



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 04:47 PM EDT

PDB ID : 9YOI / pdb_00009yoi
Title : Crystal structure of H3 hemagglutinin with HA2 N95L mutation from the influenza virus A/Hong Kong/1/1968 (H3N2)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2025-10-13
Resolution : 2.29 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

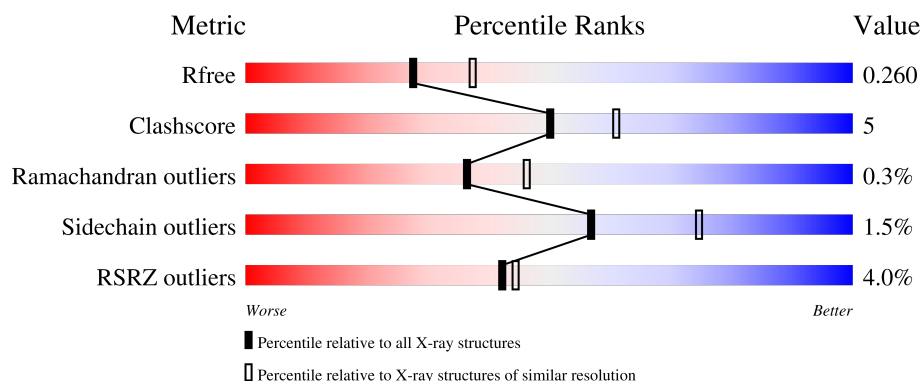
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	322	
1	C	322	
1	E	322	
2	B	196	
2	D	196	

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Mol	Chain	Length	Quality of chain
2	F	196	5% 72% 16% 12%
3	G	4	50% 50%
4	H	2	100%
4	K	2	50% 50%
5	I	5	20% 80%
6	J	6	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12133 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	319	Total	C	N	O	S	0	0	0
			2460	1541	432	474	13			
1	A	320	Total	C	N	O	S	0	0	0
			2469	1546	434	476	13			
1	E	318	Total	C	N	O	S	0	0	0
			2452	1537	431	471	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	186	Total	C	N	O	S	0	0	0
			1491	928	261	296	6			
2	B	173	Total	C	N	O	S	0	0	0
			1406	875	246	279	6			
2	F	173	Total	C	N	O	S	0	0	0
			1406	875	246	279	6			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	95	LEU	ASN	engineered mutation	UNP Q91MA7
D	176	VAL	-	expression tag	UNP Q91MA7
D	177	SER	-	expression tag	UNP Q91MA7
D	178	GLY	-	expression tag	UNP Q91MA7
D	179	GLY	-	expression tag	UNP Q91MA7
D	180	GLY	-	expression tag	UNP Q91MA7
D	181	GLY	-	expression tag	UNP Q91MA7
D	182	LEU	-	expression tag	UNP Q91MA7
D	183	ASN	-	expression tag	UNP Q91MA7
D	184	ASP	-	expression tag	UNP Q91MA7
D	185	ILE	-	expression tag	UNP Q91MA7
D	186	PHE	-	expression tag	UNP Q91MA7
D	187	GLU	-	expression tag	UNP Q91MA7
D	188	ALA	-	expression tag	UNP Q91MA7
D	189	GLN	-	expression tag	UNP Q91MA7
D	190	LYS	-	expression tag	UNP Q91MA7
D	191	ILE	-	expression tag	UNP Q91MA7
D	192	GLU	-	expression tag	UNP Q91MA7
D	193	TRP	-	expression tag	UNP Q91MA7
D	194	HIS	-	expression tag	UNP Q91MA7
D	195	GLU	-	expression tag	UNP Q91MA7
D	196	ARG	-	expression tag	UNP Q91MA7
B	95	LEU	ASN	engineered mutation	UNP Q91MA7
B	176	VAL	-	expression tag	UNP Q91MA7
B	177	SER	-	expression tag	UNP Q91MA7
B	178	GLY	-	expression tag	UNP Q91MA7
B	179	GLY	-	expression tag	UNP Q91MA7
B	180	GLY	-	expression tag	UNP Q91MA7
B	181	GLY	-	expression tag	UNP Q91MA7
B	182	LEU	-	expression tag	UNP Q91MA7
B	183	ASN	-	expression tag	UNP Q91MA7
B	184	ASP	-	expression tag	UNP Q91MA7
B	185	ILE	-	expression tag	UNP Q91MA7
B	186	PHE	-	expression tag	UNP Q91MA7
B	187	GLU	-	expression tag	UNP Q91MA7
B	188	ALA	-	expression tag	UNP Q91MA7
B	189	GLN	-	expression tag	UNP Q91MA7
B	190	LYS	-	expression tag	UNP Q91MA7
B	191	ILE	-	expression tag	UNP Q91MA7
B	192	GLU	-	expression tag	UNP Q91MA7
B	193	TRP	-	expression tag	UNP Q91MA7
B	194	HIS	-	expression tag	UNP Q91MA7
B	195	GLU	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	196	ARG	-	expression tag	UNP Q91MA7
F	95	LEU	ASN	engineered mutation	UNP Q91MA7
F	176	VAL	-	expression tag	UNP Q91MA7
F	177	SER	-	expression tag	UNP Q91MA7
F	178	GLY	-	expression tag	UNP Q91MA7
F	179	GLY	-	expression tag	UNP Q91MA7
F	180	GLY	-	expression tag	UNP Q91MA7
F	181	GLY	-	expression tag	UNP Q91MA7
F	182	LEU	-	expression tag	UNP Q91MA7
F	183	ASN	-	expression tag	UNP Q91MA7
F	184	ASP	-	expression tag	UNP Q91MA7
F	185	ILE	-	expression tag	UNP Q91MA7
F	186	PHE	-	expression tag	UNP Q91MA7
F	187	GLU	-	expression tag	UNP Q91MA7
F	188	ALA	-	expression tag	UNP Q91MA7
F	189	GLN	-	expression tag	UNP Q91MA7
F	190	LYS	-	expression tag	UNP Q91MA7
F	191	ILE	-	expression tag	UNP Q91MA7
F	192	GLU	-	expression tag	UNP Q91MA7
F	193	TRP	-	expression tag	UNP Q91MA7
F	194	HIS	-	expression tag	UNP Q91MA7
F	195	GLU	-	expression tag	UNP Q91MA7
F	196	ARG	-	expression tag	UNP Q91MA7

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



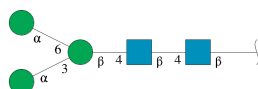
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



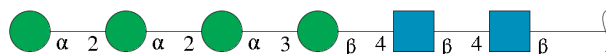
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	33	Total	O	0	0
			33	33		
8	D	6	Total	O	0	0
			6	6		
8	A	14	Total	O	0	0
			14	14		
8	B	25	Total	O	0	0
			25	25		
8	E	15	Total	O	0	0
			15	15		

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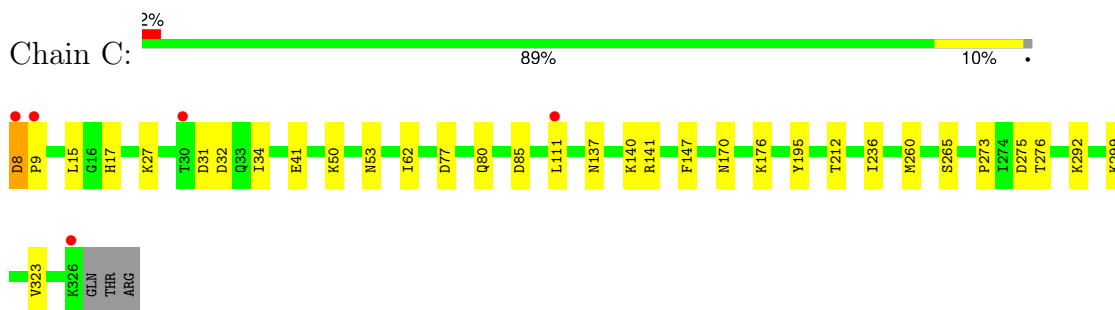
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	19	Total	O	0	0
			19	19		

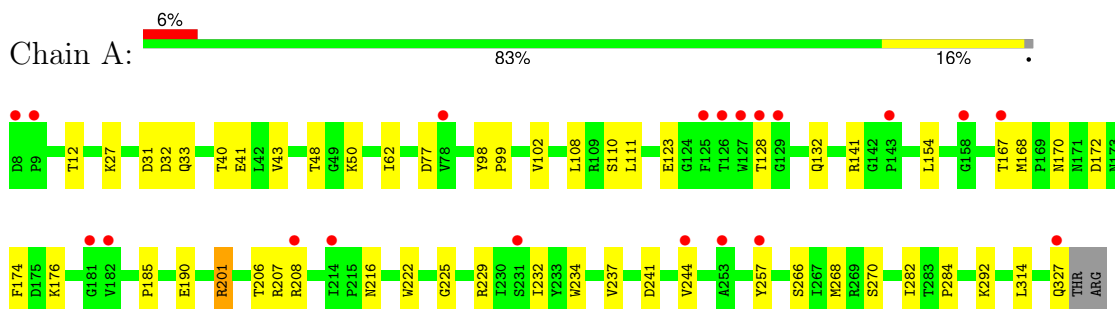
3 Residue-property plots [i](#)

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.

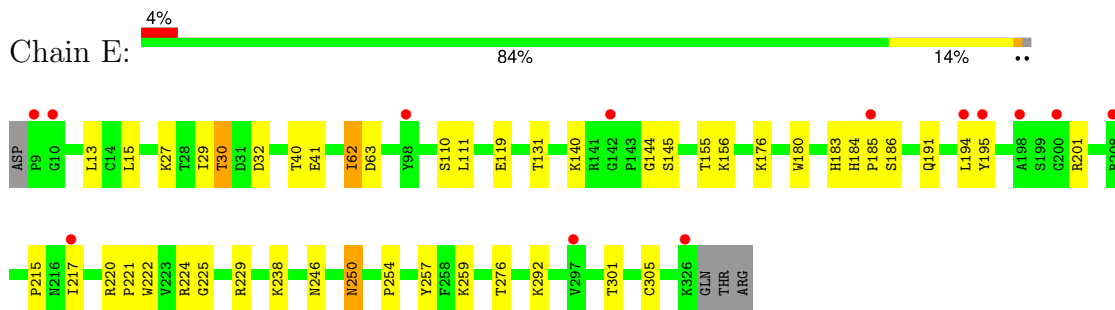
- Molecule 1: Hemagglutinin HA1



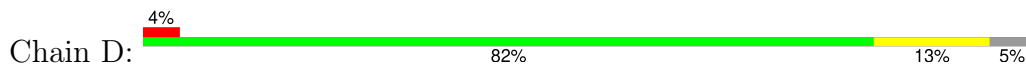
- Molecule 1: Hemagglutinin HA1

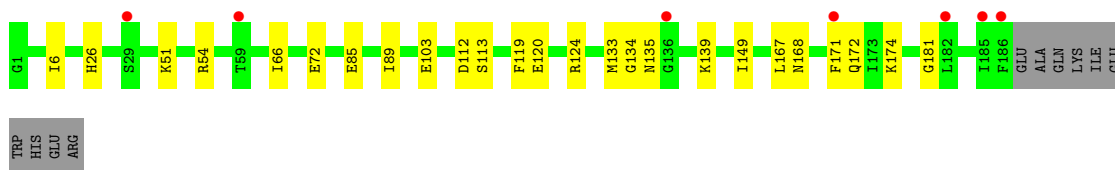


- Molecule 1: Hemagglutinin HA1

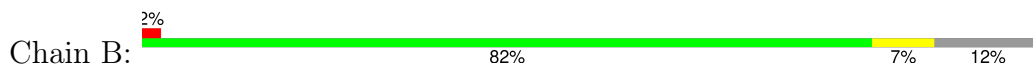


- Molecule 2: Hemagglutinin HA2

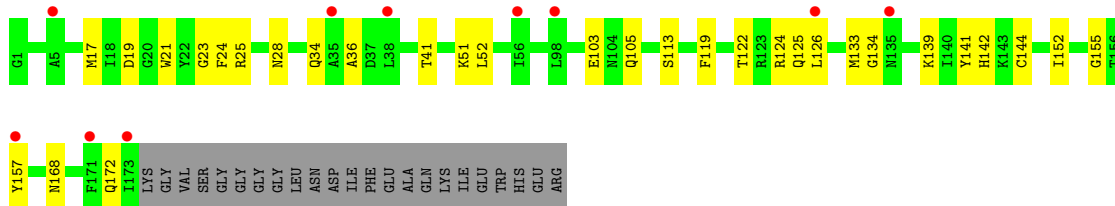




- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



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



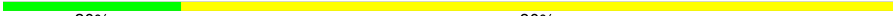
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  20% 80%

MAN1
MAN2
MAN3
MAN4
MAN5

- Molecule 6: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  50% 50%

MAN1
MAN2
MAN3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.84Å 114.16Å 235.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.16 – 2.29 45.16 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.16-2.29) 98.8 (45.16-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.224 , 0.262 0.222 , 0.260	Depositor DCC
R_{free} test set	4448 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12133	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/2526	0.38	0/3442
1	C	0.19	0/2517	0.37	0/3430
1	E	0.16	0/2509	0.38	0/3418
2	B	0.15	0/1430	0.35	0/1922
2	D	0.14	0/1516	0.35	0/2036
2	F	0.15	0/1430	0.34	0/1922
All	All	0.17	0/11928	0.37	0/16170

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	2469	0	2414	32	0
1	C	2460	0	2406	21	0
1	E	2452	0	2403	37	0
2	B	1406	0	1333	10	0
2	D	1491	0	1416	19	0
2	F	1406	0	1333	20	0
3	G	50	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	K	28	0	25	2	0
5	I	61	0	52	3	0
6	J	72	0	61	0	0
7	A	28	0	26	1	0
7	C	42	0	39	1	0
7	E	28	0	26	1	0
8	A	14	0	0	0	0
8	B	25	0	0	0	0
8	C	33	0	0	2	0
8	D	6	0	0	0	0
8	E	15	0	0	0	0
8	F	19	0	0	0	0
All	All	12133	0	11602	124	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 124 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:A:207:ARG:HD3	1:A:208:ARG:HG3	1.48	0.95
1:E:215:PRO:HG2	1:E:250:ASN:HD22	1.41	0.85
1:C:111:LEU:HD11	1:C:236:ILE:HD11	1.66	0.78
1:A:167:THR:HG22	1:A:244:VAL:HG22	1.69	0.73
1:A:185:PRO:HB3	1:A:190:GLU:HG2	1.71	0.71

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	318/322 (99%)	306 (96%)	11 (4%)	1 (0%)	36	46
1	C	317/322 (98%)	310 (98%)	5 (2%)	2 (1%)	21	27
1	E	316/322 (98%)	309 (98%)	6 (2%)	1 (0%)	36	46
2	B	171/196 (87%)	164 (96%)	7 (4%)	0	100	100
2	D	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
2	F	171/196 (87%)	161 (94%)	10 (6%)	0	100	100
All	All	1477/1554 (95%)	1428 (97%)	45 (3%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	9	PRO
1	C	62	ILE
1	A	62	ILE
1	E	62	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	281/283 (99%)	276 (98%)	5 (2%)	51	70
1	C	280/283 (99%)	277 (99%)	3 (1%)	65	81
1	E	279/283 (99%)	272 (98%)	7 (2%)	42	60
2	B	148/165 (90%)	146 (99%)	2 (1%)	59	76
2	D	156/165 (94%)	155 (99%)	1 (1%)	78	89
2	F	148/165 (90%)	146 (99%)	2 (1%)	59	76
All	All	1292/1344 (96%)	1272 (98%)	20 (2%)	57	75

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	186	SER

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Mol	Chain	Res	Type
1	E	276	THR
2	F	113	SER
2	F	28	ASN
1	A	128	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	GLN
1	E	191	GLN
1	E	188	ASN
1	E	211	GLN
2	D	135	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 ⓘ

19 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	$\# Z > 2$
3	NAG	G	1	3,1	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.53	0
3	BMA	G	3	3	11,11,12	0.57	0	15,15,17	0.74	0
3	MAN	G	4	3	11,11,12	0.78	0	15,15,17	1.07	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	4,1	14,14,15	0.37	0	17,19,21	0.53	0
4	NAG	H	2	4	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	I	1	5,1	14,14,15	0.35	0	17,19,21	0.54	0
5	NAG	I	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	I	3	5	11,11,12	0.54	0	15,15,17	0.82	0
5	MAN	I	4	5	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
5	MAN	I	5	5	11,11,12	0.76	0	15,15,17	0.90	1 (6%)
6	NAG	J	1	6,1	14,14,15	0.34	0	17,19,21	0.40	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.45	0
6	BMA	J	3	6	11,11,12	0.46	0	15,15,17	0.70	0
6	MAN	J	4	6	11,11,12	0.71	0	15,15,17	1.14	2 (13%)
6	MAN	J	5	6	11,11,12	0.85	0	15,15,17	0.93	1 (6%)
6	MAN	J	6	6	11,11,12	0.91	0	15,15,17	1.20	1 (6%)
4	NAG	K	1	4,1	14,14,15	0.40	0	17,19,21	0.43	0
4	NAG	K	2	4	14,14,15	0.43	0	17,19,21	1.36	2 (11%)

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
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	1/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	K	2	NAG	C2-N2-C7	4.68	129.18	122.90
6	J	6	MAN	C1-O5-C5	3.65	117.08	112.19
3	G	4	MAN	C1-O5-C5	3.25	116.54	112.19
5	I	4	MAN	C1-O5-C5	2.90	116.08	112.19
6	J	4	MAN	C1-O5-C5	2.88	116.04	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

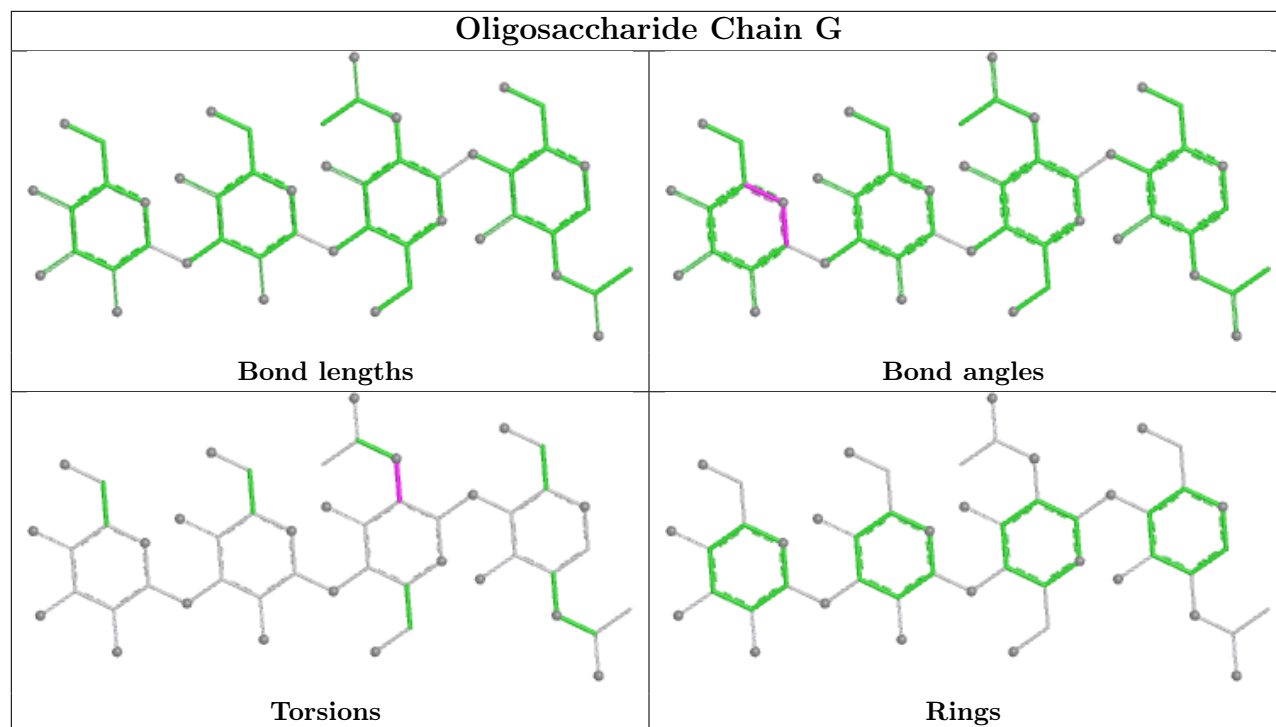
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
5	I	4	MAN	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7

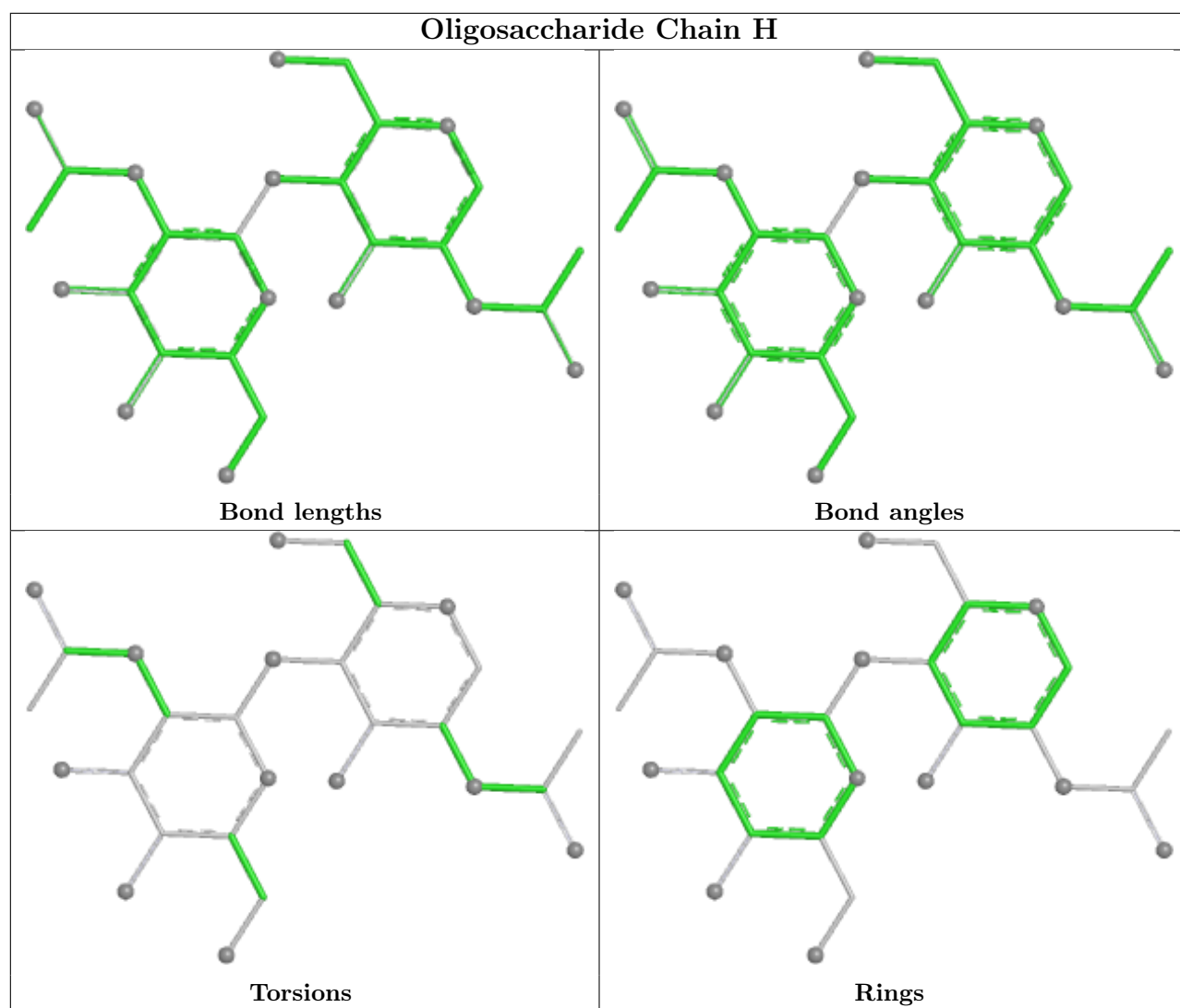
There are no ring outliers.

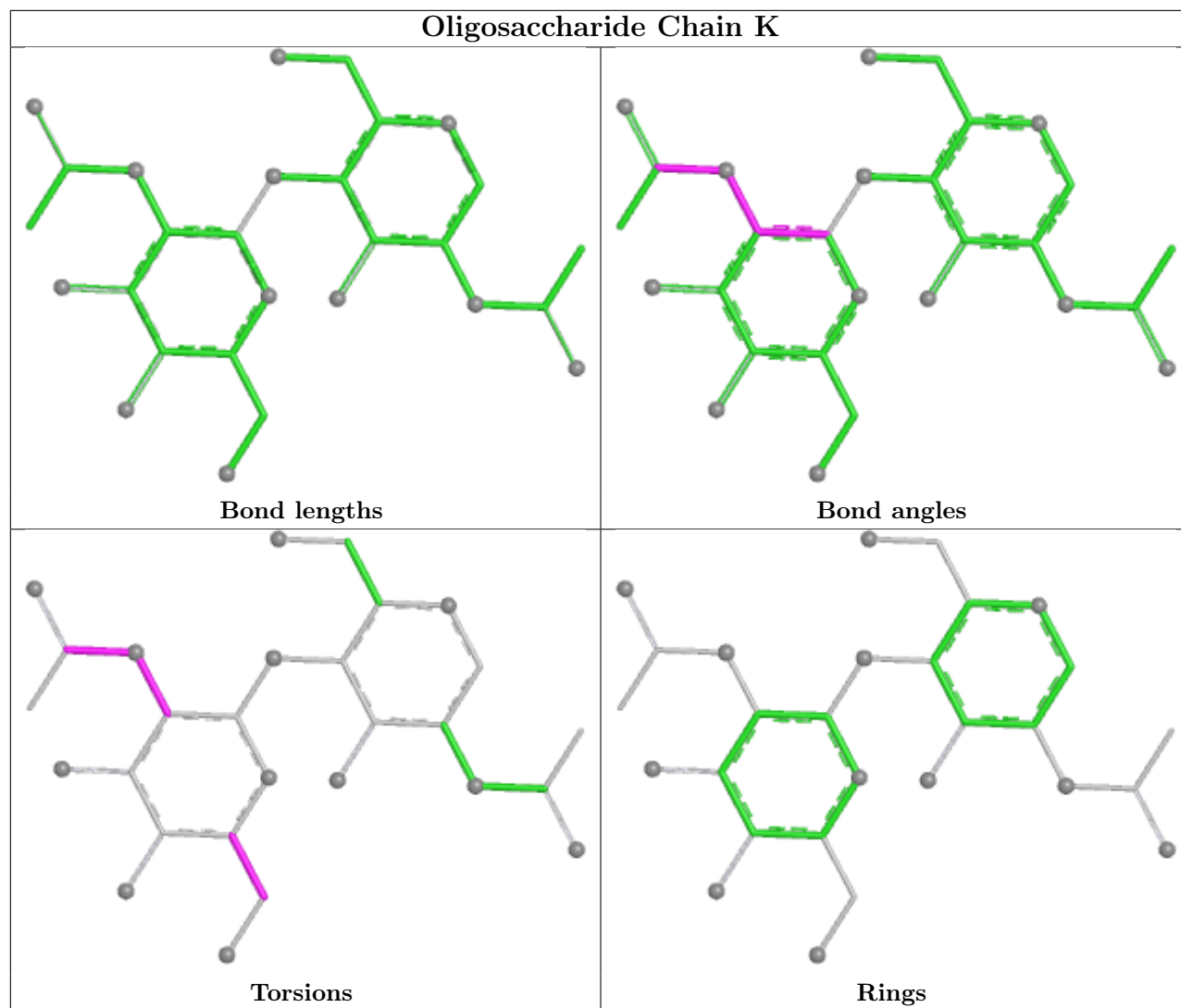
5 monomers are involved in 6 short contacts:

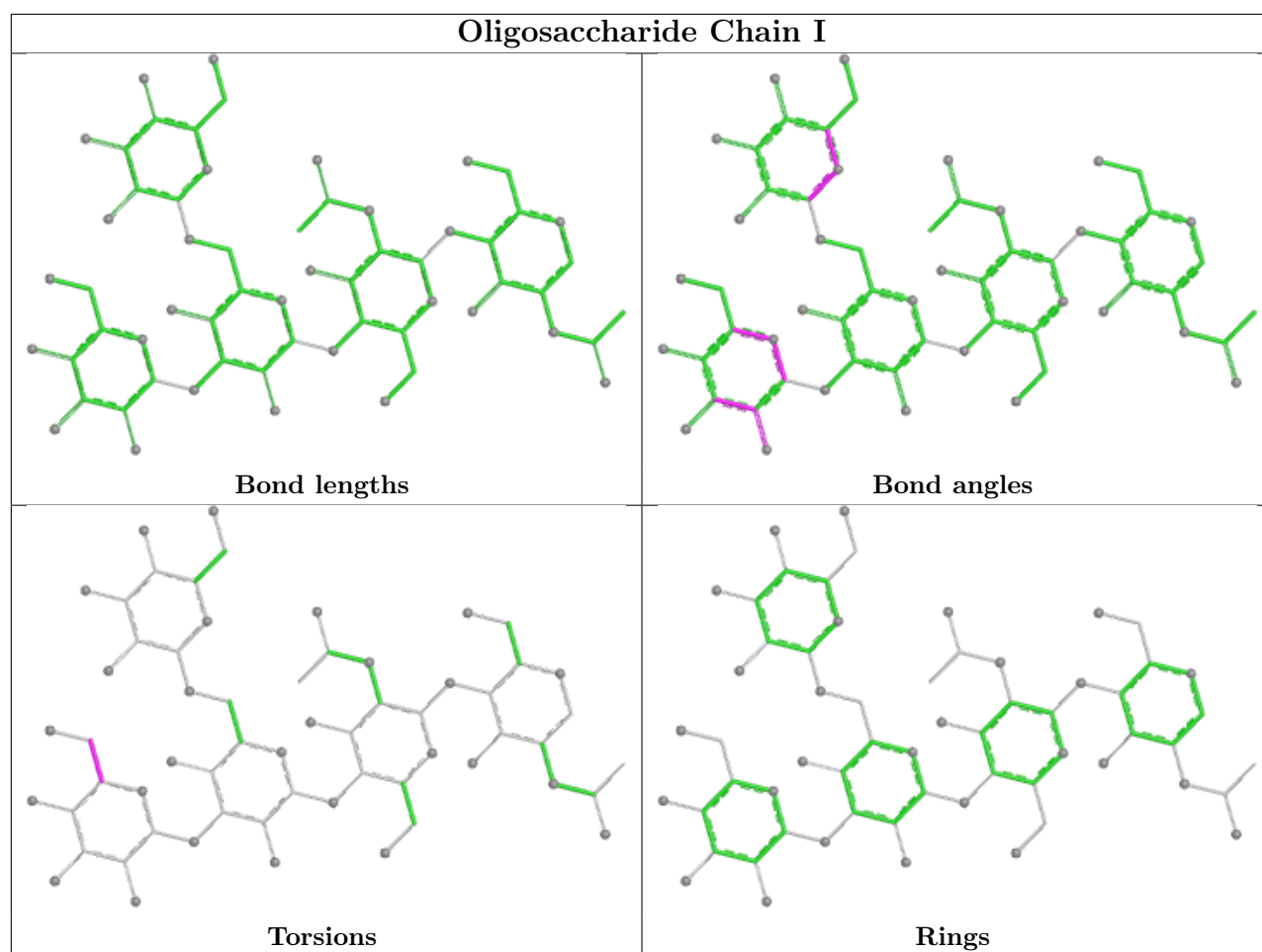
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	2	0
4	K	1	NAG	1	0
5	I	1	NAG	1	0
3	G	2	NAG	1	0
4	K	2	NAG	2	0

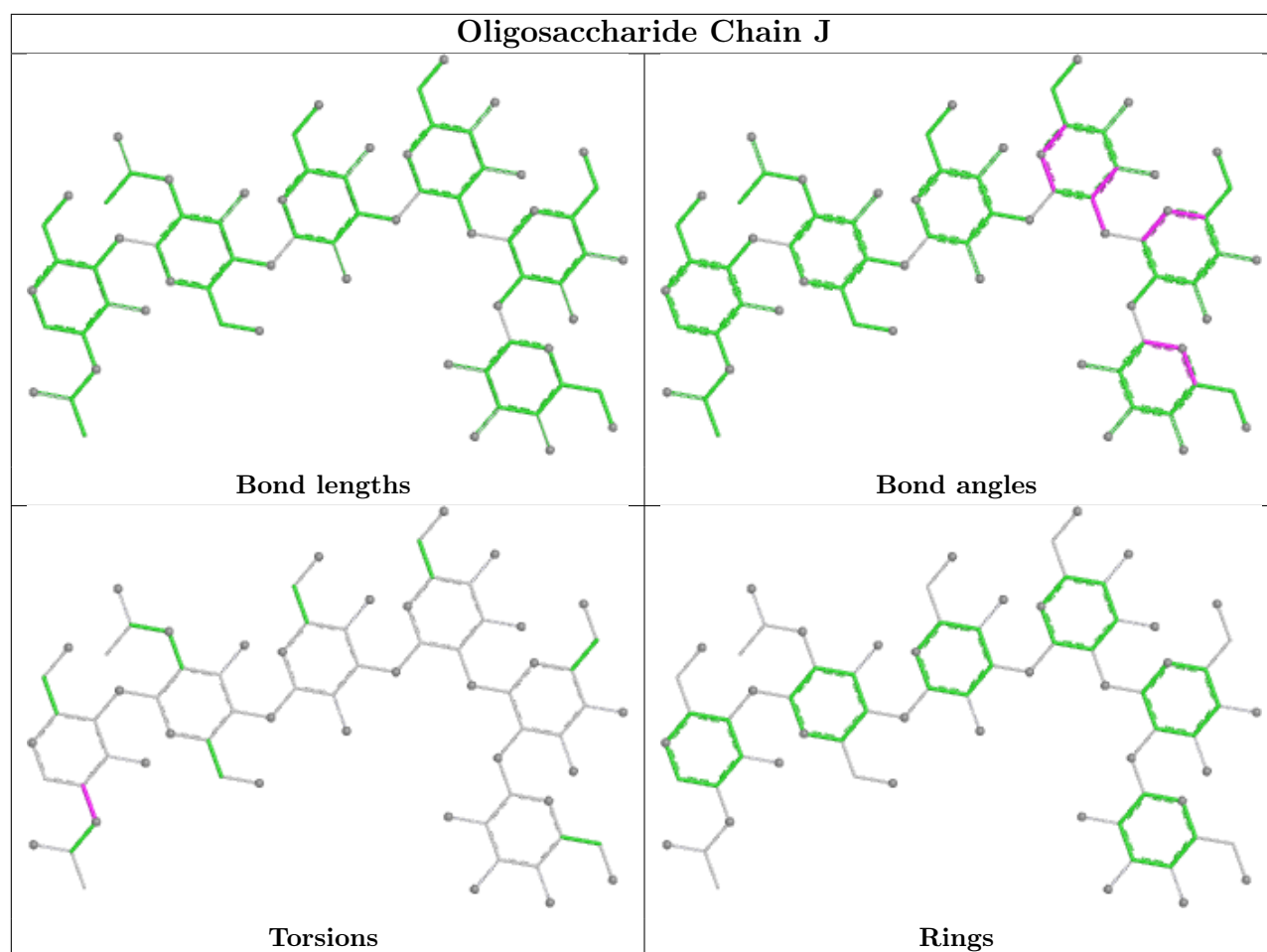
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	402	1	14,14,15	0.42	0	17,19,21	0.38	0
7	NAG	E	401	1	14,14,15	0.59	0	17,19,21	1.39	2 (11%)
7	NAG	A	402	1	14,14,15	0.41	0	17,19,21	0.52	0
7	NAG	A	401	1	14,14,15	0.54	0	17,19,21	1.40	3 (17%)
7	NAG	C	403	1	14,14,15	0.50	0	17,19,21	0.55	0
7	NAG	E	402	1	14,14,15	0.17	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	401	1	14,14,15	0.66	1 (7%)	17,19,21	1.36	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	402	1	-	2/6/23/26	0/1/1/1
7	NAG	E	401	1	-	6/6/23/26	0/1/1/1
7	NAG	A	402	1	-	0/6/23/26	0/1/1/1
7	NAG	A	401	1	-	6/6/23/26	0/1/1/1
7	NAG	C	403	1	-	2/6/23/26	0/1/1/1
7	NAG	E	402	1	-	0/6/23/26	0/1/1/1
7	NAG	C	401	1	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	NAG	C1-C2	2.06	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	401	NAG	C2-N2-C7	4.55	128.99	122.90
7	A	401	NAG	C2-N2-C7	4.54	128.98	122.90
7	C	401	NAG	C2-N2-C7	4.44	128.85	122.90
7	A	401	NAG	C1-C2-N2	2.23	113.95	110.43
7	E	401	NAG	C1-C2-N2	2.20	113.91	110.43

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	402	NAG	O5-C5-C6-O6
7	C	401	NAG	O5-C5-C6-O6
7	E	401	NAG	O5-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	C	402	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	401	NAG	1	0
7	A	401	NAG	1	0
7	C	401	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	320/322 (99%)	0.59	20 (6%) 26 28	49, 73, 106, 134	0
1	C	319/322 (99%)	0.16	5 (1%) 70 72	45, 60, 77, 131	0
1	E	318/322 (98%)	0.45	13 (4%) 41 43	53, 71, 105, 132	0
2	B	173/196 (88%)	0.38	4 (2%) 61 63	48, 66, 87, 98	0
2	D	186/196 (94%)	0.36	7 (3%) 44 46	49, 67, 88, 105	0
2	F	173/196 (88%)	0.57	10 (5%) 29 31	51, 72, 106, 120	0
All	All	1489/1554 (95%)	0.41	59 (3%) 42 44	45, 67, 101, 134	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	173	ILE	6.4
2	B	173	ILE	5.0
2	F	171	PHE	4.7
1	E	9	PRO	4.7
1	C	9	PRO	3.9

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

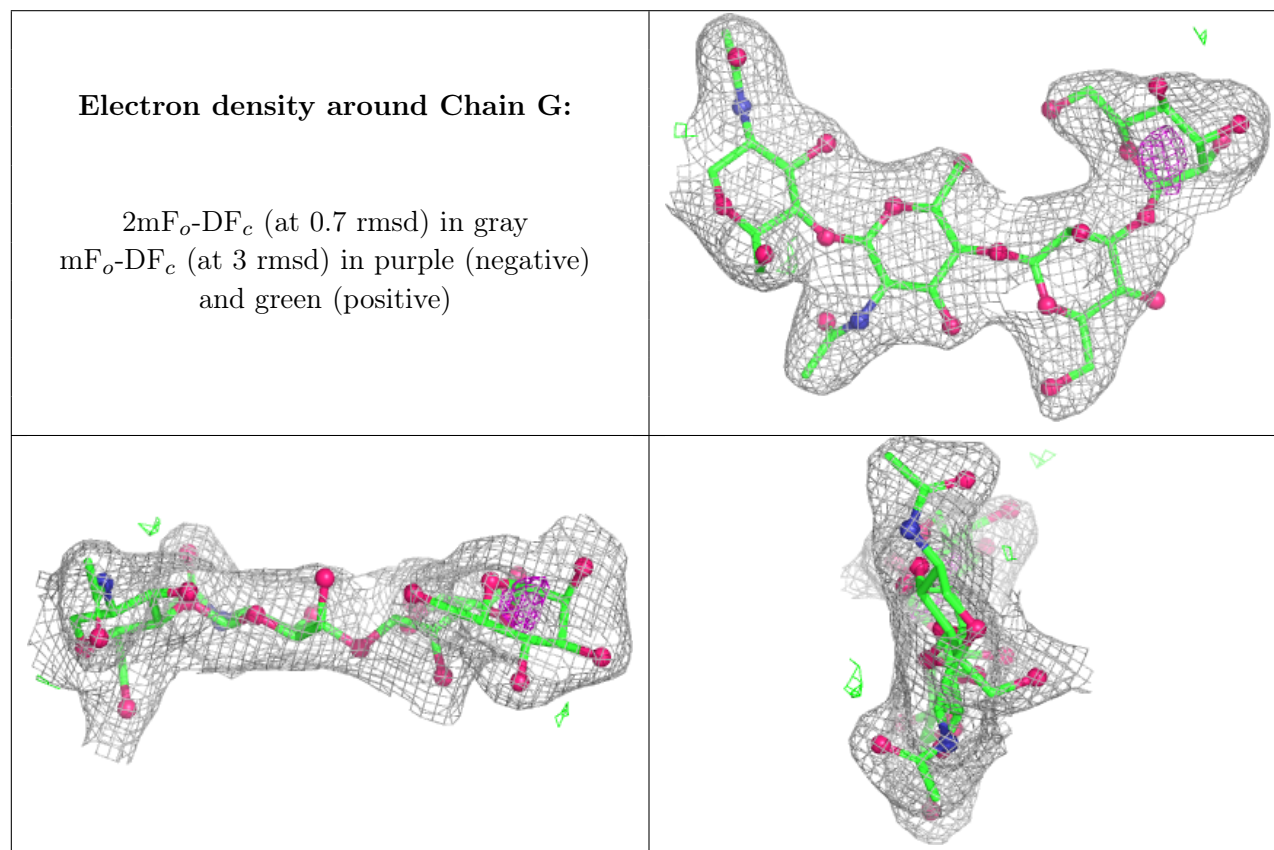
There are no non-standard protein/DNA/RNA residues in this entry.

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.

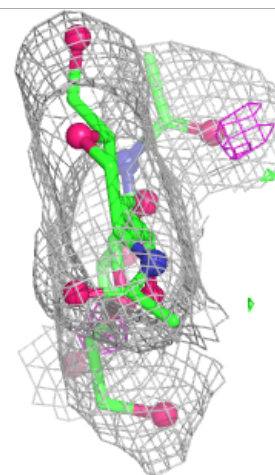
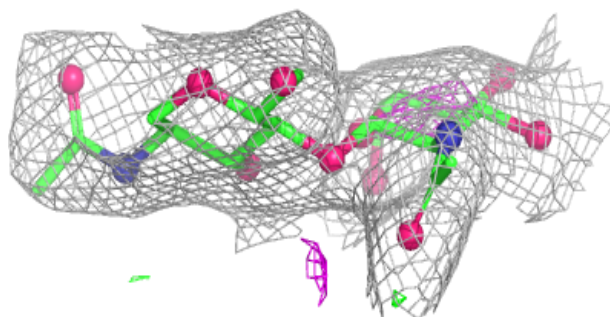
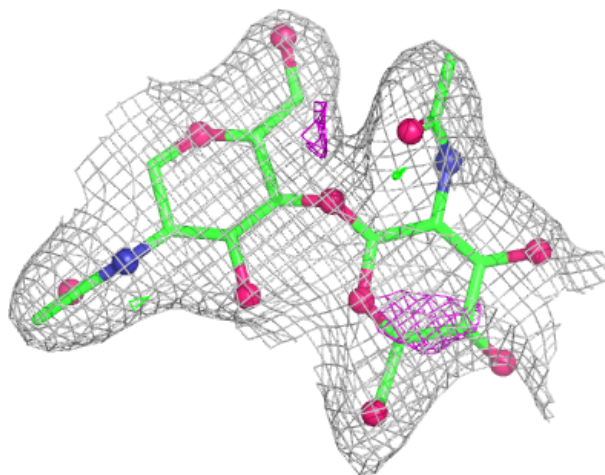
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	I	4	11/12	0.54	0.13	107,113,115,116	0
4	NAG	K	2	14/15	0.60	0.14	100,109,118,118	0
5	MAN	I	5	11/12	0.61	0.14	97,104,107,107	0
4	NAG	H	2	14/15	0.66	0.14	71,84,93,93	0
6	MAN	J	4	11/12	0.67	0.11	103,105,107,108	0
6	NAG	J	1	14/15	0.71	0.15	75,79,83,85	0
3	MAN	G	4	11/12	0.72	0.13	87,95,98,98	0
3	BMA	G	3	11/12	0.76	0.12	86,92,96,97	0
6	MAN	J	5	11/12	0.83	0.14	91,101,109,112	0
6	BMA	J	3	11/12	0.86	0.09	87,89,97,101	0
5	BMA	I	3	11/12	0.86	0.09	104,107,110,112	0
4	NAG	K	1	14/15	0.86	0.09	71,82,92,100	0
6	MAN	J	6	11/12	0.86	0.11	87,97,101,107	0
5	NAG	I	1	14/15	0.87	0.11	99,104,107,107	0
3	NAG	G	2	14/15	0.88	0.10	67,82,89,91	0
5	NAG	I	2	14/15	0.88	0.12	101,103,106,107	0
4	NAG	H	1	14/15	0.89	0.09	63,67,75,77	0
6	NAG	J	2	14/15	0.92	0.10	65,76,80,85	0
3	NAG	G	1	14/15	0.94	0.07	67,73,76,77	0

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



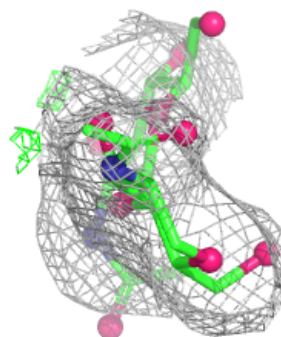
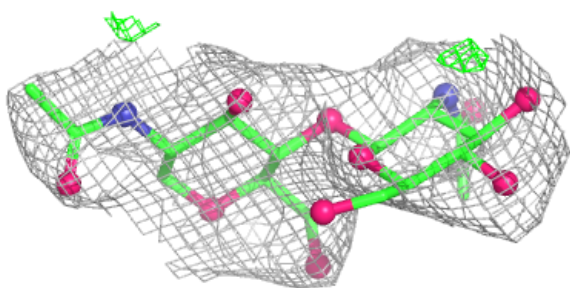
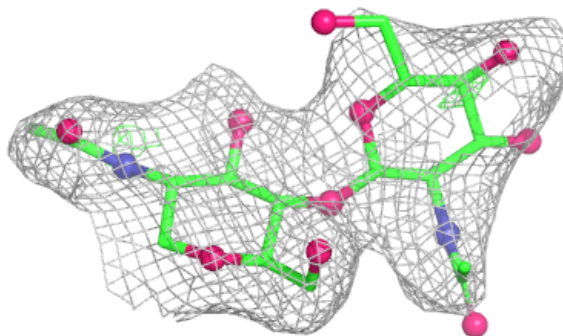
Electron density around Chain H:

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

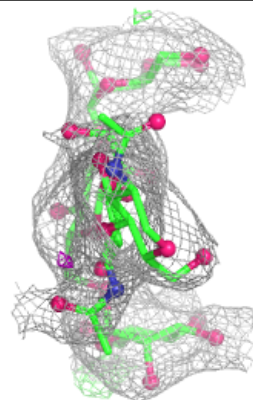
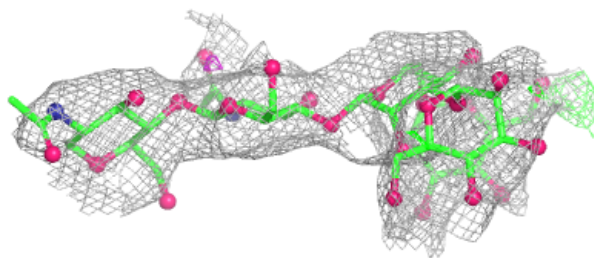
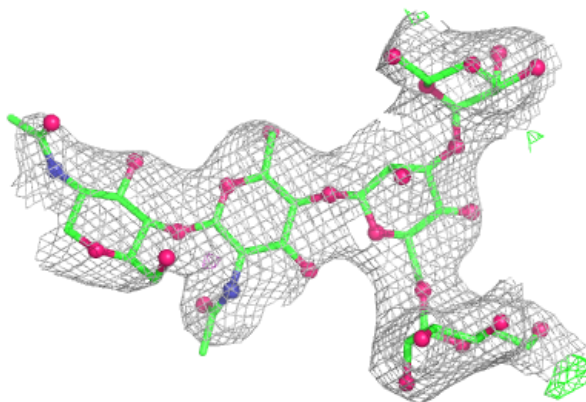


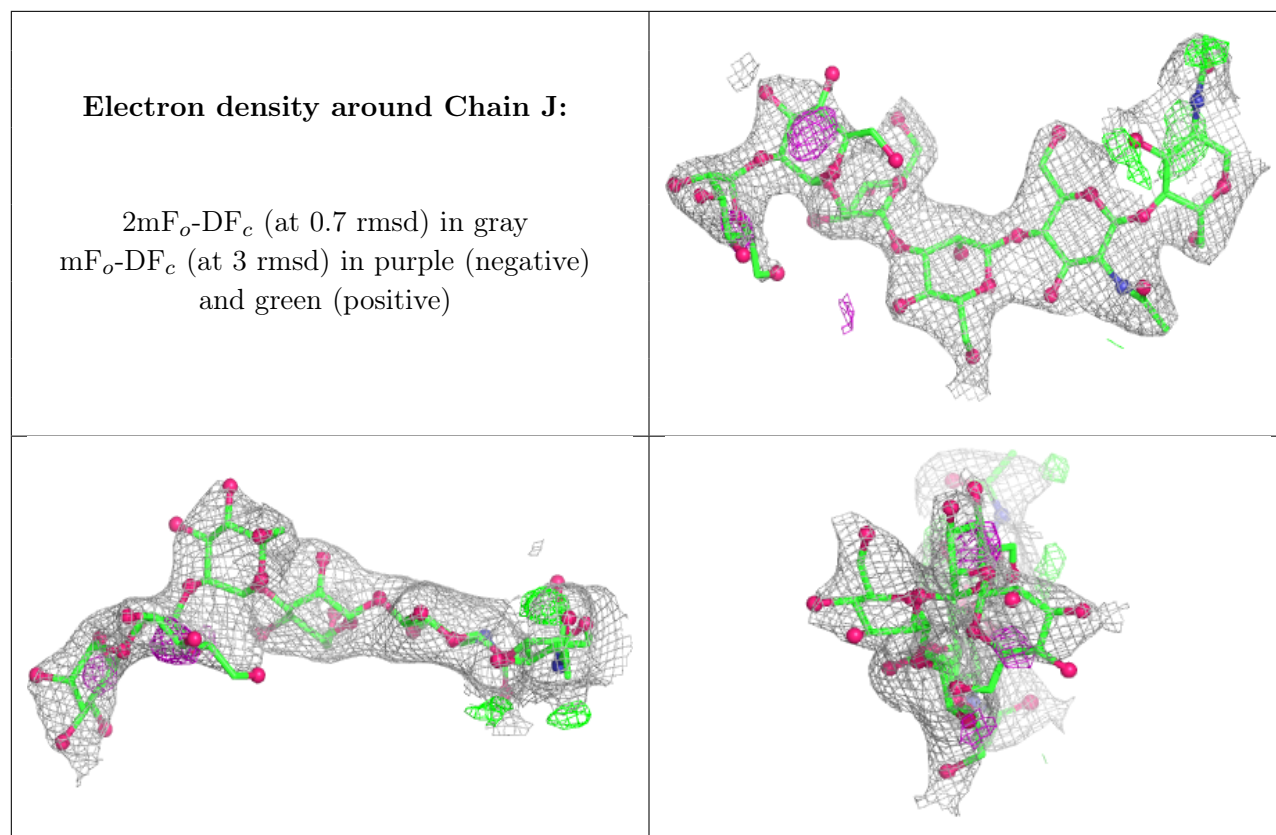
Electron density around Chain K:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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
7	NAG	C	403	14/15	0.37	0.20	93,96,104,104	0
7	NAG	A	401	14/15	0.37	0.21	122,129,132,133	0
7	NAG	E	401	14/15	0.40	0.19	88,93,99,100	0
7	NAG	C	401	14/15	0.45	0.17	94,109,115,118	0
7	NAG	E	402	14/15	0.56	0.17	85,95,101,102	0
7	NAG	A	402	14/15	0.59	0.15	84,89,95,96	0
7	NAG	C	402	14/15	0.76	0.12	64,70,75,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.