



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:36 PM UTC

PDB ID : 6ONA / pdb_00006ona
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

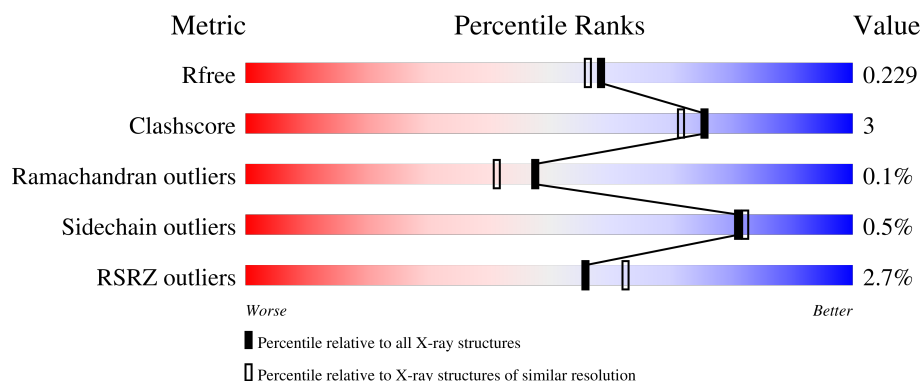
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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	538	2% 82% 7% 11%
1	B	538	2% 83% 7% 11%
1	C	538	3% 84% 7% 10%
2	D	3	100%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	G	2	 100%

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:

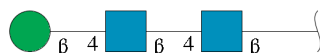
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q0HD60
A	2	SER	-	expression tag	UNP Q0HD60
A	495	PHE	-	linker	UNP Q0HD60
A	496	LEU	-	linker	UNP Q0HD60
A	497	VAL	-	linker	UNP Q0HD60
A	498	PRO	-	linker	UNP Q0HD60
A	499	ARG	-	linker	UNP Q0HD60
A	500	GLY	-	linker	UNP Q0HD60
A	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.



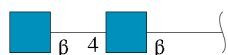
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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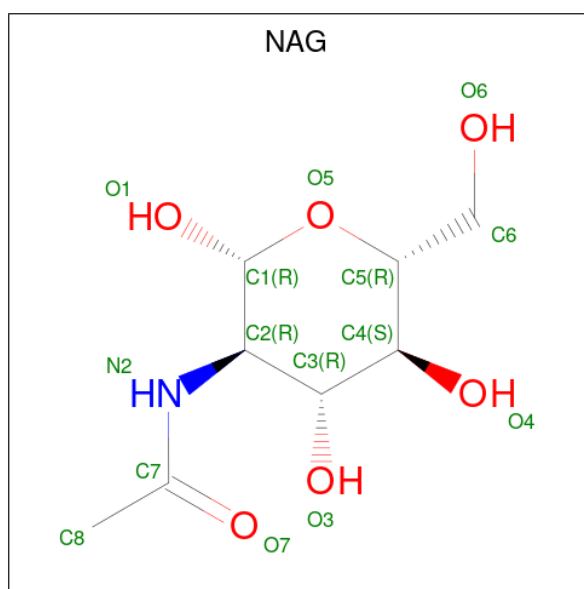
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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 (CCD ID: 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 (CCD ID: 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 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

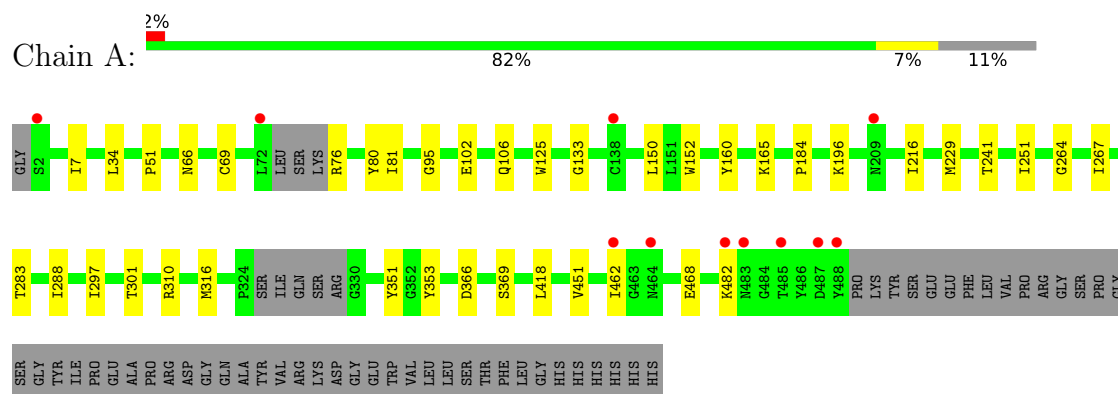
- Molecule 7 is water.

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

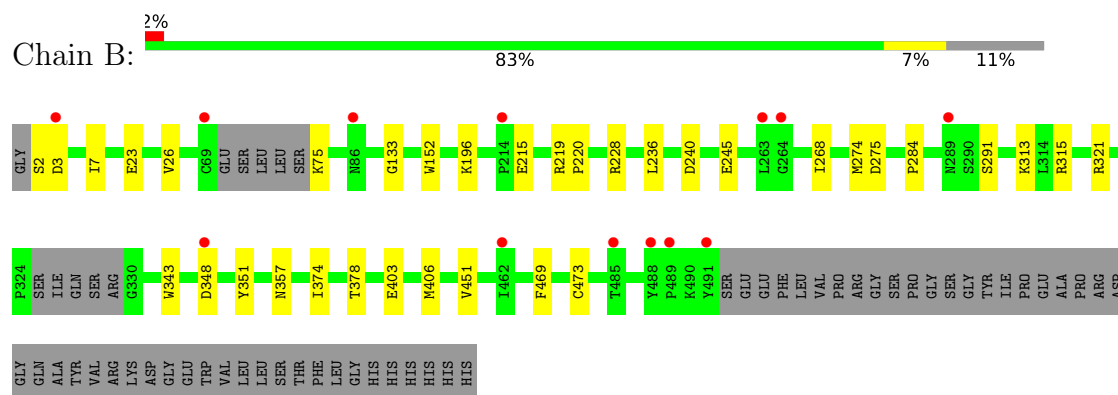
3 Residue-property plots

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.

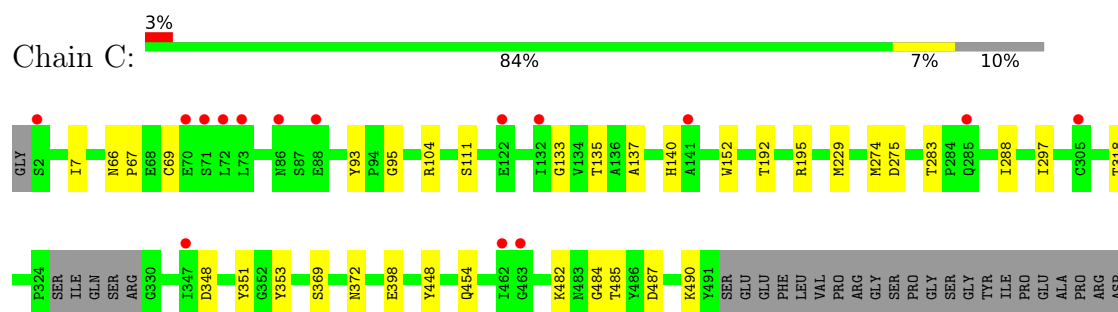
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
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%

NAG1
NAG2
BMA3

- 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%

NAG1
NAG2
BMA3

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

Chain F:  100%

NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2

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 45.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.39-1.95) 99.8 (45.39-1.95)	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 , 0.229	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)	0.36 , 53.6	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

5.1 Standard geometry

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

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	0.29	0/3793	0.50	0/5150
1	B	0.32	0/3804	0.53	0/5170
1	C	0.29	0/3846	0.49	0/5227
All	All	0.30	0/11443	0.51	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

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	23	0
1	C	3757	0	3493	23	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	67	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.

All (67) 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:23:GLU:CD	1:B:321:ARG:HH22	2.00	0.69
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:A:288:ILE:HG21	1:A:297:ILE:HD13	1.81	0.61
1:B:23:GLU:OE1	1:B:321:ARG:NH2	2.31	0.60
1:B:215:GLU:O	1:B:219:ARG:NH2	2.36	0.58
4:B:504:NAG:H83	4:B:504:NAG:H3	1.85	0.58
1:C:454:GLN:NE2	1:C:484:GLY:O	2.35	0.58
1:A:160:TYR:O	1:A:196:LYS:NZ	2.38	0.57
1:B:196:LYS:NZ	7:B:604:HOH:O	2.39	0.56
1:A:7:ILE:HD11	1:A:451:VAL:HG21	1.88	0.55
1:C:7:ILE:HG13	1:C:448:TYR:HA	1.88	0.54
1:C:95:GLY:HA3	1:C:229:MET:O	2.09	0.54
1:B:7:ILE:HD11	1:B:451:VAL:HG21	1.90	0.53
1:C:485:THR:HG21	4:C:506:NAG:H2	1.91	0.52
1:C:192:THR:O	1:C:195:ARG:NH1	2.43	0.52
1:A:241:THR:HB	1:B:220:PRO:HG3	1.92	0.52
1:B:2:SER:HA	1:B:357:ASN:HA	1.92	0.52
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.92	0.51
1:A:76:ARG:NH1	7:A:602:HOH:O	2.39	0.51
1:C:353:TYR:HB2	1:C:482:LYS:HZ2	1.76	0.51
1:B:2:SER:CB	1:B:473:CYS:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:GLN:HE22	1:C:484:GLY:HA2	1.76	0.50
1:C:369:SER:HA	5:C:509:PEG:H42	1.93	0.50
1:C:348:ASP:OD1	1:C:348:ASP:N	2.46	0.49
1:A:95:GLY:HA3	1:A:229:MET:O	2.13	0.49
1:A:184:PRO:HD2	1:A:216:ILE:HD13	1.94	0.49
1:B:403:GLU:HB3	1:B:406[B]:MET:HE2	1.95	0.49
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.95	0.48
1:C:372:ASN:HB3	5:C:509:PEG:C1	2.44	0.47
1:C:318:THR:HG21	5:C:510:PEG:H22	1.96	0.47
1:C:454:GLN:HE22	1:C:484:GLY:C	2.21	0.47
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.97	0.47
1:C:487:ASP:OD2	1:C:490:LYS:HB2	2.15	0.47
1:B:313:LYS:HE3	1:B:315:ARG:HD3	1.96	0.46
1:A:125:TRP:CZ3	1:A:165:LYS:HG3	2.49	0.46
1:B:268:ILE:HD12	1:B:284:PRO:HG3	1.97	0.46
1:B:236:LEU:HD22	1:B:240:ASP:HB3	1.98	0.46
1:C:454:GLN:HE22	1:C:484:GLY:CA	2.30	0.45
1:A:462:ILE:HD11	1:A:468:GLU:HB2	1.99	0.45
1:B:245:GLU:OE2	4:B:505:NAG:H82	2.16	0.45
1:C:66:ASN:HB3	1:C:69:CYS:SG	2.57	0.44
1:C:67:PRO:HB2	1:C:140:HIS:HB2	2.00	0.44
1:C:288:ILE:HG21	1:C:297:ILE:HG13	1.99	0.44
1:A:196:LYS:HE3	1:A:196:LYS:HB2	1.62	0.44
1:C:274:MET:HE3	1:C:275:ASP:O	2.18	0.44
1:A:34:LEU:HD11	1:A:316:MET:SD	2.58	0.44
1:A:66:ASN:HB3	1:A:69:CYS:SG	2.57	0.43
1:A:51:PRO:HB3	1:A:80:TYR:CZ	2.53	0.43
1:B:274:MET:HE3	1:B:275:ASP:O	2.19	0.43
1:B:348:ASP:OD1	1:B:348:ASP:N	2.51	0.43
1:C:104:ARG:NH2	1:C:398:GLU:OE1	2.35	0.43
1:B:75:LYS:HD3	7:B:663:HOH:O	2.18	0.43
1:A:150:LEU:HB3	1:A:251:ILE:HG22	2.01	0.42
1:A:353:TYR:CD1	1:A:482:LYS:HG2	2.54	0.42
1:A:81:ILE:HB	1:A:267:ILE:HD12	2.00	0.42
1:A:310:ARG:HG2	1:A:418:LEU:HD11	2.00	0.42
1:A:366:ASP:OD2	1:A:369:SER:HB2	2.20	0.42
1:A:102:GLU:O	1:A:106:GLN:HG3	2.21	0.41
1:A:283:THR:HG22	1:A:301:THR:HG22	2.01	0.41
1:B:219:ARG:HD2	1:B:228:ARG:HG2	2.02	0.41
1:B:3:ASP:O	1:B:469:PHE:N	2.45	0.41
1:C:93:TYR:CD1	1:C:229:MET:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:HG3	1:B:26:VAL:CG2	2.51	0.40
7:A:707:HOH:O	1:B:406[B]:MET:HG3	2.21	0.40

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	473/538 (88%)	458 (97%)	14 (3%)	1 (0%)	43	36
1	B	475/538 (88%)	464 (98%)	11 (2%)	0	100	100
1	C	481/538 (89%)	471 (98%)	10 (2%)	0	100	100
All	All	1429/1614 (88%)	1393 (98%)	35 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLY

5.3.2 Protein sidechains [i](#)

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%)	86	87
1	B	388/465 (83%)	386 (100%)	2 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	394/465 (85%)	391 (99%)	3 (1%)	73	74
All	All	1172/1395 (84%)	1166 (100%)	6 (0%)	81	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	TYR
1	B	291	SER
1	B	351	TYR
1	C	111	SER
1	C	283	THR
1	C	351	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	ASN
1	C	454	GLN
1	C	458	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.35	0	17,19,21	0.60	0
2	NAG	D	2	2	14,14,15	0.53	0	17,19,21	0.50	0
2	BMA	D	3	2	11,11,12	1.02	0	15,15,17	0.78	0
2	NAG	E	1	1,2	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	0.66	0
2	BMA	E	3	2	11,11,12	0.25	0	15,15,17	0.75	0
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	G	1	1,3	14,14,15	0.41	0	17,19,21	0.51	0
3	NAG	G	2	3	14,14,15	0.33	0	17,19,21	0.37	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
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.

All (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
2	D	1	NAG	C4-C5-C6-O6

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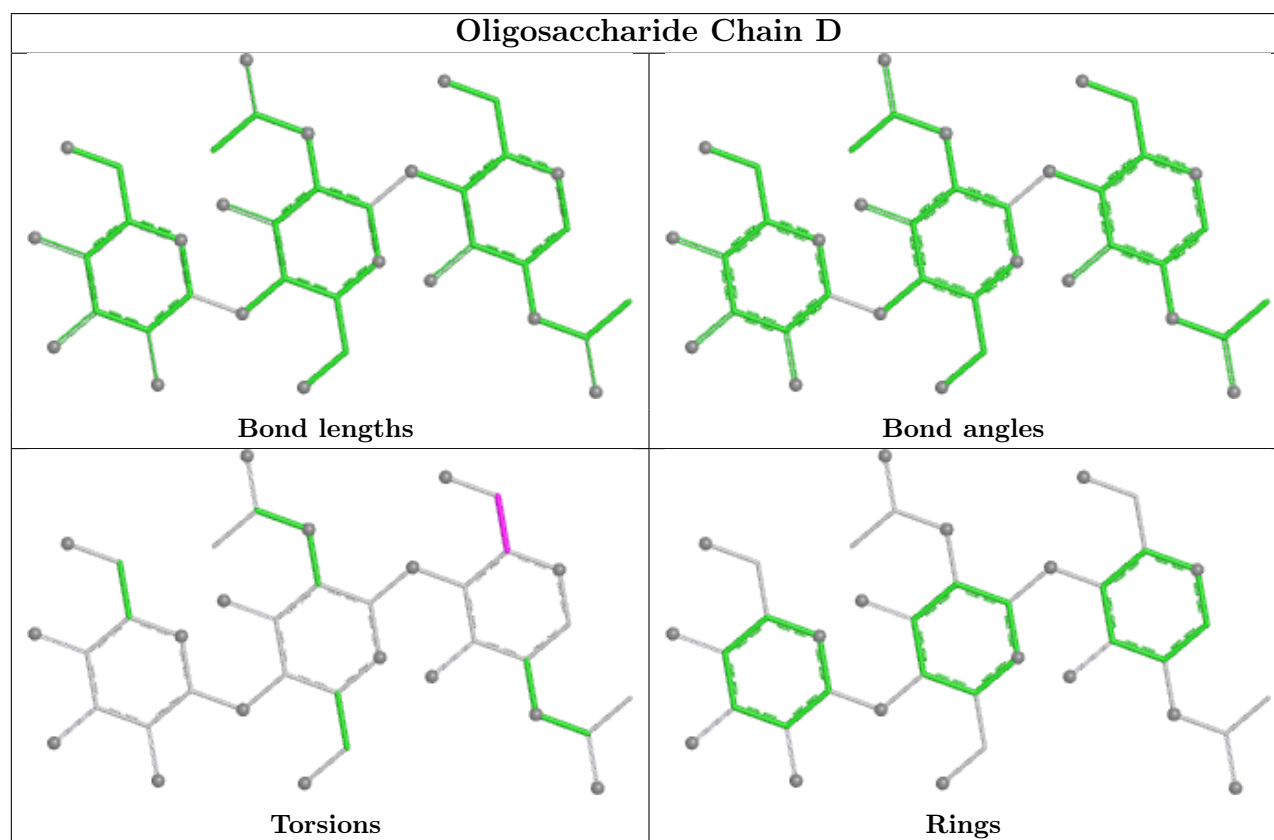
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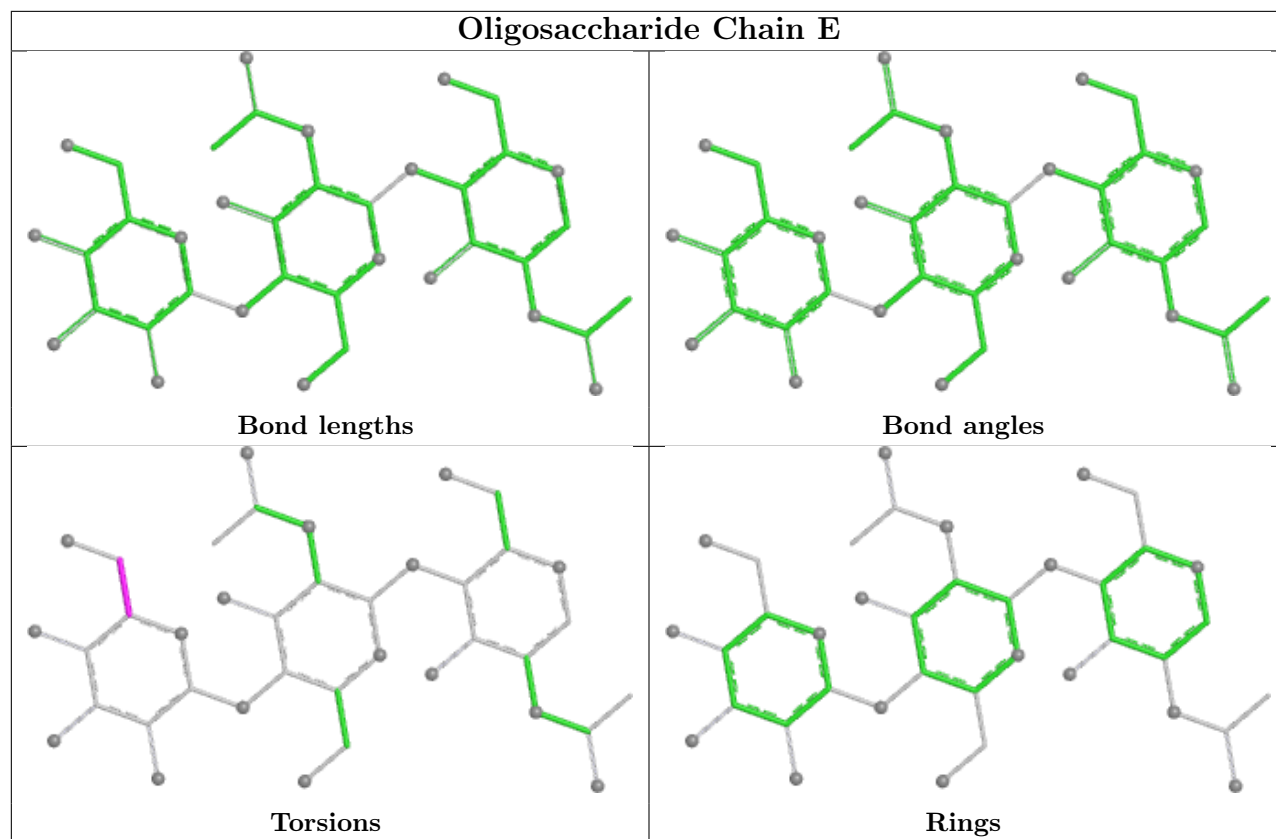
Mol	Chain	Res	Type	Atoms
2	E	3	BMA	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

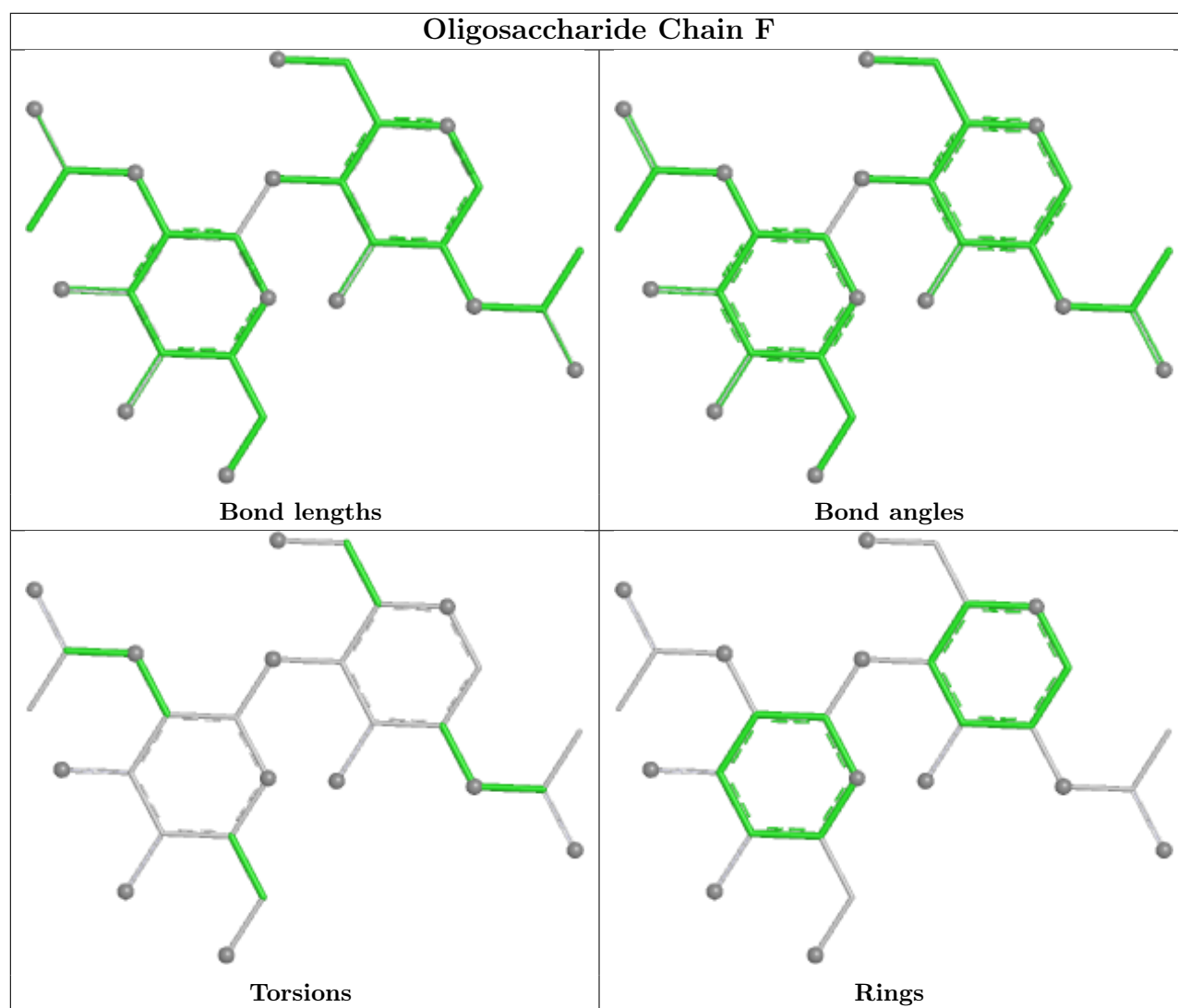
There are no ring outliers.

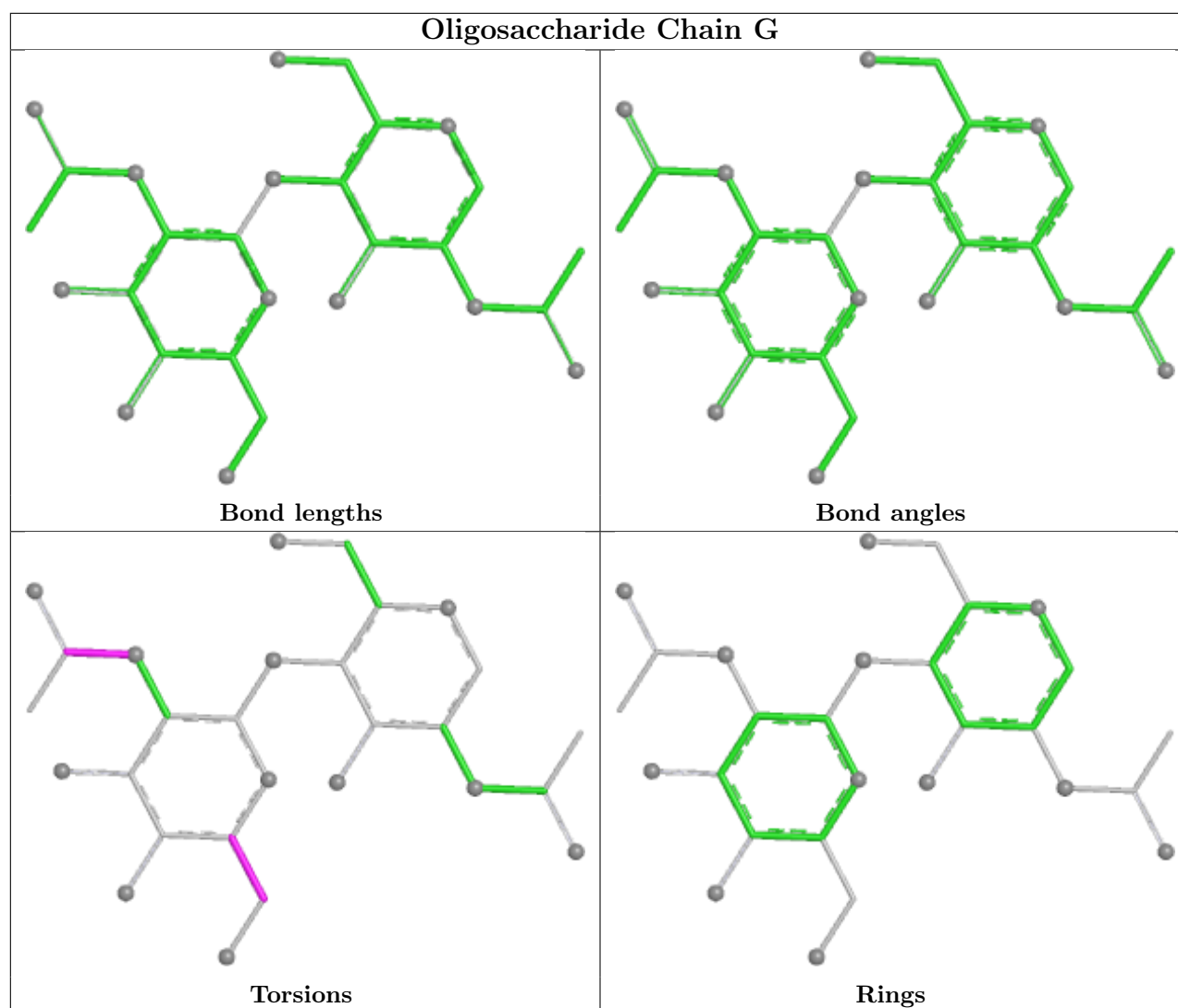
No monomer is involved in short contacts.

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 [i](#)

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	C	513	1	14,14,15	0.46	0	17,19,21	0.40	0
4	NAG	A	502	1	14,14,15	0.30	0	17,19,21	0.45	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	B	507	1	14,14,15	0.73	1 (7%)	17,19,21	0.64	1 (5%)
4	NAG	B	506	1	14,14,15	0.65	0	17,19,21	0.67	1 (5%)
5	PEG	A	507	-	6,6,6	0.47	0	5,5,5	1.00	0
5	PEG	A	508	-	6,6,6	0.47	0	5,5,5	0.96	0
5	PEG	C	510	-	6,6,6	0.52	0	5,5,5	0.81	0
5	PEG	B	509	-	6,6,6	0.50	0	5,5,5	0.96	0
4	NAG	B	504	1	14,14,15	0.43	0	17,19,21	1.47	2 (11%)
4	NAG	C	505	1	14,14,15	0.51	0	17,19,21	0.53	0
5	PEG	C	508	-	6,6,6	0.52	0	5,5,5	0.83	0
5	PEG	C	509	-	6,6,6	0.53	0	5,5,5	0.70	0
4	NAG	A	501	1	14,14,15	0.24	0	17,19,21	0.34	0
4	NAG	C	507	1	14,14,15	0.51	0	17,19,21	0.65	0
4	NAG	B	505	1	14,14,15	0.68	0	17,19,21	0.67	0
4	NAG	A	506	1	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	C	506	1	14,14,15	0.74	0	17,19,21	0.77	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	513	1	-	1/6/23/26	0/1/1/1
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	PEG	B	508	-	-	2/4/4/4	-
4	NAG	B	507	1	-	0/6/23/26	0/1/1/1
4	NAG	B	506	1	-	0/6/23/26	0/1/1/1
5	PEG	A	507	-	-	3/4/4/4	-
5	PEG	A	508	-	-	1/4/4/4	-
5	PEG	C	510	-	-	2/4/4/4	-
5	PEG	B	509	-	-	4/4/4/4	-
4	NAG	B	504	1	-	4/6/23/26	0/1/1/1
4	NAG	C	505	1	-	2/6/23/26	0/1/1/1
5	PEG	C	508	-	-	2/4/4/4	-
5	PEG	C	509	-	-	3/4/4/4	-
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
4	NAG	C	507	1	-	4/6/23/26	0/1/1/1
4	NAG	B	505	1	-	2/6/23/26	0/1/1/1
4	NAG	A	506	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	506	1	-	4/6/23/26	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	2.30	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	4.71	129.21	122.90
4	B	504	NAG	C1-C2-N2	2.35	114.14	110.43
4	B	506	NAG	C1-O5-C5	2.31	115.28	112.19
4	B	507	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (40) 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
4	A	502	NAG	C4-C5-C6-O6
4	B	504	NAG	C8-C7-N2-C2
4	B	504	NAG	O7-C7-N2-C2
4	C	505	NAG	O5-C5-C6-O6
5	A	507	PEG	O1-C1-C2-O2
5	A	508	PEG	O2-C3-C4-O4
4	C	505	NAG	C4-C5-C6-O6
5	B	508	PEG	O1-C1-C2-O2
4	A	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
5	B	509	PEG	O1-C1-C2-O2
4	A	502	NAG	O5-C5-C6-O6
5	C	508	PEG	O1-C1-C2-O2
4	C	507	NAG	C4-C5-C6-O6
5	B	509	PEG	O2-C3-C4-O4
5	C	509	PEG	O1-C1-C2-O2
5	C	510	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	C	513	NAG	O5-C5-C6-O6
4	C	506	NAG	C1-C2-N2-C7
5	A	507	PEG	C4-C3-O2-C2
5	B	508	PEG	O2-C3-C4-O4
5	C	510	PEG	C1-C2-O2-C3
4	A	506	NAG	C4-C5-C6-O6
5	B	509	PEG	C4-C3-O2-C2
4	B	504	NAG	C3-C2-N2-C7
4	C	506	NAG	C3-C2-N2-C7
4	C	507	NAG	C3-C2-N2-C7
5	C	509	PEG	O2-C3-C4-O4
5	C	508	PEG	C4-C3-O2-C2
4	A	506	NAG	O5-C5-C6-O6
4	B	504	NAG	C1-C2-N2-C7
4	C	507	NAG	C1-C2-N2-C7
5	B	509	PEG	C1-C2-O2-C3
5	A	507	PEG	C1-C2-O2-C3
5	C	509	PEG	C1-C2-O2-C3

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
5	C	510	PEG	1	0
4	B	504	NAG	1	0
5	C	509	PEG	3	0
4	B	505	NAG	1	0
4	C	506	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

6.1 Protein, DNA and RNA chains

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%)	0.20	11 (2%) 61 68	26, 42, 67, 94	0
1	B	480/538 (89%)	0.09	13 (2%) 56 62	19, 39, 63, 89	1 (0%)
1	C	485/538 (90%)	0.21	15 (3%) 51 58	24, 42, 72, 93	0
All	All	1444/1614 (89%)	0.17	39 (2%) 56 62	19, 41, 68, 94	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	5.4
1	A	488	TYR	4.2
1	C	305	CYS	3.8
1	C	72	LEU	3.5
1	B	489	PRO	3.4
1	C	71	SER	3.4
1	C	347	ILE	3.3
1	C	70	GLU	3.2
1	A	462	ILE	3.2
1	B	462	ILE	3.1
1	B	491	TYR	3.0
1	C	462	ILE	3.0
1	C	463	GLY	3.0
1	C	73	LEU	2.9
1	C	141	ALA	2.9
1	B	348	ASP	2.8
1	A	483	ASN	2.7
1	C	88	GLU	2.6
1	C	285	GLN	2.6
1	B	69	CYS	2.5
1	C	86	ASN	2.4
1	C	132	ILE	2.4
1	C	122	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASN	2.3
1	B	488	TYR	2.3
1	A	487	ASP	2.3
1	B	264	GLY	2.3
1	B	214	PRO	2.2
1	C	2	SER	2.2
1	A	464	ASN	2.2
1	B	485	THR	2.2
1	B	263	LEU	2.2
1	B	289	ASN	2.1
1	A	2	SER	2.1
1	A	485	THR	2.1
1	B	3	ASP	2.1
1	A	482	LYS	2.0
1	A	138	CYS	2.0
1	A	209	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.

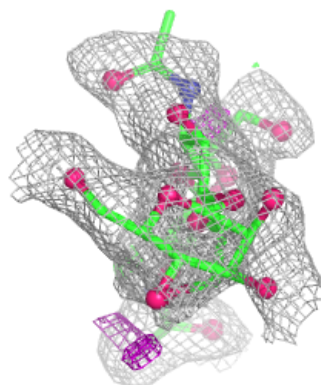
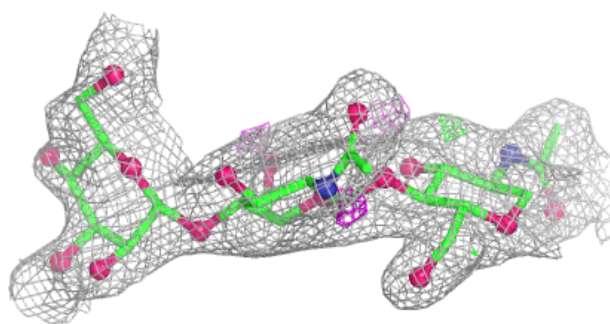
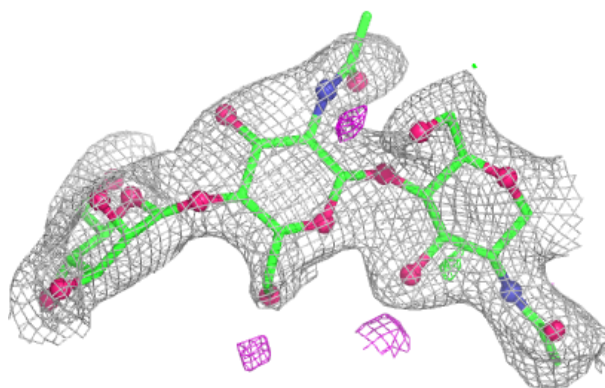
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.42	0.15	72,88,92,96	0
3	NAG	G	2	14/15	0.59	0.14	64,74,80,84	0
2	BMA	E	3	11/12	0.60	0.12	67,74,81,81	0
2	BMA	D	3	11/12	0.63	0.12	65,75,77,79	0
3	NAG	F	1	14/15	0.64	0.14	56,67,82,89	0
2	NAG	D	2	14/15	0.81	0.12	54,67,72,75	0
2	NAG	E	2	14/15	0.85	0.10	55,62,68,77	0
2	NAG	D	1	14/15	0.89	0.09	36,48,55,55	0
3	NAG	G	1	14/15	0.91	0.09	41,53,67,71	0
2	NAG	E	1	14/15	0.91	0.10	31,41,62,71	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

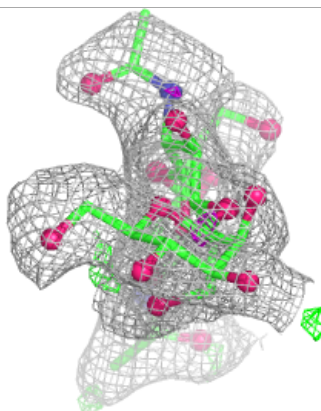
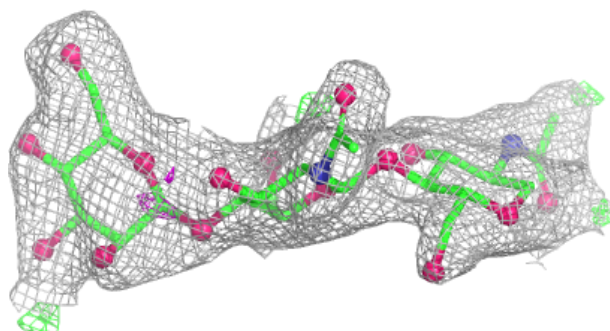
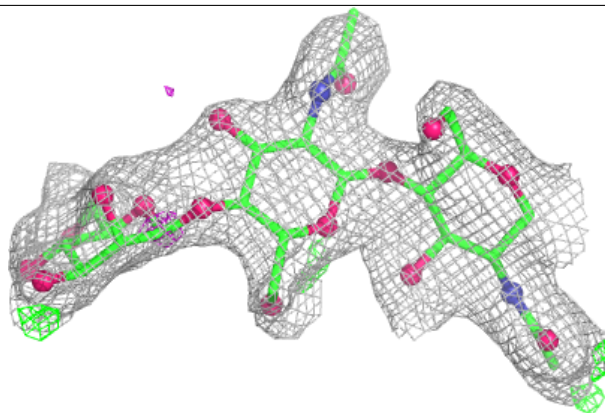
Electron density around Chain D:

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



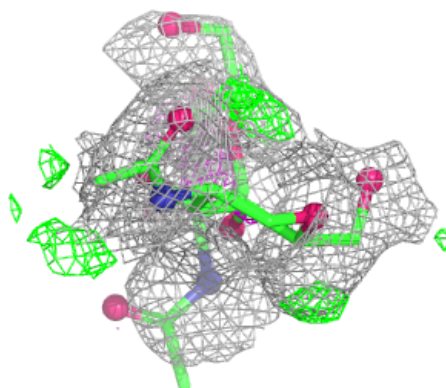
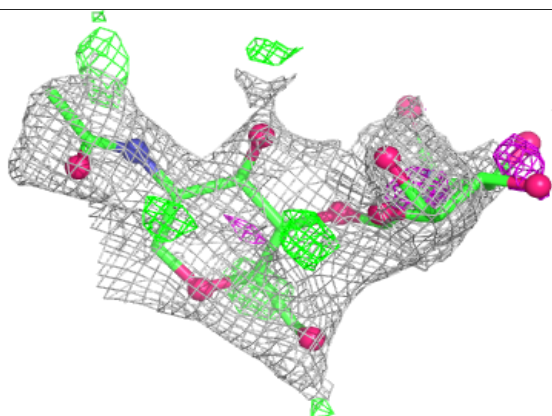
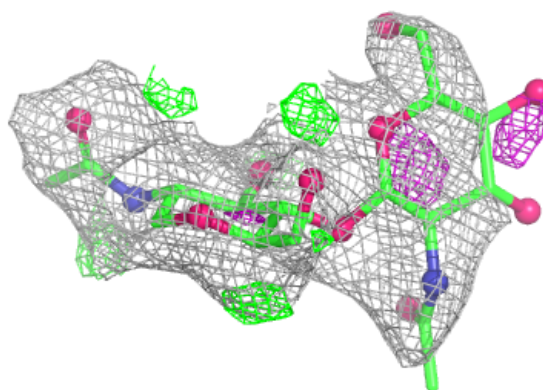
Electron density around Chain E:

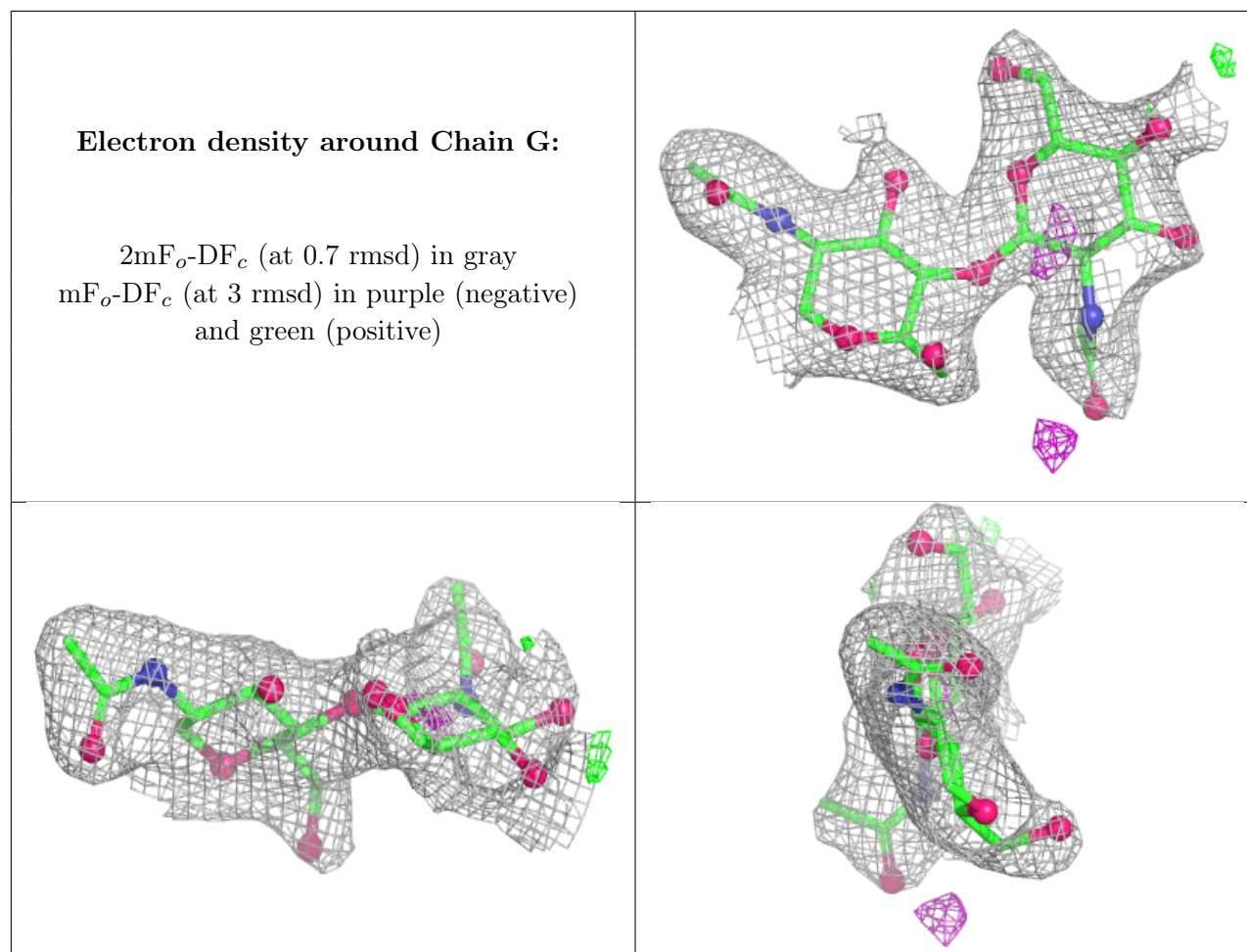
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
4	NAG	C	513	14/15	0.44	0.15	66,79,89,91	0
4	NAG	B	507	14/15	0.48	0.16	63,73,77,77	0
4	NAG	B	505	14/15	0.55	0.15	68,82,89,90	0
4	NAG	A	501	14/15	0.55	0.15	59,76,83,91	0
4	NAG	B	504	14/15	0.55	0.14	64,76,89,93	0
4	NAG	C	506	14/15	0.56	0.15	64,76,81,82	0
4	NAG	A	506	14/15	0.69	0.12	67,80,88,91	0
5	PEG	C	510	7/7	0.76	0.17	56,62,63,65	0
4	NAG	C	507	14/15	0.77	0.12	62,79,85,86	0
4	NAG	C	505	14/15	0.77	0.12	57,69,71,75	0
4	NAG	A	502	14/15	0.77	0.11	46,59,76,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	B	509	7/7	0.83	0.14	54,56,61,63	0
5	PEG	B	508	7/7	0.86	0.13	53,55,57,63	0
5	PEG	C	509	7/7	0.87	0.13	51,55,60,65	0
5	PEG	A	507	7/7	0.87	0.12	58,58,59,59	0
4	NAG	B	506	14/15	0.88	0.10	54,63,65,70	0
5	PEG	A	508	7/7	0.91	0.10	51,54,62,65	0
5	PEG	C	508	7/7	0.92	0.10	53,53,59,60	0
6	CL	A	509	1/1	0.96	0.14	37,37,37,37	0
6	CL	B	510	1/1	0.96	0.09	39,39,39,39	0
6	CL	C	511	1/1	0.96	0.10	41,41,41,41	0
6	CL	C	512	1/1	0.96	0.06	52,52,52,52	0
6	CL	A	511	1/1	0.97	0.09	37,37,37,37	0
6	CL	B	511	1/1	0.97	0.09	49,49,49,49	0
6	CL	A	510	1/1	0.98	0.07	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.