



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:28 AM BST

PDB ID : 6ONA
Title : Crystal structure of Influenza hemagglutinin from strain A/Hickox/JY2/1940
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2019-04-20
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

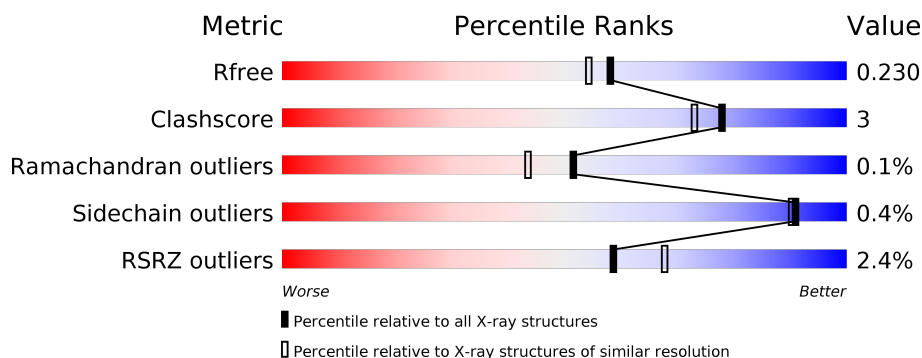
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	538	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 82% 7% 11% </div> </div>
1	B	538	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 83% 6% 11% </div> </div>
1	C	538	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 6% 10% </div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="text-align: center;">100%</div> </div>
2	E	3	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="text-align: center;">100%</div> </div>
3	F	2	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="text-align: center;">100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%

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	F	2	-	-	-	X
4	NAG	A	501	-	-	-	X
4	NAG	A	506	-	-	-	X
4	NAG	C	513	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12176 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3708	2333	649	707	19			
1	B	480	Total	C	N	O	S	0	1	0
			3713	2344	642	707	20			
1	C	485	Total	C	N	O	S	0	0	0
			3757	2365	648	725	19			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q0HD60
A	2	SER	-	expression tag	UNP Q0HD60
A	495	PHE	-	linker	UNP Q0HD60
A	496	LEU	-	linker	UNP Q0HD60
A	497	VAL	-	linker	UNP Q0HD60
A	498	PRO	-	linker	UNP Q0HD60
A	499	ARG	-	linker	UNP Q0HD60
A	500	GLY	-	linker	UNP Q0HD60
A	501	SER	-	linker	UNP Q0HD60
A	502	PRO	-	linker	UNP Q0HD60
A	503	GLY	-	linker	UNP Q0HD60
A	504	SER	-	linker	UNP Q0HD60
A	533	HIS	-	expression tag	UNP M1E1E4
A	534	HIS	-	expression tag	UNP M1E1E4
A	535	HIS	-	expression tag	UNP M1E1E4
A	536	HIS	-	expression tag	UNP M1E1E4
A	537	HIS	-	expression tag	UNP M1E1E4
A	538	HIS	-	expression tag	UNP M1E1E4
B	1	GLY	-	expression tag	UNP Q0HD60
B	2	SER	-	expression tag	UNP Q0HD60
B	495	PHE	-	linker	UNP Q0HD60
B	496	LEU	-	linker	UNP Q0HD60
B	497	VAL	-	linker	UNP Q0HD60

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	PRO	-	linker	UNP Q0HD60
B	499	ARG	-	linker	UNP Q0HD60
B	500	GLY	-	linker	UNP Q0HD60
B	501	SER	-	linker	UNP Q0HD60
B	502	PRO	-	linker	UNP Q0HD60
B	503	GLY	-	linker	UNP Q0HD60
B	504	SER	-	linker	UNP Q0HD60
B	533	HIS	-	expression tag	UNP M1E1E4
B	534	HIS	-	expression tag	UNP M1E1E4
B	535	HIS	-	expression tag	UNP M1E1E4
B	536	HIS	-	expression tag	UNP M1E1E4
B	537	HIS	-	expression tag	UNP M1E1E4
B	538	HIS	-	expression tag	UNP M1E1E4
C	1	GLY	-	expression tag	UNP Q0HD60
C	2	SER	-	expression tag	UNP Q0HD60
C	495	PHE	-	linker	UNP Q0HD60
C	496	LEU	-	linker	UNP Q0HD60
C	497	VAL	-	linker	UNP Q0HD60
C	498	PRO	-	linker	UNP Q0HD60
C	499	ARG	-	linker	UNP Q0HD60
C	500	GLY	-	linker	UNP Q0HD60
C	501	SER	-	linker	UNP Q0HD60
C	502	PRO	-	linker	UNP Q0HD60
C	503	GLY	-	linker	UNP Q0HD60
C	504	SER	-	linker	UNP Q0HD60
C	533	HIS	-	expression tag	UNP M1E1E4
C	534	HIS	-	expression tag	UNP M1E1E4
C	535	HIS	-	expression tag	UNP M1E1E4
C	536	HIS	-	expression tag	UNP M1E1E4
C	537	HIS	-	expression tag	UNP M1E1E4
C	538	HIS	-	expression tag	UNP M1E1E4

- Molecule 2 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
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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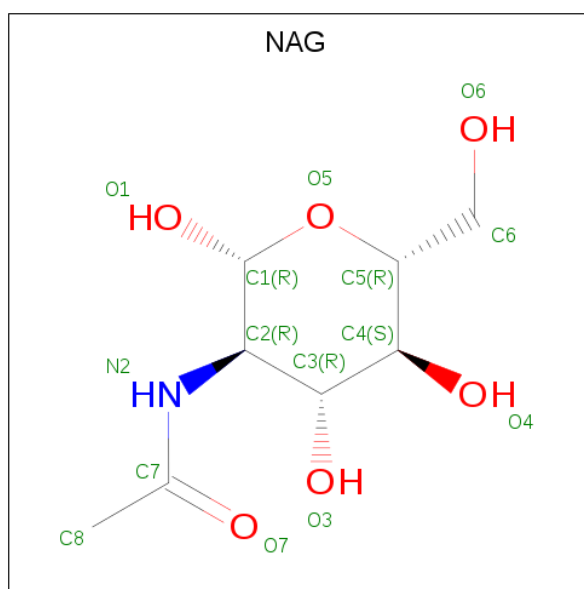
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



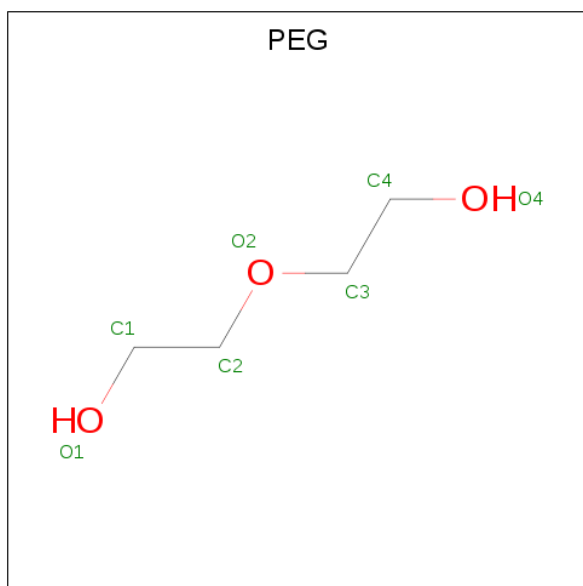
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl	0	0
			2	2		
6	A	3	Total	Cl	0	0
			3	3		
6	C	2	Total	Cl	0	0
			2	2		

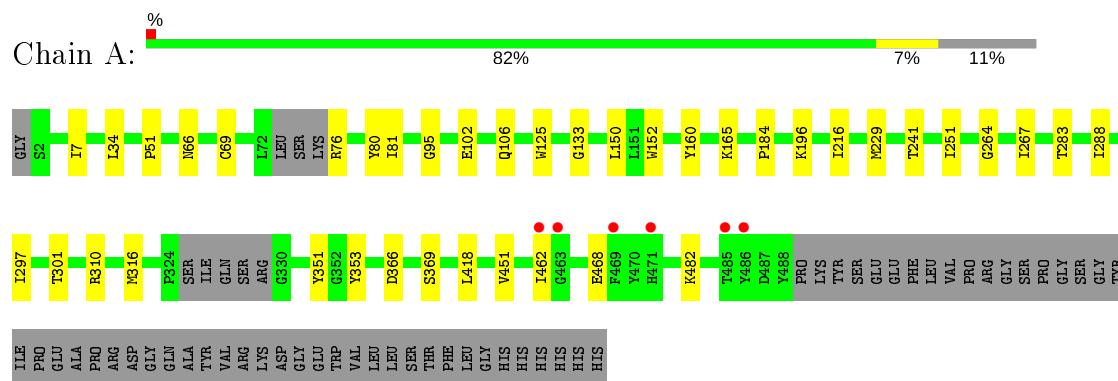
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total	O	0	1
			215	215		
7	B	246	Total	O	0	1
			247	247		
7	C	192	Total	O	0	0
			192	192		

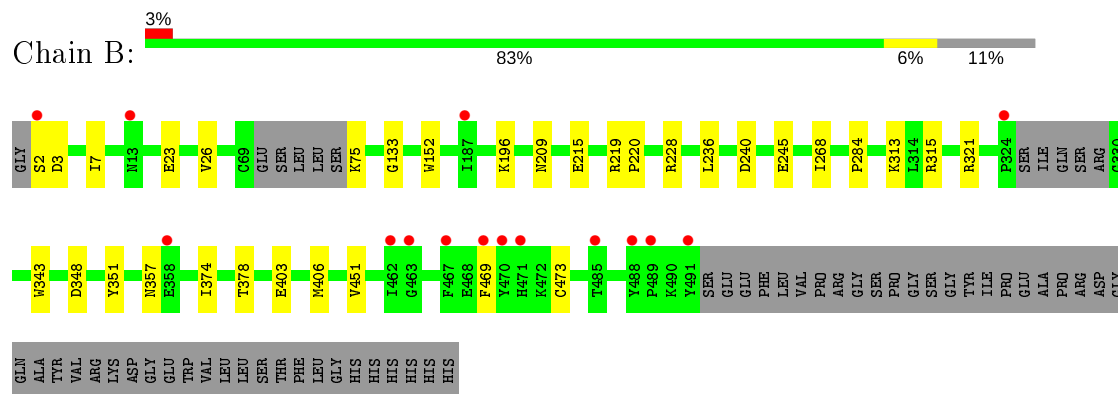
3 Residue-property plots [i](#)

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.

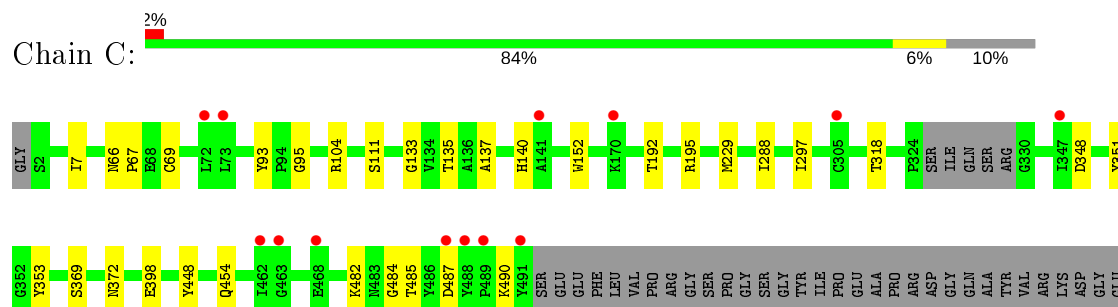
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
HIS
HIS
HIS
HIS
HIS
HIS

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

Chain D:  100%

NA61
NA62
BM43

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

Chain E:  100%

NA61
NA62
BM43

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

Chain F:  100%

NA61
NA62

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

Chain G:  100%

NA61
NA62

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.56Å 102.25Å 160.95Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	45.39 – 1.95 48.73 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.39-1.95) 99.9 (48.73-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_3409	Depositor
R, R_{free}	0.193 , 0.230 0.193 , 0.230	Depositor DCC
R_{free} test set	2048 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12176	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: CL, PEG, BMA, NAG

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	0.37	0/3793	0.55	0/5150
1	B	0.39	0/3804	0.57	0/5170
1	C	0.37	0/3846	0.54	0/5227
All	All	0.38	0/11443	0.55	0/15547

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	3708	0	3481	21	0
1	B	3713	0	3467	22	0
1	C	3757	0	3493	22	0
2	D	39	0	34	0	0
2	E	39	0	34	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
4	A	42	0	39	0	0
4	B	56	0	52	2	0
4	C	56	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	20	0	0
5	B	14	0	20	1	0
5	C	21	0	30	4	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
7	A	215	0	0	2	0
7	B	247	0	0	2	0
7	C	192	0	0	0	0
All	All	12176	0	10772	65	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 3.

The worst 5 of 65 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:C:135:THR:HG22	1:C:137:ALA:H	1.54	0.71
1:B:374:ILE:O	1:B:378:THR:HG23	1.93	0.67
1:B:343:TRP:HE1	5:B:508:PEG:H22	1.57	0.67
1:C:372:ASN:HB3	5:C:509:PEG:H12	1.76	0.65
1:B:23:GLU:CD	1:B:321:ARG:HH22	2.00	0.65

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	473/538 (88%)	458 (97%)	14 (3%)	1 (0%)	47 38
1	B	475/538 (88%)	464 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	481/538 (89%)	471 (98%)	10 (2%)	0	100	100
All	All	1429/1614 (88%)	1393 (98%)	35 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLY

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	390/465 (84%)	389 (100%)	1 (0%)	92	92
1	B	388/465 (83%)	386 (100%)	2 (0%)	88	88
1	C	394/465 (85%)	392 (100%)	2 (0%)	88	88
All	All	1172/1395 (84%)	1167 (100%)	5 (0%)	91	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	TYR
1	B	209	ASN
1	B	351	TYR
1	C	111	SER
1	C	351	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	454	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 ⓘ

10 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	D	1	1,2	14,14,15	0.33	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	0.48	0
2	BMA	D	3	2	11,11,12	1.06	0	15,15,17	0.83	0
2	NAG	E	1	1,2	14,14,15	0.41	0	17,19,21	0.80	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	0.66	0
2	BMA	E	3	2	11,11,12	0.26	0	15,15,17	0.85	0
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	G	1	1,3	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.34	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	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

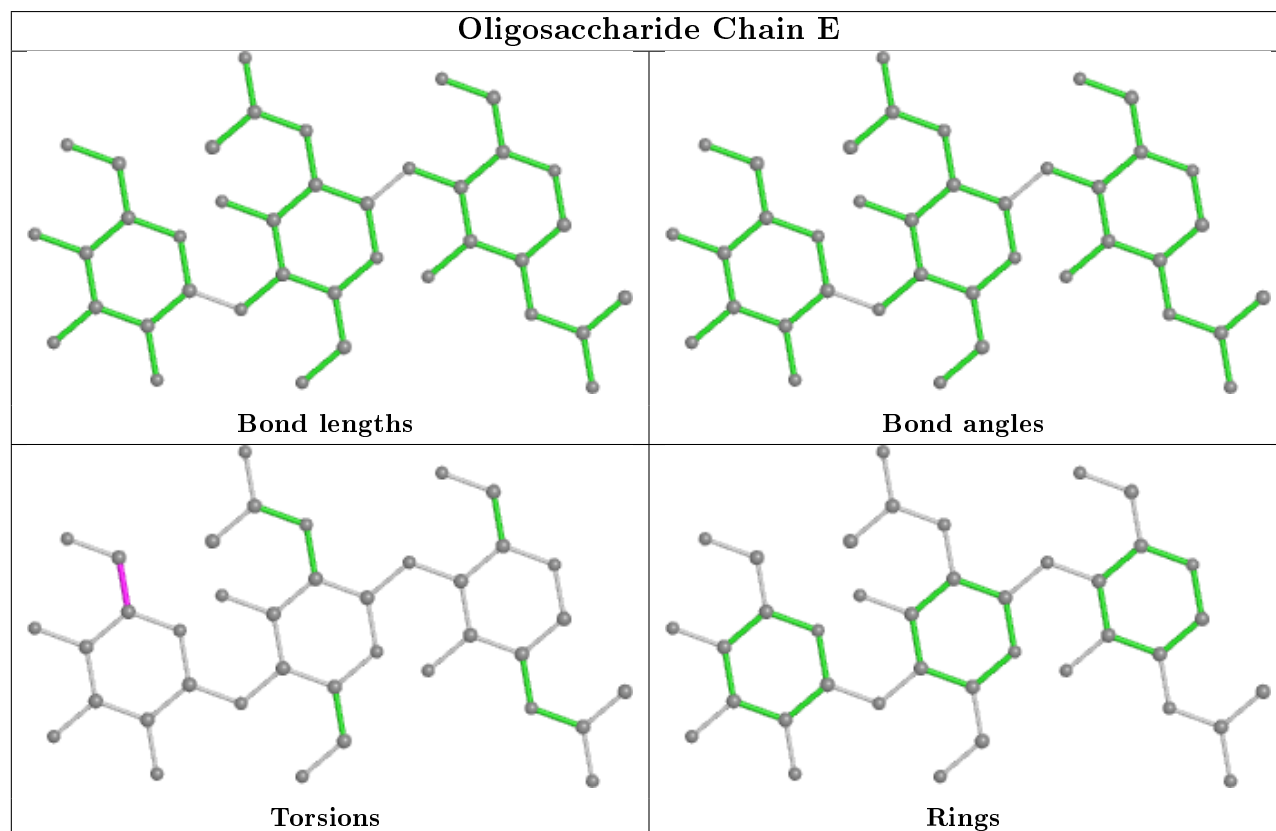
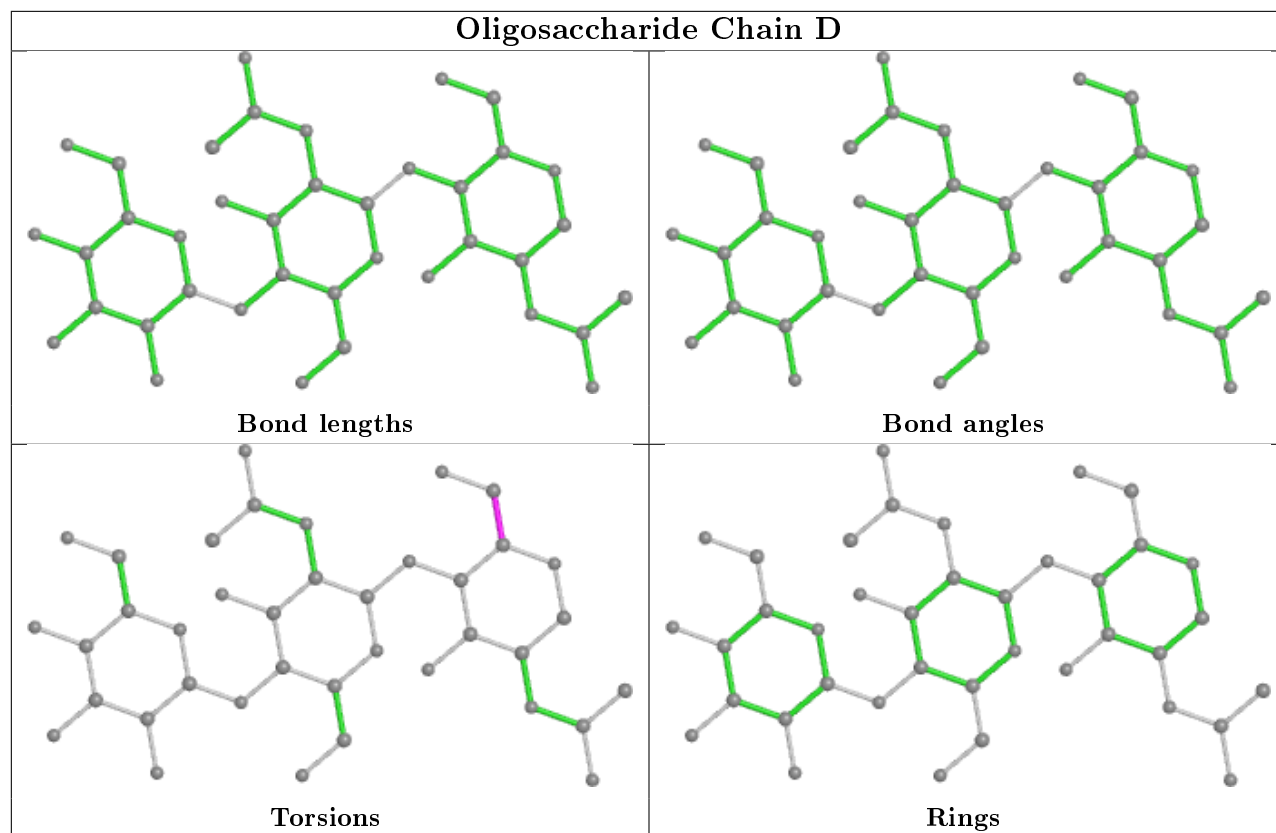
5 of 8 torsion outliers are listed below:

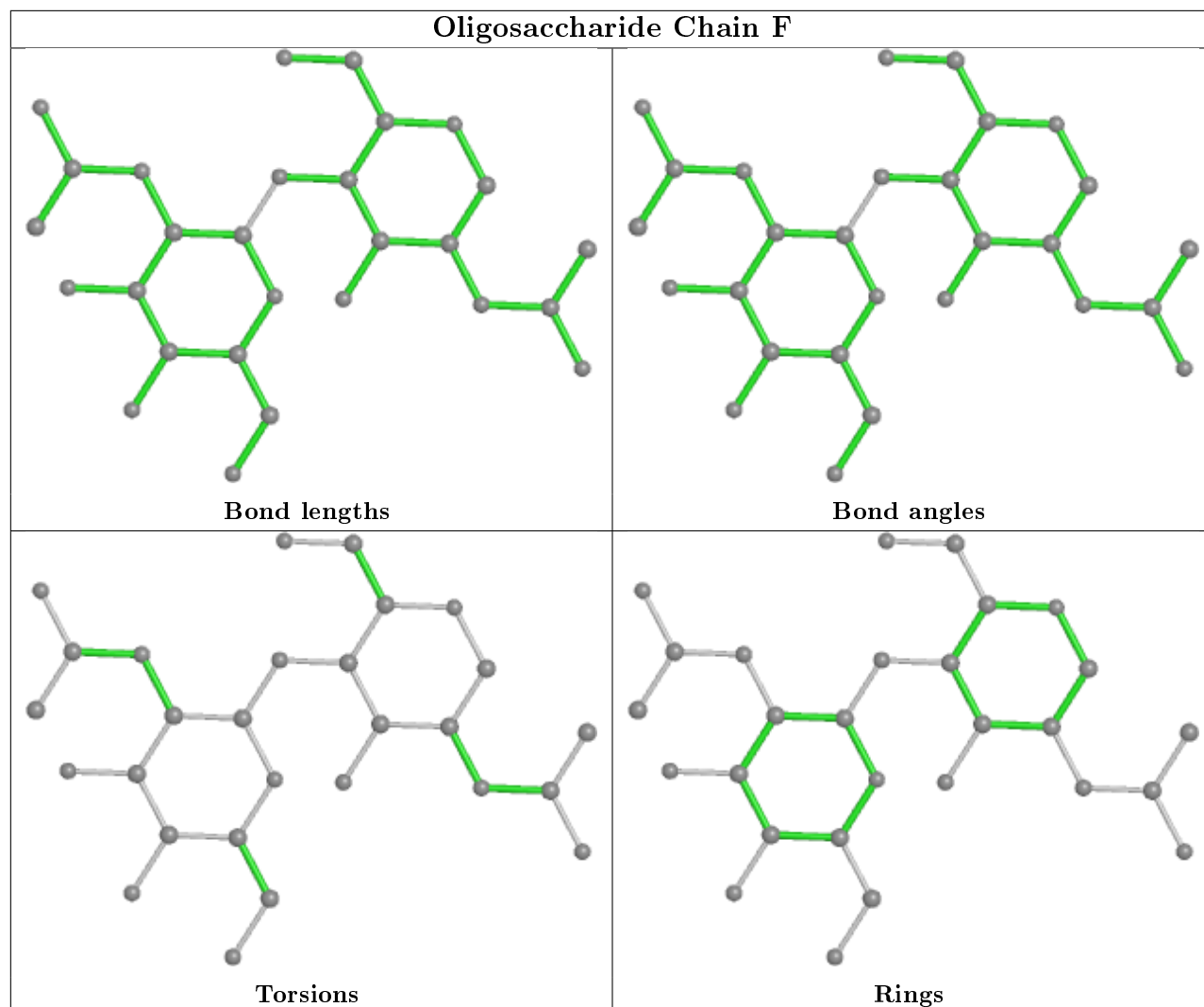
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6

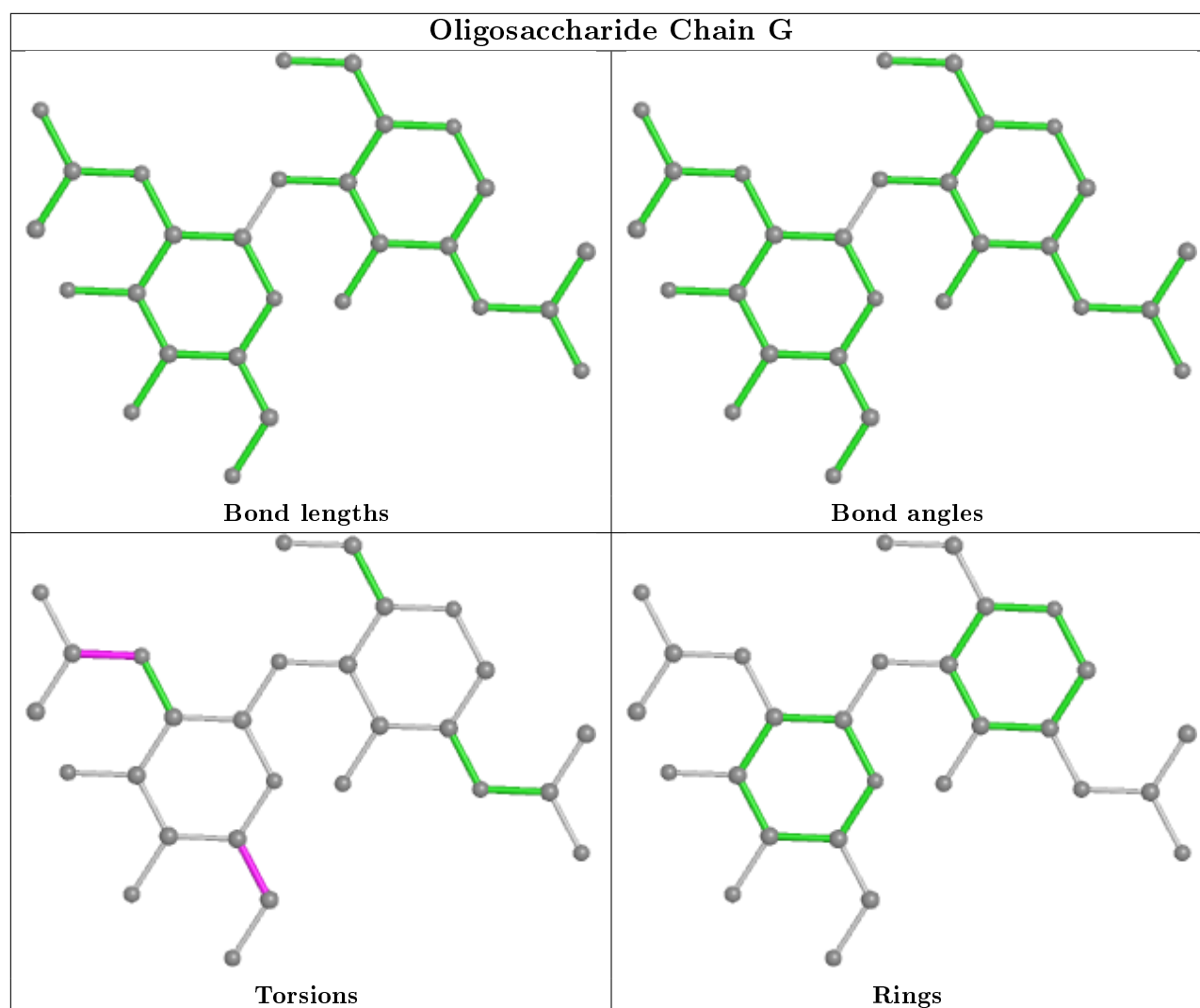
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	507	1	14,14,15	0.74	1 (7%)	17,19,21	0.63	1 (5%)
4	NAG	C	513	1	14,14,15	0.43	0	17,19,21	0.39	0
5	PEG	B	508	-	6,6,6	0.54	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	502	1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	B	504	1	14,14,15	0.45	0	17,19,21	1.39	2 (11%)
4	NAG	C	506	1	14,14,15	0.73	0	17,19,21	0.74	0
5	PEG	A	507	-	6,6,6	0.46	0	5,5,5	1.01	0
5	PEG	C	510	-	6,6,6	0.52	0	5,5,5	0.81	0
5	PEG	C	509	-	6,6,6	0.52	0	5,5,5	0.70	0
4	NAG	C	505	1	14,14,15	0.47	0	17,19,21	0.51	0
4	NAG	A	501	1	14,14,15	0.23	0	17,19,21	0.32	0
4	NAG	A	506	1	14,14,15	0.35	0	17,19,21	0.51	0
5	PEG	B	509	-	6,6,6	0.50	0	5,5,5	0.97	0
4	NAG	B	506	1	14,14,15	0.63	0	17,19,21	0.66	1 (5%)
5	PEG	A	508	-	6,6,6	0.47	0	5,5,5	0.96	0
4	NAG	B	505	1	14,14,15	0.67	0	17,19,21	0.64	0
5	PEG	C	508	-	6,6,6	0.52	0	5,5,5	0.84	0
4	NAG	C	507	1	14,14,15	0.50	0	17,19,21	0.62	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
4	NAG	B	507	1	-	0/6/23/26	0/1/1/1
4	NAG	C	513	1	-	1/6/23/26	0/1/1/1
5	PEG	B	508	-	-	2/4/4/4	-
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
4	NAG	B	504	1	-	3/6/23/26	0/1/1/1
4	NAG	C	506	1	-	4/6/23/26	0/1/1/1
5	PEG	A	507	-	-	3/4/4/4	-
5	PEG	C	510	-	-	2/4/4/4	-
5	PEG	C	509	-	-	2/4/4/4	-
4	NAG	C	505	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	PEG	B	509	-	-	4/4/4/4	-
4	NAG	B	506	1	-	0/6/23/26	0/1/1/1
5	PEG	A	508	-	-	1/4/4/4	-
4	NAG	B	505	1	-	2/6/23/26	0/1/1/1
5	PEG	C	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	507	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	507	NAG	O5-C1	2.41	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	NAG	C2-N2-C7	4.43	129.21	122.90
4	B	506	NAG	C1-O5-C5	2.28	115.28	112.19
4	B	504	NAG	C1-C2-N2	2.14	114.14	110.49
4	B	507	NAG	C1-O5-C5	2.11	115.06	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	506	NAG	C4-C5-C6-O6
4	B	505	NAG	C4-C5-C6-O6
4	C	507	NAG	O5-C5-C6-O6
4	C	506	NAG	O5-C5-C6-O6
4	B	505	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	508	PEG	1	0
4	B	504	NAG	1	0
4	C	506	NAG	1	0
5	C	510	PEG	1	0
5	C	509	PEG	3	0
4	B	505	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	479/538 (89%)	0.10	6 (1%) 77 83	26, 42, 67, 94	0
1	B	480/538 (89%)	0.10	15 (3%) 49 58	23, 39, 63, 89	0
1	C	485/538 (90%)	0.24	13 (2%) 54 63	24, 42, 72, 93	0
All	All	1444/1614 (89%)	0.15	34 (2%) 59 68	23, 41, 68, 94	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	ALA	6.3
1	B	489	PRO	5.8
1	B	491	TYR	5.3
1	C	73	LEU	4.8
1	B	488	TYR	4.8

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.

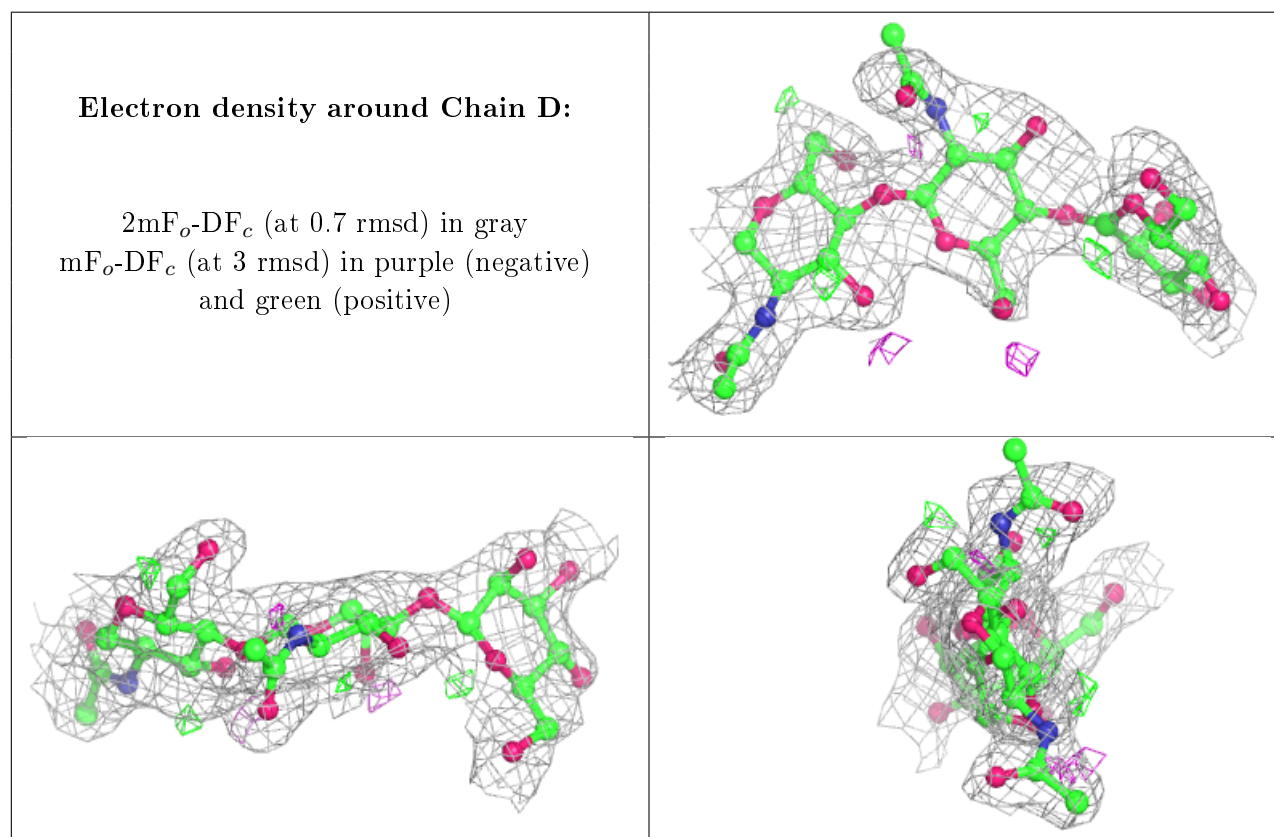
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.63	0.47	72,88,92,96	0
3	NAG	G	2	14/15	0.72	0.37	64,74,80,84	0
2	BMA	D	3	11/12	0.74	0.31	65,75,77,79	0

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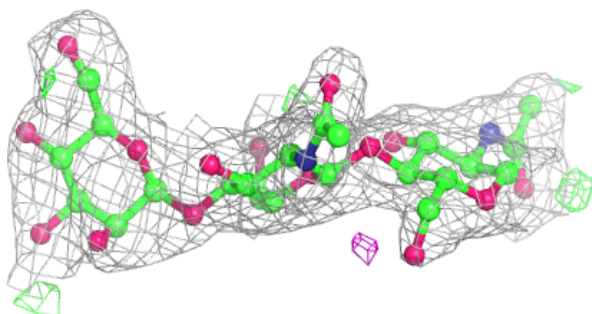
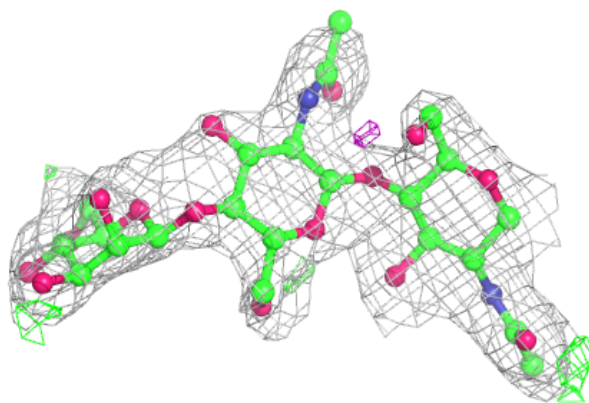
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	E	3	11/12	0.76	0.33	67,74,81,81	0
3	NAG	F	1	14/15	0.78	0.24	56,67,82,89	0
2	NAG	D	2	14/15	0.84	0.21	54,67,72,75	0
2	NAG	E	2	14/15	0.88	0.23	55,62,68,77	0
3	NAG	G	1	14/15	0.91	0.20	41,53,67,71	0
2	NAG	D	1	14/15	0.92	0.12	36,48,55,55	0
2	NAG	E	1	14/15	0.93	0.15	31,41,62,71	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.

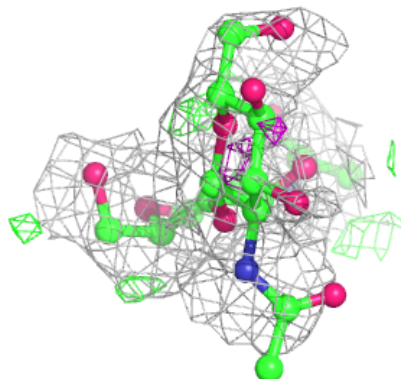
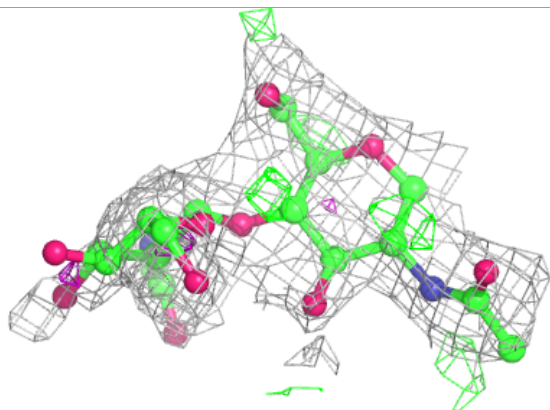
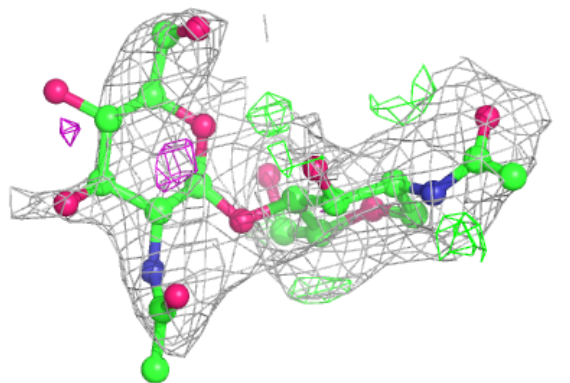


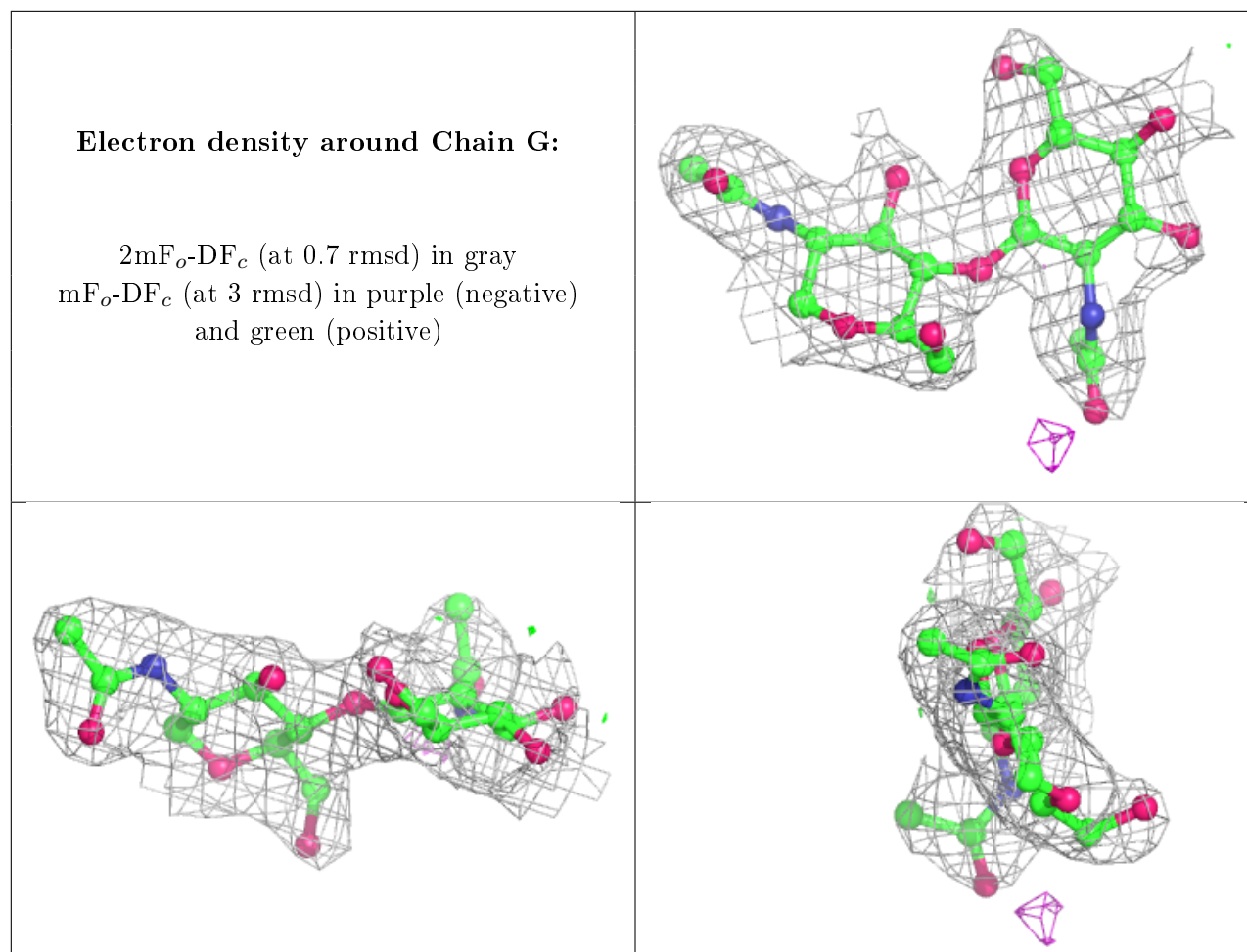
Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	NAG	B	507	14/15	0.60	0.36	63,73,77,77	0
4	NAG	C	506	14/15	0.67	0.35	64,76,81,82	0
4	NAG	C	513	14/15	0.72	0.45	66,79,89,91	0
4	NAG	A	501	14/15	0.76	0.40	59,76,83,91	0
4	NAG	B	504	14/15	0.77	0.33	64,76,89,93	0
4	NAG	B	505	14/15	0.78	0.34	68,82,89,90	0
4	NAG	A	506	14/15	0.79	0.44	67,80,88,91	0
5	PEG	B	509	7/7	0.80	0.15	54,56,61,63	0
4	NAG	A	502	14/15	0.81	0.23	46,59,76,82	0
4	NAG	C	505	14/15	0.82	0.25	57,69,71,75	0
5	PEG	C	510	7/7	0.82	0.18	56,62,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	507	14/15	0.83	0.35	62,79,85,86	0
5	PEG	C	509	7/7	0.85	0.18	51,55,60,65	0
5	PEG	A	507	7/7	0.86	0.19	58,58,59,59	0
5	PEG	B	508	7/7	0.89	0.26	53,55,57,63	0
5	PEG	A	508	7/7	0.92	0.12	51,54,62,65	0
4	NAG	B	506	14/15	0.92	0.20	54,63,65,70	0
5	PEG	C	508	7/7	0.93	0.12	53,53,59,60	0
6	CL	C	512	1/1	0.95	0.10	52,52,52,52	0
6	CL	A	511	1/1	0.96	0.11	37,37,37,37	0
6	CL	C	511	1/1	0.96	0.09	41,41,41,41	0
6	CL	B	511	1/1	0.97	0.07	49,49,49,49	0
6	CL	A	509	1/1	0.98	0.06	37,37,37,37	0
6	CL	B	510	1/1	0.98	0.09	39,39,39,39	0
6	CL	A	510	1/1	0.98	0.06	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.