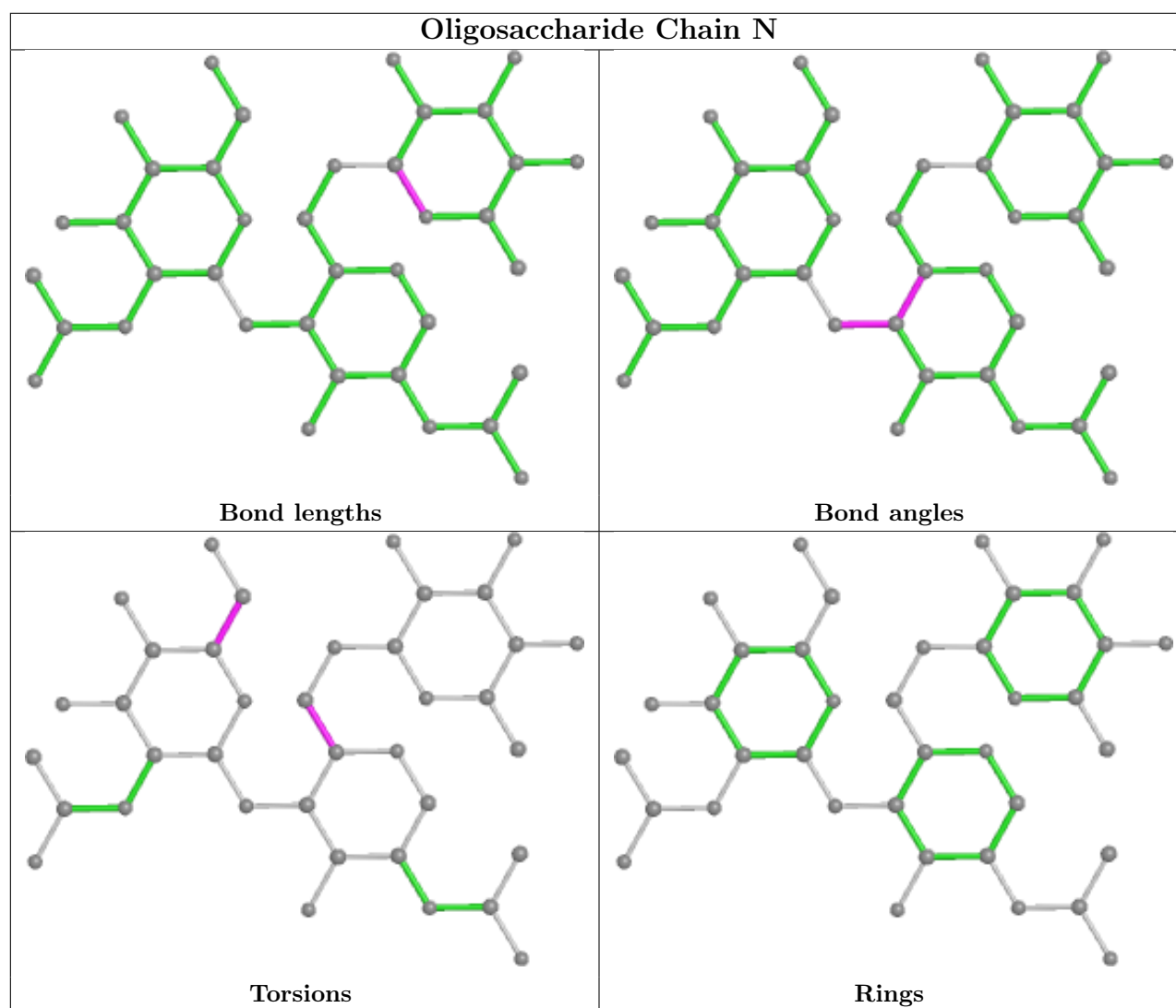
6 monomers are involved in 5 short contacts:

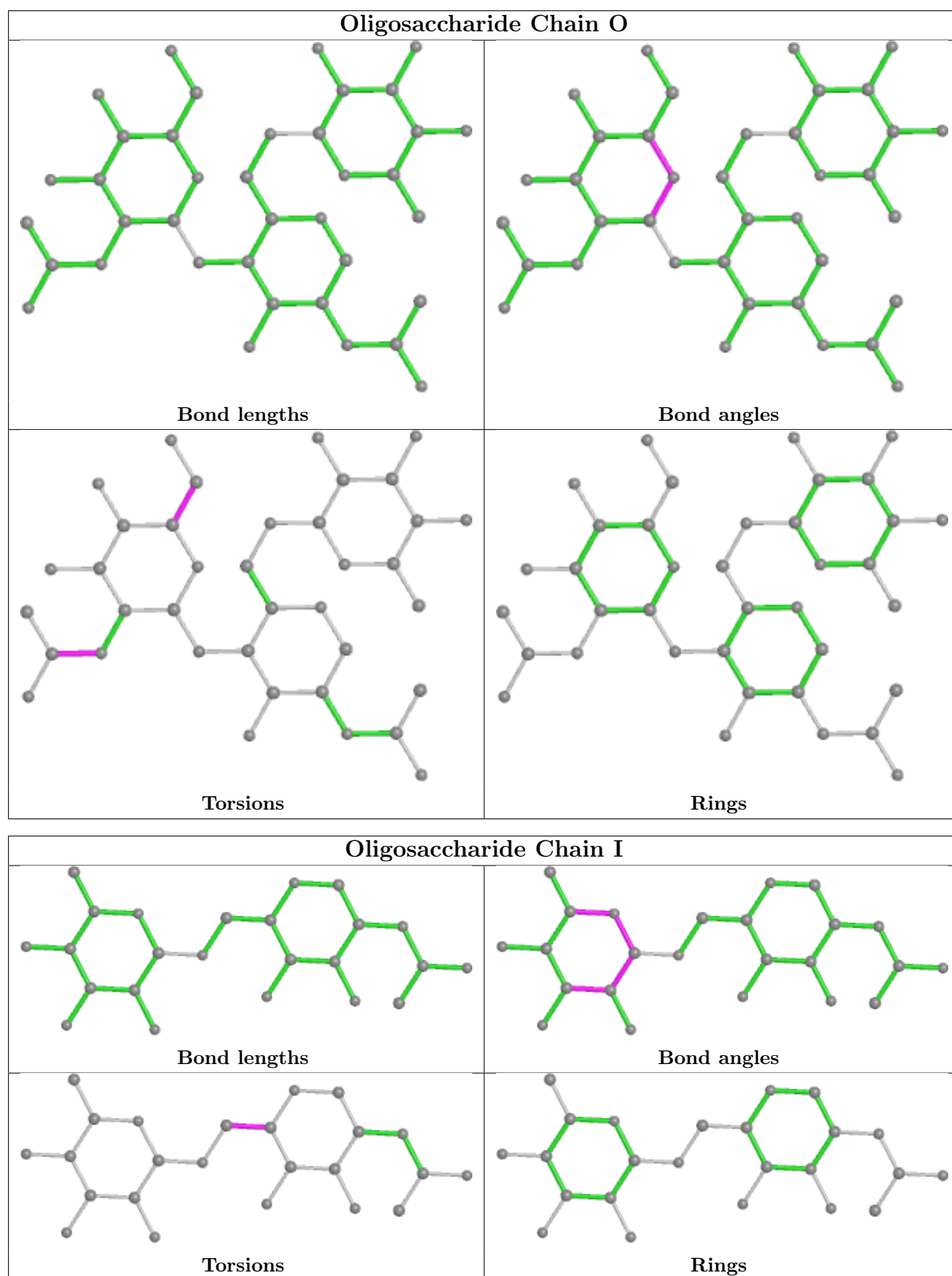
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0
7	M	1	NAG	1	0
3	K	1	NAG	1	0
6	L	2	NAG	2	0
6	L	1	NAG	1	0
3	N	2	NAG	1	0

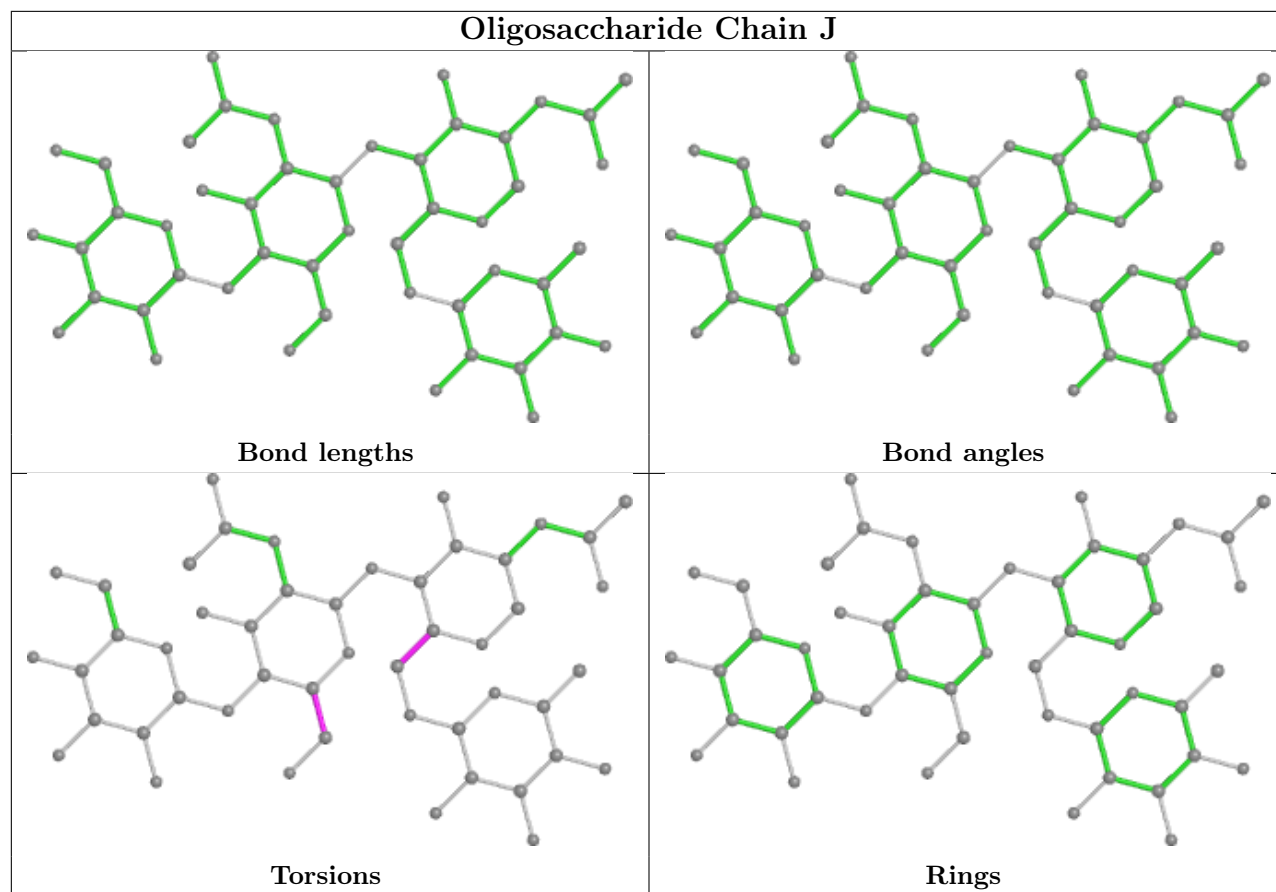
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

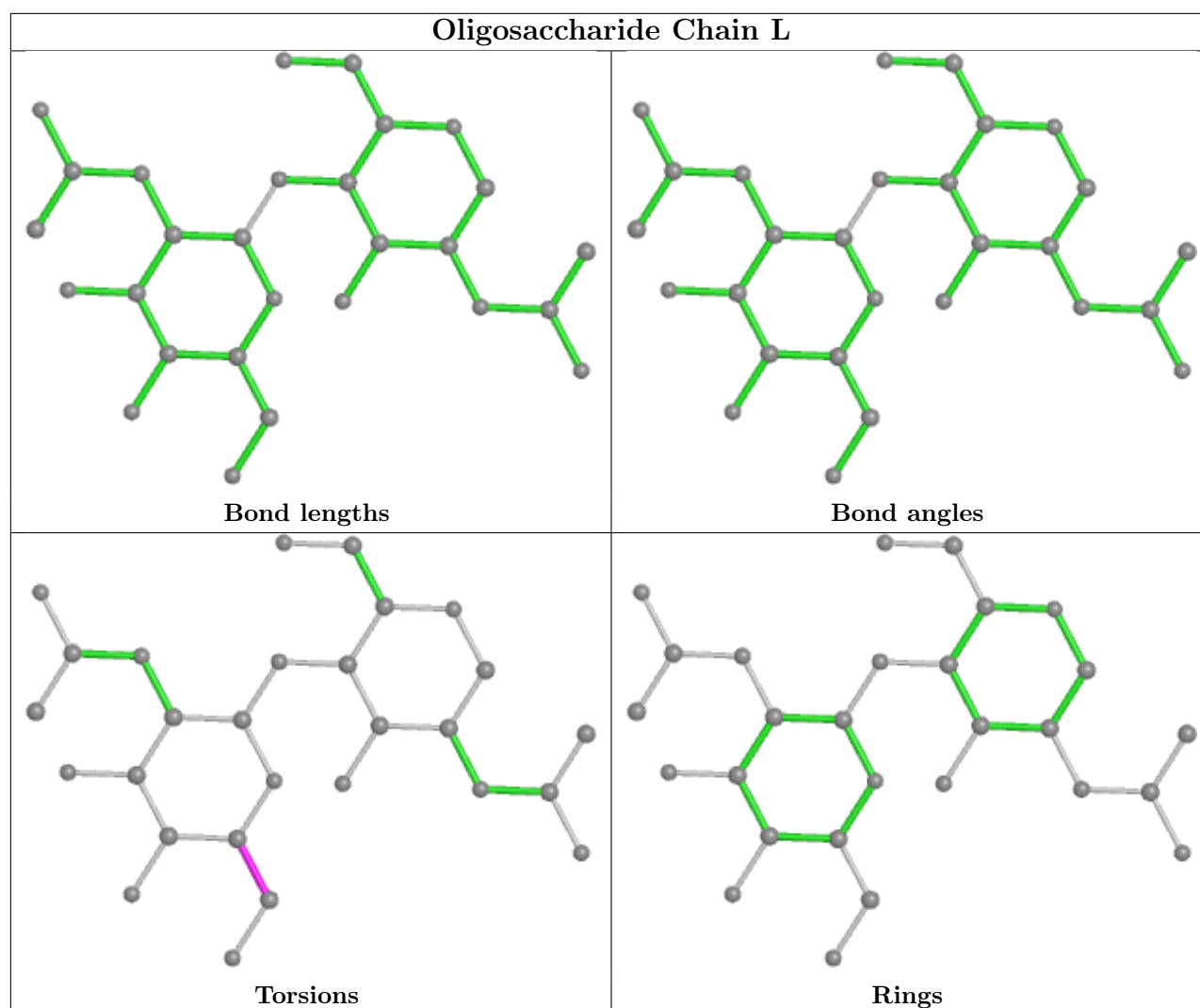


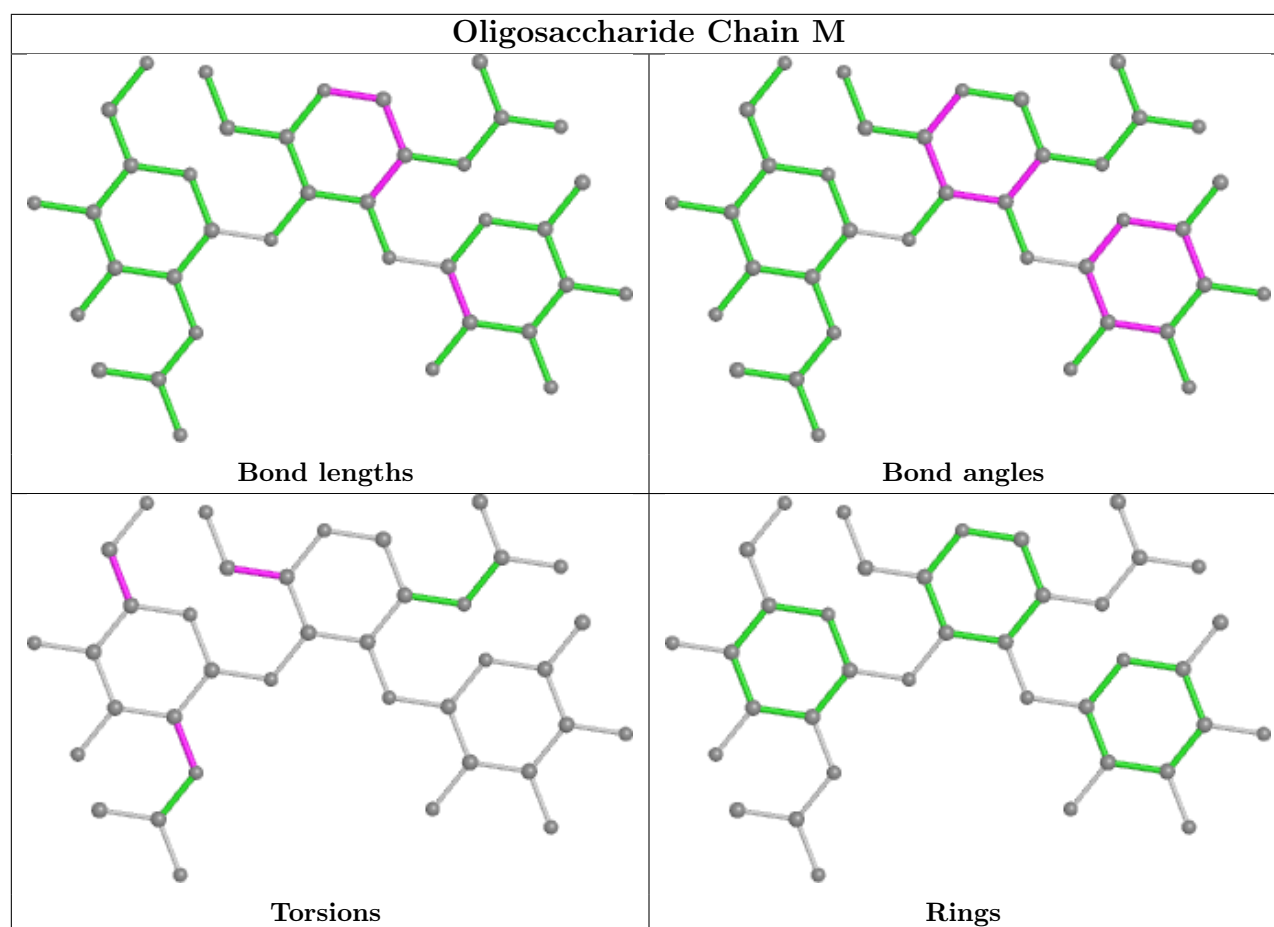












5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
9	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.15	0
8	GOL	B	304	-	5,5,5	1.16	0	5,5,5	0.93	0
8	GOL	A	301	-	5,5,5	1.03	0	5,5,5	0.93	0
9	SO4	D	302	-	4,4,4	0.16	0	6,6,6	0.12	0
8	GOL	D	301	-	5,5,5	1.11	0	5,5,5	0.97	0
8	GOL	B	305	-	5,5,5	1.01	0	5,5,5	0.94	0
8	GOL	C	301	-	5,5,5	1.03	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	C	302	-	4,4,4	0.16	0	6,6,6	0.08	0
8	GOL	B	303	-	5,5,5	1.03	0	5,5,5	1.00	0
9	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.17	0
9	SO4	C	303	-	4,4,4	0.18	0	6,6,6	0.10	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
8	GOL	B	304	-	-	2/4/4/4	-
8	GOL	A	301	-	-	2/4/4/4	-
8	GOL	D	301	-	-	3/4/4/4	-
8	GOL	B	305	-	-	2/4/4/4	-
8	GOL	C	301	-	-	0/4/4/4	-
8	GOL	B	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	301	GOL	O1-C1-C2-C3
8	A	301	GOL	O1-C1-C2-C3
8	B	303	GOL	O1-C1-C2-C3
8	B	304	GOL	O1-C1-C2-C3
8	B	305	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	301	SO4	1	0
8	A	301	GOL	1	0
8	C	301	GOL	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	218/267 (81%)	3.73	193 (88%) 0 0	16, 24, 38, 50	0
1	B	218/267 (81%)	3.39	176 (80%) 0 0	17, 24, 29, 37	0
1	C	218/267 (81%)	3.90	195 (89%) 0 0	19, 27, 38, 56	0
1	D	218/267 (81%)	3.70	195 (89%) 0 0	15, 25, 31, 40	0
2	E	8/8 (100%)	4.03	7 (87%) 0 0	27, 31, 35, 36	0
2	F	8/8 (100%)	4.33	8 (100%) 0 0	22, 28, 32, 32	0
2	G	8/8 (100%)	4.53	8 (100%) 0 0	27, 37, 40, 44	0
2	H	8/8 (100%)	3.73	8 (100%) 0 0	22, 32, 35, 37	0
All	All	904/1100 (82%)	3.70	790 (87%) 0 0	15, 25, 35, 56	0

The worst 5 of 790 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	16.5
1	A	37	GLY	13.6
1	A	141	GLY	11.5
1	D	138	GLY	11.4
1	B	121	ALA	10.9

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,

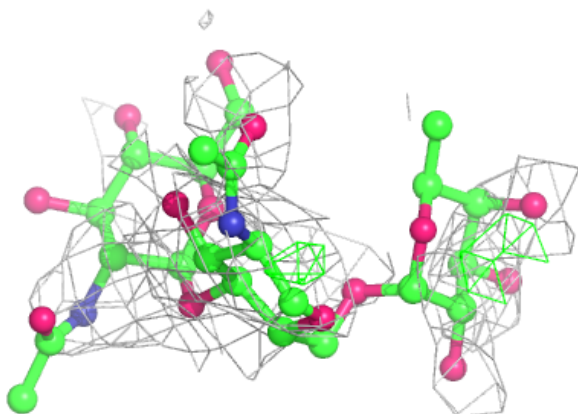
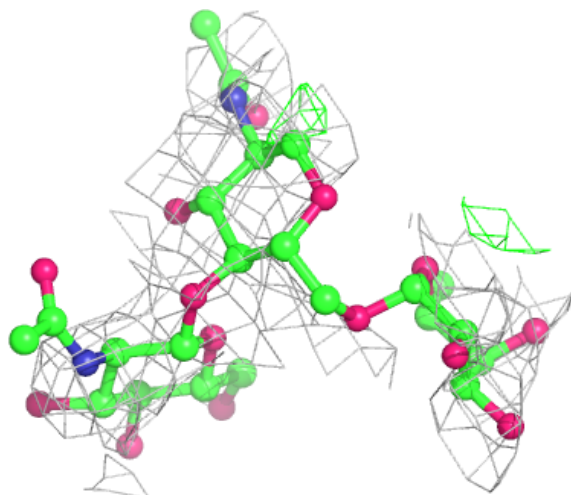
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	P	3	10/11	0.11	0.74	28,33,35,37	0
4	NAG	I	1	14/15	0.11	0.83	31,38,50,53	0
3	FUC	K	3	10/11	0.12	0.76	35,39,42,44	0
6	NAG	L	1	14/15	0.12	0.59	32,35,39,39	0
5	NAG	J	1	14/15	0.19	0.56	38,41,47,48	0
5	BMA	J	3	11/12	0.23	0.49	65,69,72,72	0
7	NAG	M	3	14/15	0.25	1.03	46,48,50,50	0
4	FUC	I	2	10/11	0.27	0.76	44,47,49,50	0
3	NAG	N	2	14/15	0.33	0.52	38,39,42,42	0
3	NAG	P	2	14/15	0.34	0.76	45,47,49,49	0
3	NAG	K	1	14/15	0.34	0.58	31,35,39,46	0
3	FUC	O	3	10/11	0.35	0.73	26,31,33,34	0
7	NAG	M	1	14/15	0.39	0.42	35,41,45,46	0
6	NAG	L	2	14/15	0.40	0.55	37,41,45,48	0
5	NAG	J	2	14/15	0.41	0.58	45,55,61,65	0
3	NAG	P	1	14/15	0.42	0.46	38,42,45,46	0
3	NAG	N	1	14/15	0.43	0.44	37,40,42,48	0
3	NAG	K	2	14/15	0.43	0.56	38,41,42,43	0
7	FUC	M	2	10/11	0.44	0.39	44,47,51,65	0
3	NAG	O	2	14/15	0.47	0.74	50,54,58,58	0
3	FUC	N	3	10/11	0.53	0.44	36,39,42,45	0
3	NAG	O	1	14/15	0.53	0.54	36,41,45,47	0
5	FUC	J	4	10/11	0.64	0.45	27,33,38,39	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.

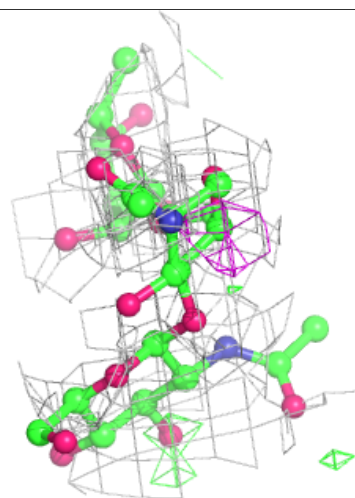
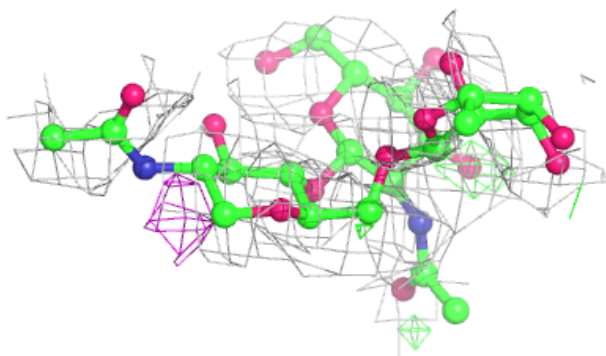
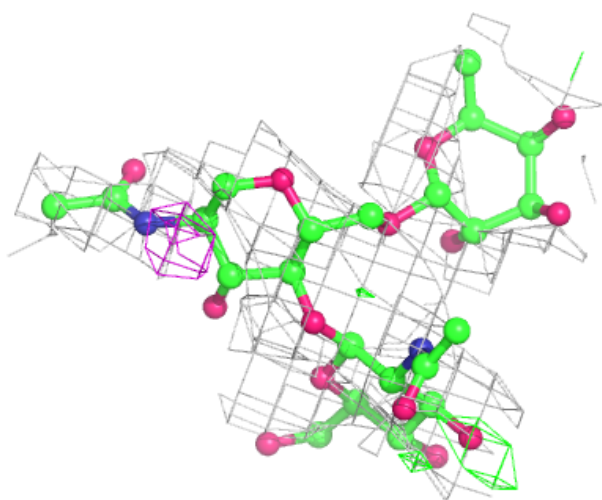
Electron density around Chain P:

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



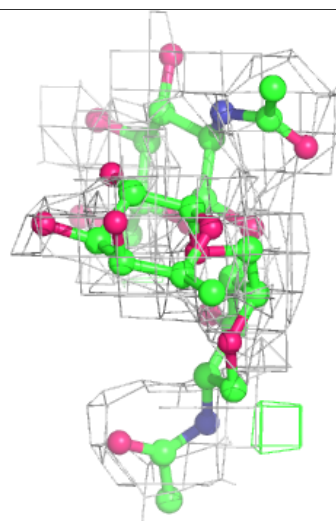
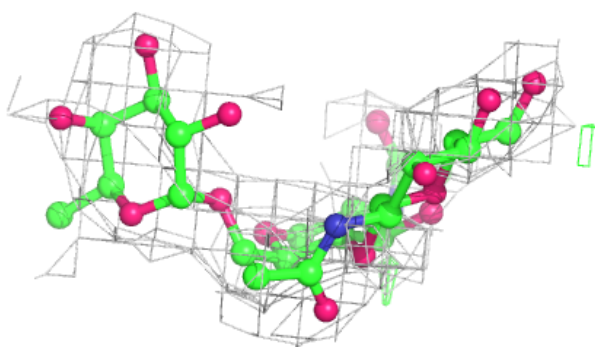
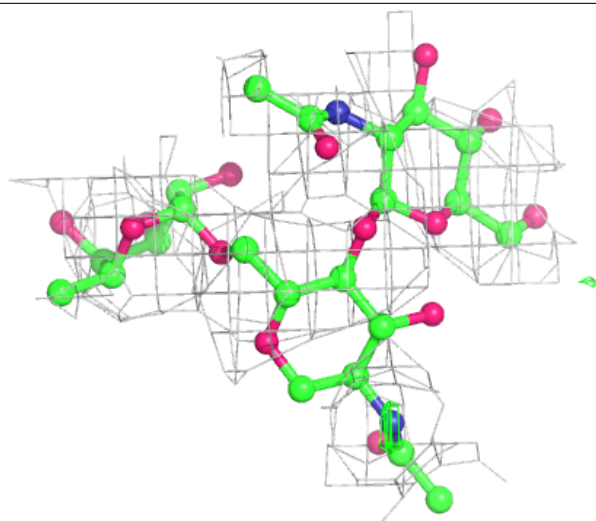
Electron density around Chain K:

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



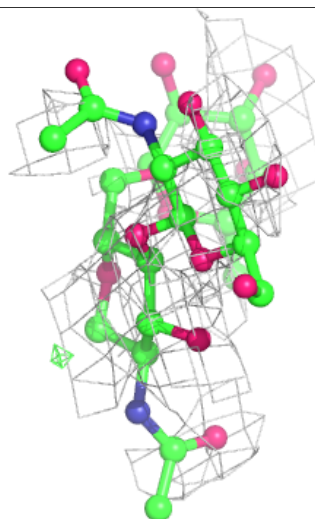
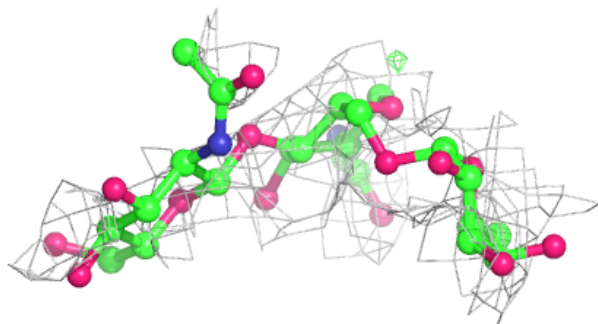
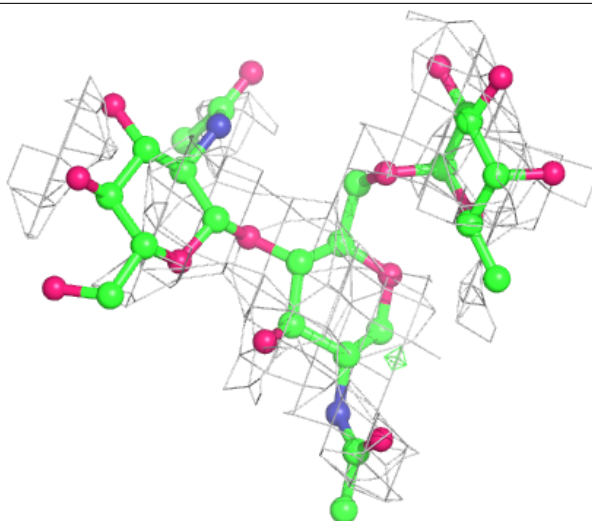
Electron density around Chain N:

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



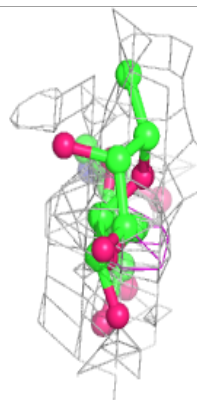
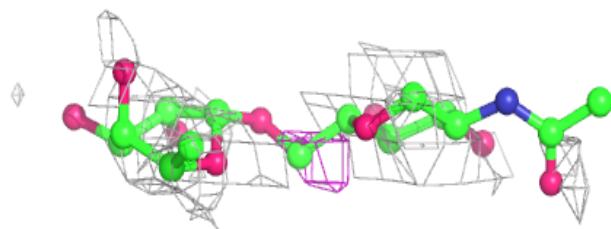
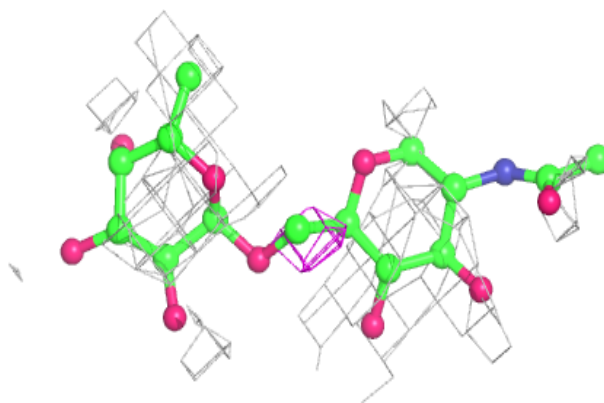
Electron density around Chain O:

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



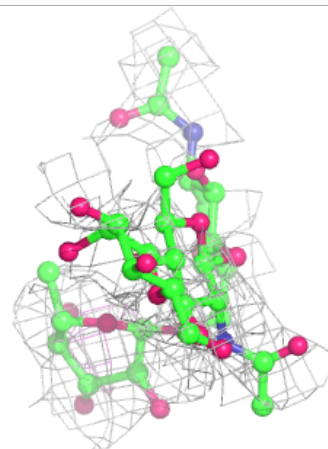
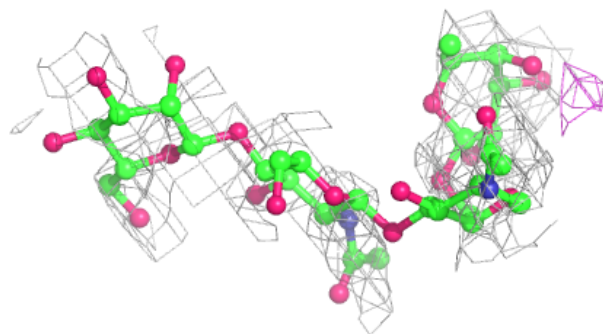
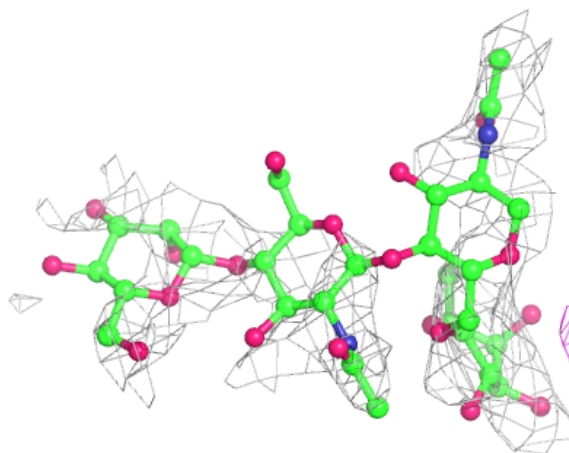
Electron density around Chain I:

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



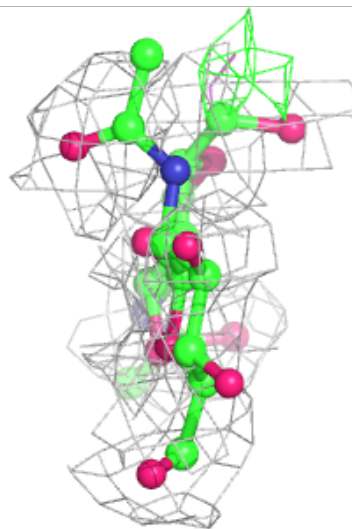
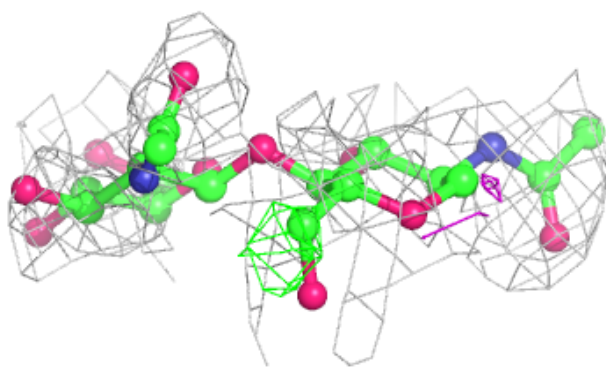
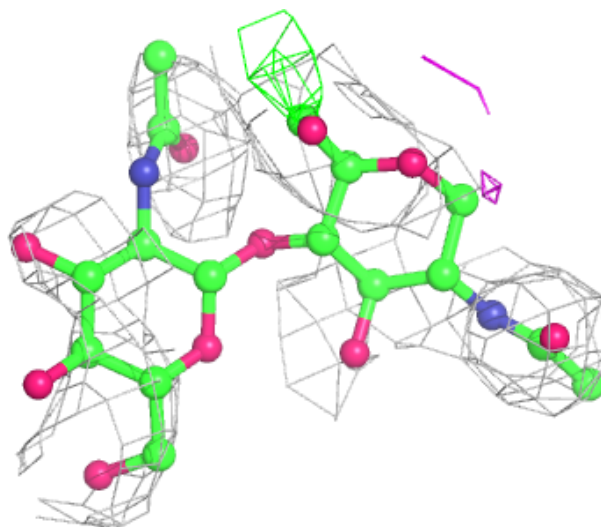
Electron density around Chain J:

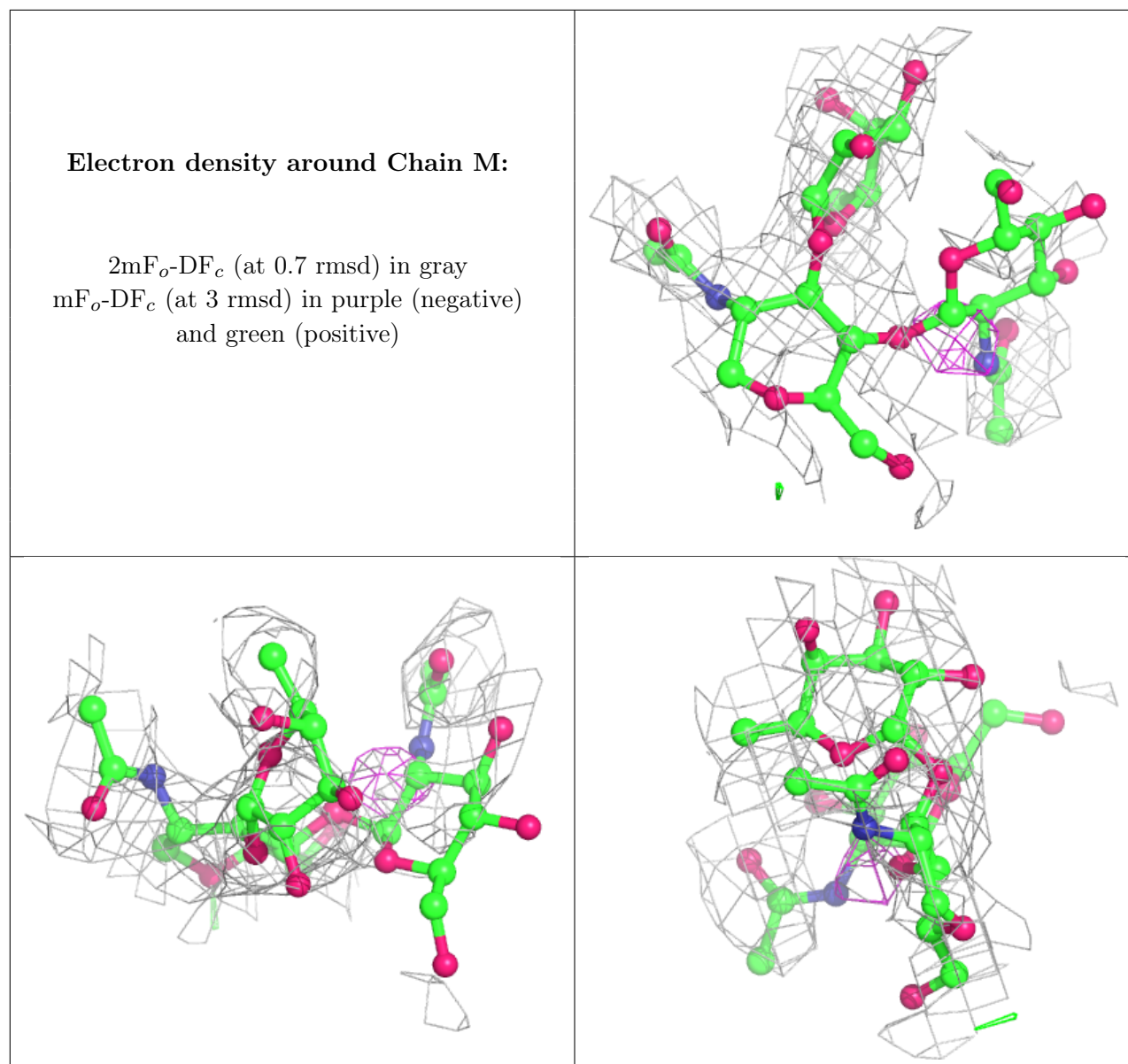
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o-DF_c$ (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
9	SO4	C	302	5/5	0.21	0.89	58,58,67,70	0
8	GOL	C	301	6/6	0.26	0.77	31,33,33,34	0
8	GOL	B	305	6/6	0.30	0.44	14,15,15,15	0
9	SO4	B	302	5/5	0.34	0.67	31,31,37,40	0
9	SO4	D	302	5/5	0.42	0.77	40,53,54,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	303	6/6	0.47	0.49	20,22,26,33	0
8	GOL	A	301	6/6	0.50	0.54	24,26,28,28	0
8	GOL	D	301	6/6	0.56	0.55	17,20,20,21	0
8	GOL	B	304	6/6	0.57	0.34	12,13,15,15	0
9	SO4	B	301	5/5	0.66	0.50	39,42,44,56	0
9	SO4	C	303	5/5	0.67	0.45	41,43,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.