



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:27 PM BST

PDB ID : 4WE4
Title : The crystal structure of hemagglutinin from 1968 H3N2 influenza virus
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Guo, Z.; Villanueva, J.M.; Stevens, J.
Deposited on : 2014-09-09
Resolution : 2.35 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 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
buster-report : 1.1.7 (2018)
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

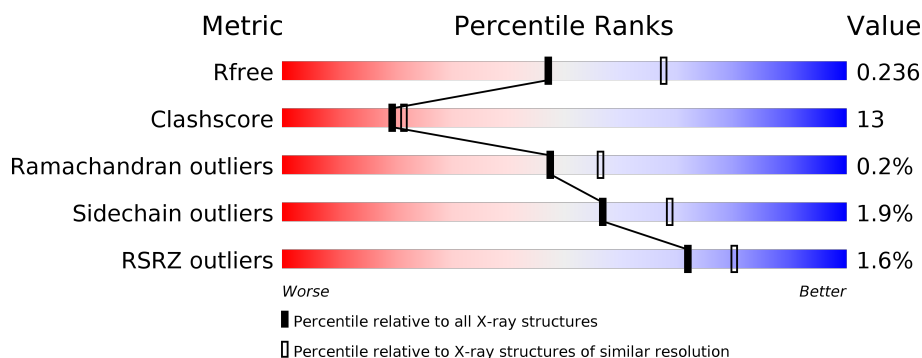
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	321	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
2	B	172	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>21%</div> </div> </div>
3	C	6	<div> <div>33%</div> <div>67%</div> </div>
4	D	5	<div> <div>40%</div> <div>60%</div> </div>
5	E	3	<div> <div>67%</div> <div>33%</div> </div>
6	F	2	<div> <div>50%</div> <div>50%</div> </div>

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	C	5	X	-	-	-
8	PEG	A	417	-	-	X	-
8	PEG	A	418	-	-	X	-
8	PEG	B	203	-	-	X	-
8	PEG	B	204	-	-	X	-
8	PEG	B	206	-	-	X	-
9	PE5	B	208	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4484 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2480	1552	436	479	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	ILE	VAL	conflict	UNP Q91MA7
A	329	GLN	ARG	conflict	UNP Q91MA7

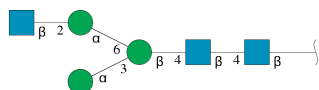
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1399	868	247	278	6			

There are 2 discrepancies between the modelled and reference sequences:

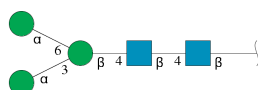
Chain	Residue	Modelled	Actual	Comment	Reference
B	132	GLU	ASP	conflict	UNP Q91MA7
B	164	ASN	ASP	conflict	UNP Q91MA7

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



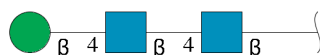
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 4 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
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



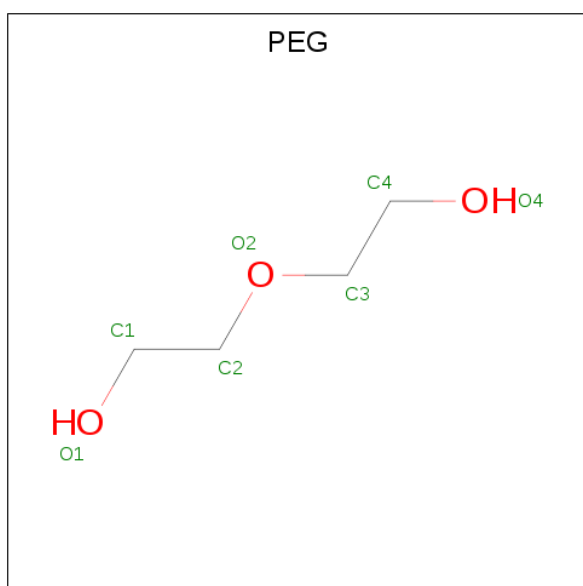
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



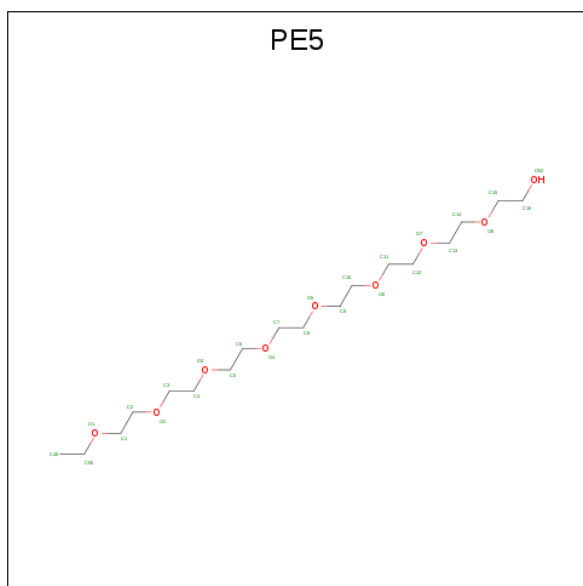
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 9 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			25	16	9		

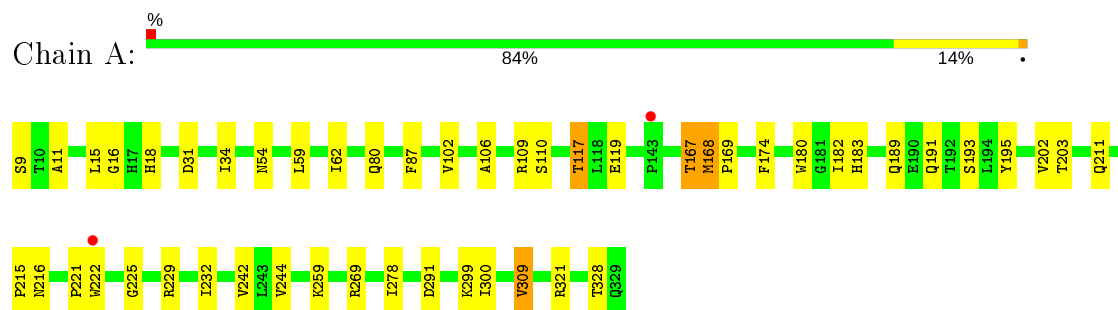
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	223	Total	O	0	0
			223	223		
10	B	77	Total	O	0	0
			77	77		

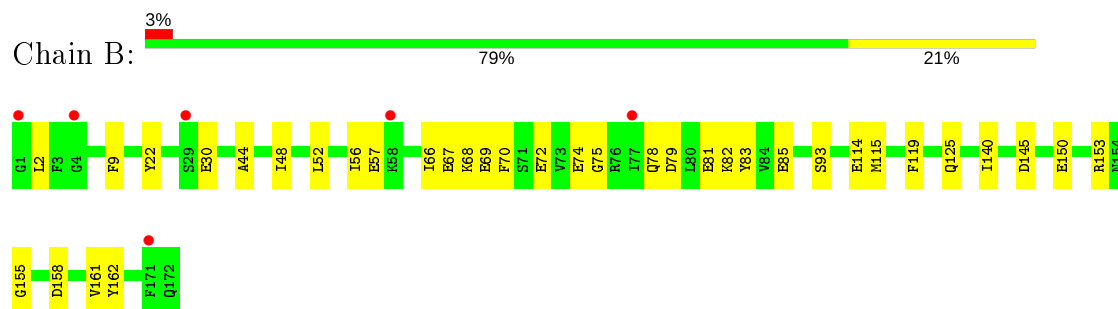
3 Residue-property plots

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 HA1 chain



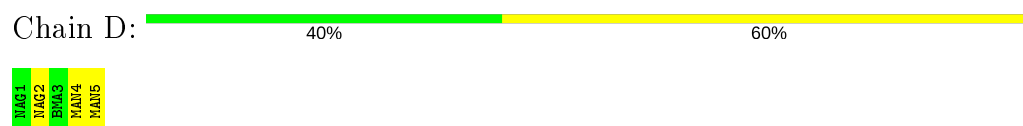
- Molecule 2: Hemagglutinin HA2 chain



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



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




- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%

MAG1
MAG2
BMA3

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

Chain F:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	155.51Å 155.51Å 155.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.50 – 2.35 49.18 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.50-2.35) 98.1 (49.18-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.193 , 0.236 0.193 , 0.236	Depositor DCC
R_{free} test set	1308 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4484	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: PEG, PE5, 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	0.25	0/2536	0.45	0/3455
2	B	0.26	0/1423	0.41	0/1912
All	All	0.26	0/3959	0.44	0/5367

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	2480	0	2428	44	0
2	B	1399	0	1319	55	0
3	C	75	0	64	0	0
4	D	61	0	52	1	0
5	E	39	0	34	0	0
6	F	28	0	25	1	0
7	A	28	0	26	1	0
8	A	14	0	18	13	0
8	B	35	0	45	22	0
9	B	25	0	33	26	0
10	A	223	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	77	0	0	5	0
All	All	4484	0	4044	105	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 13.

All (105) 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:229:ARG:NH1	10:A:501:HOH:O	1.84	1.08
2:B:82:LYS:HA	8:B:204:PEG:H21	1.43	0.99
1:A:211:GLN:OE1	10:A:502:HOH:O	1.88	0.92
2:B:67:GLU:HB2	9:B:208:PE5:H121	1.52	0.91
2:B:66:ILE:HA	9:B:208:PE5:H101	1.54	0.90
8:A:417:PEG:H42	2:B:69:GLU:H	1.34	0.90
1:A:269:ARG:HB2	8:A:417:PEG:H21	1.58	0.85
1:A:299:LYS:HE3	8:B:204:PEG:H32	1.58	0.85
1:A:191:GLN:O	10:A:503:HOH:O	1.95	0.82
1:A:80:GLN:O	10:A:504:HOH:O	2.01	0.79
1:A:269:ARG:HH22	9:B:208:PE5:H42	1.48	0.77
7:A:401:NAG:O6	10:A:505:HOH:O	2.03	0.76
1:A:117:THR:HG23	1:A:119:GLU:H	1.51	0.75
1:A:9:SER:N	10:A:507:HOH:O	2.20	0.74
1:A:215:PRO:O	10:A:506:HOH:O	2.06	0.74
8:A:418:PEG:H32	2:B:68:LYS:HE3	1.70	0.73
9:B:208:PE5:H41	9:B:208:PE5:H131	1.70	0.72
10:A:654:HOH:O	9:B:208:PE5:H11	1.91	0.70
2:B:145:ASP:OD1	10:B:301:HOH:O	2.09	0.70
8:A:417:PEG:H12	8:A:418:PEG:H12	1.76	0.67
2:B:68:LYS:HG2	8:B:204:PEG:H11	1.76	0.67
1:A:300:ILE:HD13	8:A:417:PEG:H12	1.75	0.67
1:A:321:ARG:NH1	10:A:510:HOH:O	2.25	0.66
9:B:208:PE5:H12	9:B:208:PE5:H142	1.76	0.66
9:B:208:PE5:H12	9:B:208:PE5:C14	2.26	0.65
2:B:70:PHE:CE1	9:B:208:PE5:H132	2.34	0.63
2:B:85:GLU:HB2	8:B:204:PEG:H12	1.80	0.63
2:B:83:TYR:HA	8:B:205:PEG:H32	1.81	0.63
1:A:309:VAL:HG22	2:B:93:SER:HA	1.82	0.62
8:A:417:PEG:H32	2:B:69:GLU:HB2	1.81	0.61
1:A:109:ARG:HH11	9:B:208:PE5:H61	1.66	0.61
8:A:417:PEG:C3	2:B:69:GLU:HB2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LYS:HA	8:B:204:PEG:H11	1.85	0.59
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.85	0.59
2:B:82:LYS:HD2	8:B:206:PEG:H31	1.84	0.59
1:A:16:GLY:HA2	2:B:9:PHE:HB3	1.84	0.58
1:A:106:ALA:HA	9:B:208:PE5:H32	1.86	0.58
2:B:74:GLU:N	8:B:206:PEG:O1	2.33	0.57
1:A:191:GLN:C	10:A:503:HOH:O	2.42	0.57
2:B:75:GLY:N	8:B:206:PEG:O1	2.36	0.56
2:B:85:GLU:CB	8:B:204:PEG:H12	2.35	0.56
2:B:22:TYR:HD1	2:B:115:MET:HE2	1.71	0.56
2:B:70:PHE:N	8:B:203:PEG:O4	2.34	0.55
9:B:208:PE5:C4	9:B:208:PE5:H131	2.36	0.54
2:B:162:TYR:OH	10:B:302:HOH:O	2.18	0.54
8:A:417:PEG:C4	2:B:69:GLU:H	2.14	0.54
2:B:81:GLU:OE2	9:B:208:PE5:H122	2.07	0.54
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.37	0.53
2:B:52:LEU:HG	2:B:56:ILE:HD12	1.90	0.53
2:B:74:GLU:OE1	9:B:208:PE5:H151	2.08	0.53
1:A:109:ARG:NH1	9:B:208:PE5:H61	2.23	0.53
1:A:189:GLN:O	1:A:193:SER:OG	2.19	0.52
1:A:269:ARG:HH22	9:B:208:PE5:C4	2.18	0.52
1:A:180:TRP:HZ3	1:A:182:ILE:HD11	1.74	0.52
2:B:78:GLN:CD	8:B:206:PEG:H12	2.30	0.51
2:B:72:GLU:H	9:B:208:PE5:H162	1.76	0.51
2:B:150:GLU:HB3	6:F:1:NAG:H82	1.94	0.50
1:A:59:LEU:HD23	1:A:87:PHE:CD1	2.46	0.50
1:A:168:MET:HE1	10:A:716:HOH:O	2.11	0.49
1:A:300:ILE:HD13	8:A:417:PEG:C1	2.41	0.49
1:A:221:PRO:O	1:A:229:ARG:NH2	2.46	0.49
2:B:82:LYS:HZ2	8:B:206:PEG:C4	2.26	0.49
8:A:418:PEG:H22	2:B:67:GLU:HA	1.94	0.48
8:A:418:PEG:H31	10:B:342:HOH:O	2.14	0.48
2:B:68:LYS:HA	8:B:204:PEG:C1	2.42	0.48
2:B:44:ALA:O	2:B:48:ILE:HG12	2.14	0.48
2:B:70:PHE:HB3	9:B:208:PE5:H161	1.96	0.48
2:B:114:GLU:HG2	10:B:306:HOH:O	2.14	0.47
9:B:208:PE5:H12	9:B:208:PE5:H152	1.96	0.47
9:B:208:PE5:C13	9:B:208:PE5:H41	2.41	0.47
2:B:82:LYS:HA	8:B:204:PEG:H41	1.95	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.97	0.47
1:A:291:ASP:O	2:B:56:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:208:PE5:H12	9:B:208:PE5:C15	2.46	0.46
8:A:417:PEG:H42	2:B:69:GLU:N	2.16	0.46
1:A:11:ALA:HB3	2:B:140:ILE:HB	1.97	0.46
2:B:70:PHE:HE1	9:B:208:PE5:H132	1.79	0.46
8:A:417:PEG:H41	2:B:67:GLU:OE1	2.15	0.46
1:A:169:PRO:HA	1:A:242:VAL:HG23	1.97	0.45
1:A:167:THR:HG21	4:D:2:NAG:H82	1.99	0.45
2:B:78:GLN:HB3	8:B:206:PEG:H21	1.98	0.45
1:A:106:ALA:HB2	9:B:208:PE5:H22	1.98	0.45
1:A:59:LEU:HD23	1:A:87:PHE:CE1	2.52	0.45
2:B:82:LYS:HZ1	8:B:203:PEG:C2	2.29	0.44
1:A:31:ASP:HB2	1:A:34:ILE:HG12	2.00	0.44
2:B:70:PHE:CD1	9:B:208:PE5:H132	2.53	0.43
1:A:203:THR:HG22	10:A:542:HOH:O	2.18	0.43
1:A:54:ASN:HB3	1:A:278:ILE:HG12	1.99	0.43
2:B:79:ASP:OD1	8:B:206:PEG:H32	2.19	0.43
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.54	0.43
9:B:208:PE5:H12	9:B:208:PE5:O8	2.18	0.43
2:B:82:LYS:CA	8:B:204:PEG:H41	2.49	0.43
2:B:150:GLU:OE1	2:B:153:ARG:NH2	2.48	0.43
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.18	0.43
2:B:158:ASP:OD2	10:B:303:HOH:O	2.22	0.42
2:B:78:GLN:HB3	8:B:206:PEG:C2	2.49	0.42
1:A:167:THR:HG23	1:A:244:VAL:HG22	2.01	0.42
1:A:182:ILE:HG13	1:A:202:VAL:HG21	2.02	0.42
2:B:125:GLN:OE1	2:B:155:GLY:HA2	2.20	0.41
1:A:328:THR:HB	2:B:2:LEU:HD12	2.02	0.41
1:A:174:PHE:CD2	1:A:259:LYS:HE3	2.55	0.41
1:A:106:ALA:HA	9:B:208:PE5:H51	2.03	0.41
1:A:110:SER:CB	9:B:208:PE5:H72	2.51	0.41
2:B:82:LYS:HZ3	8:B:203:PEG:H31	1.86	0.40
2:B:70:PHE:H	8:B:203:PEG:HO4	1.63	0.40

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	319/321 (99%)	308 (97%)	10 (3%)	1 (0%)	41	47
2	B	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
All	All	489/493 (99%)	469 (96%)	19 (4%)	1 (0%)	47	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	283/283 (100%)	277 (98%)	6 (2%)	53	65
2	B	147/147 (100%)	145 (99%)	2 (1%)	67	78
All	All	430/430 (100%)	422 (98%)	8 (2%)	57	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	117	THR
1	A	167	THR
1	A	168	MET
1	A	216	ASN
1	A	309	VAL
2	B	57	GLU
2	B	161	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
2	B	65	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 ⓘ

16 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	C	1	1,3	14,14,15	0.69	0	17,19,21	1.13	2 (11%)
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.44	0
3	BMA	C	3	3	11,11,12	0.91	0	15,15,17	1.13	0
3	MAN	C	4	3	11,11,12	1.56	4 (36%)	15,15,17	1.82	2 (13%)
3	NAG	C	5	3	14,14,15	0.87	1 (7%)	17,19,21	0.76	1 (5%)
3	MAN	C	6	3	11,11,12	1.28	1 (9%)	15,15,17	0.97	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	D	2	4	14,14,15	0.56	0	17,19,21	0.57	0
4	BMA	D	3	4	11,11,12	0.92	0	15,15,17	0.98	0
4	MAN	D	4	4	11,11,12	0.78	1 (9%)	15,15,17	1.42	3 (20%)
4	MAN	D	5	4	11,11,12	0.89	0	15,15,17	1.40	3 (20%)
5	NAG	E	1	1,5	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	0.62	0
5	BMA	E	3	5	11,11,12	0.73	0	15,15,17	1.34	2 (13%)
6	NAG	F	1	2,6	14,14,15	0.68	1 (7%)	17,19,21	0.66	0
6	NAG	F	2	6	14,14,15	1.15	2 (14%)	17,19,21	0.88	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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	1/1/1/1
3	NAG	C	5	3	1/1/5/7	2/6/23/26	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	1/1/1/1
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	MAN	O5-C1	-3.30	1.38	1.43
3	C	5	NAG	O5-C1	3.02	1.48	1.43
6	F	2	NAG	C1-C2	2.95	1.56	1.52
6	F	2	NAG	O5-C1	-2.61	1.39	1.43
3	C	4	MAN	C1-C2	2.49	1.57	1.52
6	F	1	NAG	O5-C1	-2.43	1.39	1.43
3	C	4	MAN	C4-C5	2.35	1.58	1.53
3	C	4	MAN	O2-C2	2.27	1.48	1.43
3	C	4	MAN	C4-C3	2.20	1.57	1.52
4	D	4	MAN	C1-C2	2.03	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	O2-C2-C1	4.76	118.89	109.15
3	C	4	MAN	C1-C2-C3	-4.17	104.54	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	C1-O5-C5	3.83	117.38	112.19
4	D	4	MAN	C1-O5-C5	3.60	117.07	112.19
4	D	5	MAN	C1-O5-C5	3.49	116.92	112.19
3	C	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	C	5	NAG	C1-O5-C5	2.70	115.85	112.19
4	D	4	MAN	O5-C1-C2	2.31	114.34	110.77
6	F	2	NAG	C4-C3-C2	2.27	114.35	111.02
3	C	1	NAG	C3-C4-C5	2.20	114.17	110.24
4	D	5	MAN	O2-C2-C3	-2.14	105.84	110.14
6	F	2	NAG	O5-C5-C4	-2.03	105.89	110.83
3	C	6	MAN	O2-C2-C3	-2.03	106.07	110.14
5	E	3	BMA	O5-C1-C2	2.02	113.88	110.77
4	D	5	MAN	O5-C1-C2	2.01	113.88	110.77
4	D	4	MAN	O2-C2-C3	-2.01	106.11	110.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	5	NAG	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6

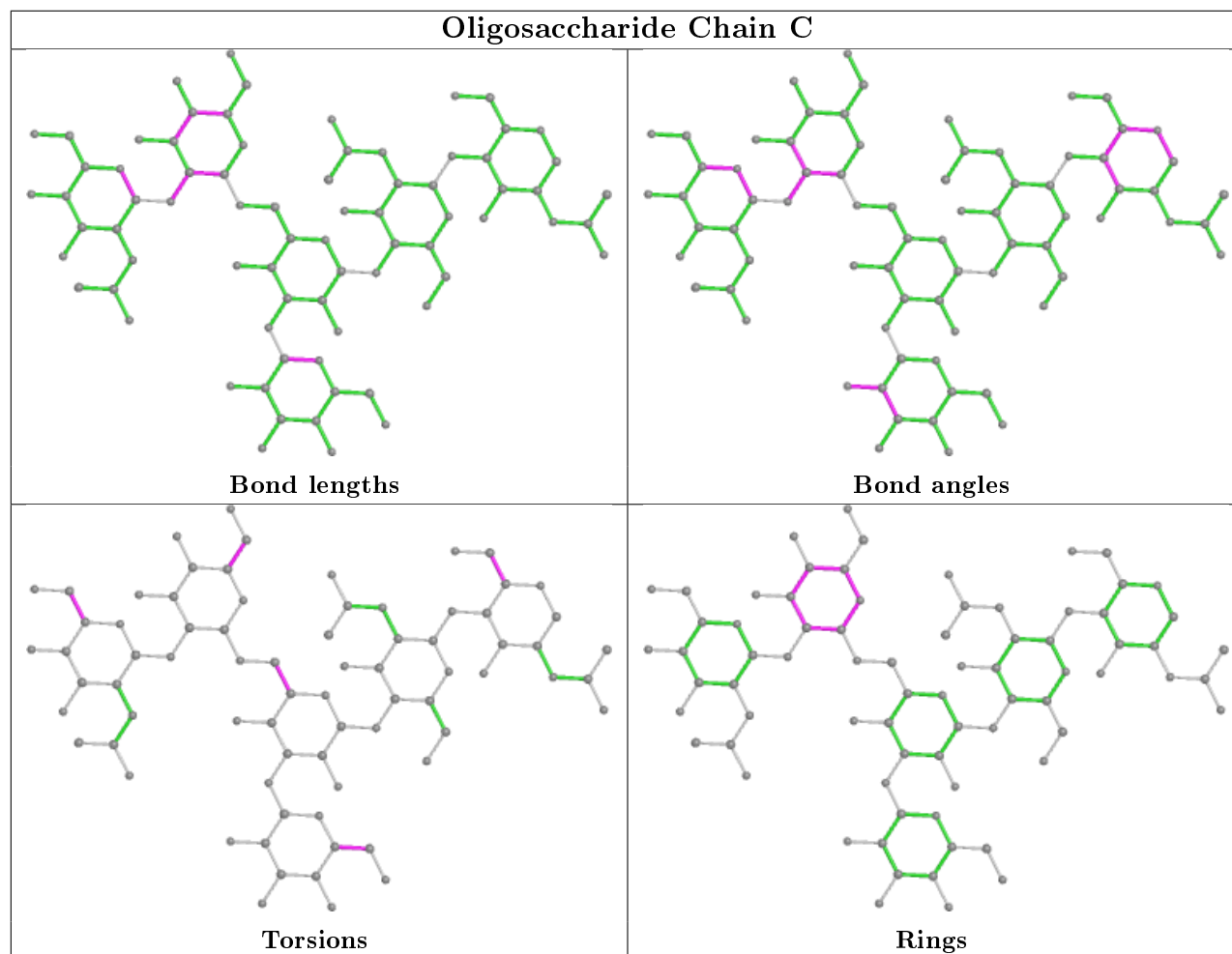
All (2) ring outliers are listed below:

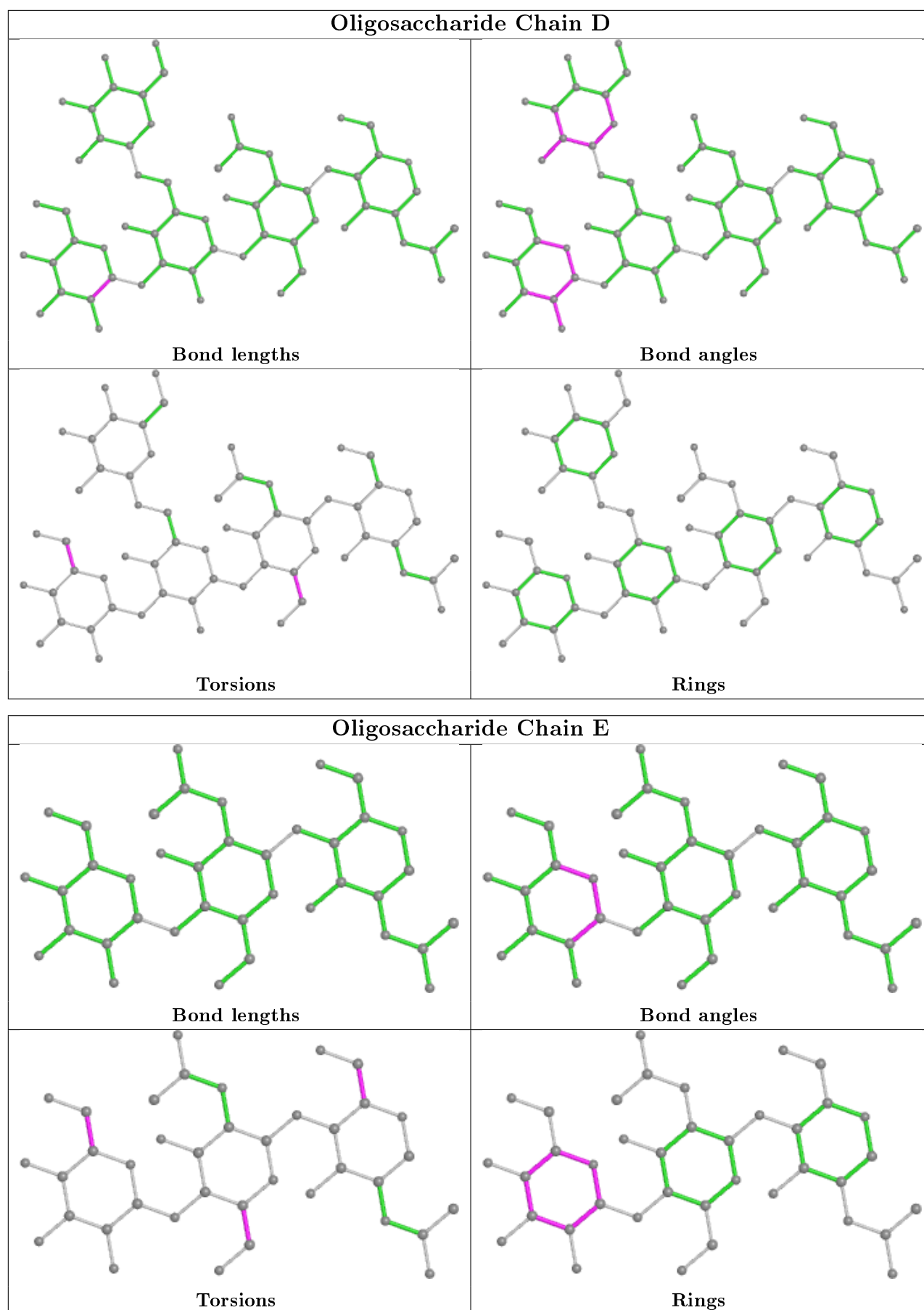
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	C1-C2-C3-C4-C5-O5
3	C	4	MAN	C1-C2-C3-C4-C5-O5

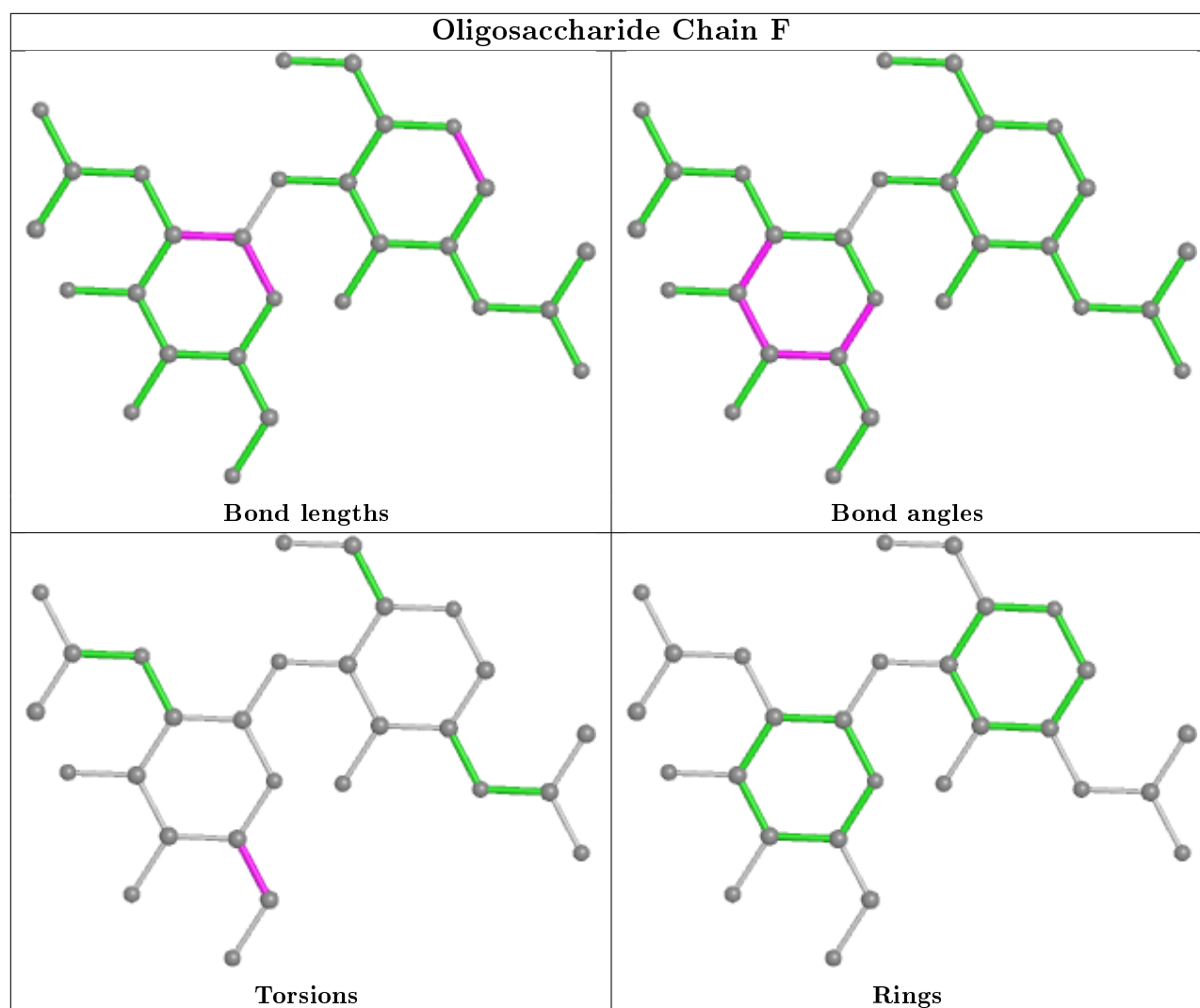
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0
4	D	2	NAG	1	0

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







5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
8	PEG	B	207	-	6,6,6	0.58	0	5,5,5	0.24	0
7	NAG	A	416	1	14,14,15	0.20	0	17,19,21	0.56	0
8	PEG	B	203	-	6,6,6	0.60	0	5,5,5	0.45	0
8	PEG	A	418	-	6,6,6	0.58	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PE5	B	208	-	24,24,26	0.64	0	23,23,25	0.43	0
8	PEG	B	206	-	6,6,6	0.64	0	5,5,5	0.32	0
8	PEG	B	205	-	6,6,6	0.57	0	5,5,5	0.35	0
7	NAG	A	401	1	14,14,15	0.24	0	17,19,21	0.46	0
8	PEG	A	417	-	6,6,6	0.62	0	5,5,5	0.28	0
8	PEG	B	204	-	6,6,6	0.66	0	5,5,5	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	207	-	-	3/4/4/4	-
7	NAG	A	416	1	-	2/6/23/26	0/1/1/1
8	PEG	B	203	-	-	2/4/4/4	-
8	PEG	A	418	-	-	3/4/4/4	-
9	PE5	B	208	-	-	11/22/22/24	-
8	PEG	B	206	-	-	1/4/4/4	-
8	PEG	B	205	-	-	3/4/4/4	-
7	NAG	A	401	1	-	2/6/23/26	0/1/1/1
8	PEG	A	417	-	-	2/4/4/4	-
8	PEG	B	204	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	416	NAG	O5-C5-C6-O6
7	A	416	NAG	C4-C5-C6-O6
9	B	208	PE5	O6-C10-C9-O5
8	A	418	PEG	O2-C3-C4-O4
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
8	B	207	PEG	O1-C1-C2-O2
8	B	205	PEG	O1-C1-C2-O2
8	B	205	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
9	B	208	PE5	C9-C10-O6-C11
8	B	207	PEG	O2-C3-C4-O4
8	B	203	PEG	O1-C1-C2-O2
9	B	208	PE5	O1-C1-C2-O2
8	B	203	PEG	O2-C3-C4-O4
8	B	205	PEG	C4-C3-O2-C2
8	A	418	PEG	C4-C3-O2-C2
8	A	417	PEG	C4-C3-O2-C2
8	B	207	PEG	C1-C2-O2-C3
8	A	418	PEG	C1-C2-O2-C3
9	B	208	PE5	C4-C3-O2-C2
8	A	417	PEG	C1-C2-O2-C3
9	B	208	PE5	C11-C12-O7-C13
9	B	208	PE5	O6-C11-C12-O7
9	B	208	PE5	C1-C2-O2-C3
9	B	208	PE5	C13-C14-O8-C15
8	B	206	PEG	O2-C3-C4-O4
9	B	208	PE5	C10-C9-O5-C8
9	B	208	PE5	O7-C13-C14-O8
9	B	208	PE5	O2-C3-C4-O3

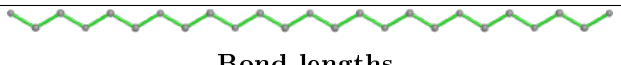
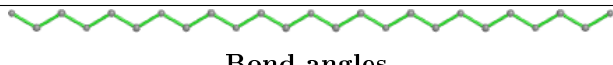
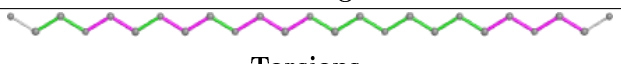
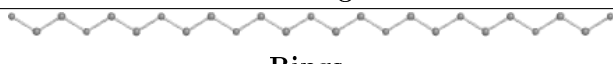
There are no ring outliers.

8 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	203	PEG	4	0
8	A	418	PEG	4	0
9	B	208	PE5	26	0
8	B	206	PEG	8	0
8	B	205	PEG	1	0
7	A	401	NAG	1	0
8	A	417	PEG	10	0
8	B	204	PEG	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PE5 B 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	321/321 (100%)	-0.15	2 (0%) 89 93	14, 28, 49, 71	0
2	B	172/172 (100%)	0.09	6 (3%) 44 56	11, 35, 56, 88	0
All	All	493/493 (100%)	-0.06	8 (1%) 72 80	11, 31, 53, 88	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	GLY	3.4
2	B	29	SER	3.1
2	B	58	LYS	2.6
2	B	171	PHE	2.5
2	B	77	ILE	2.4
1	A	143	PRO	2.1
2	B	1	GLY	2.1
1	A	222	TRP	2.1

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.

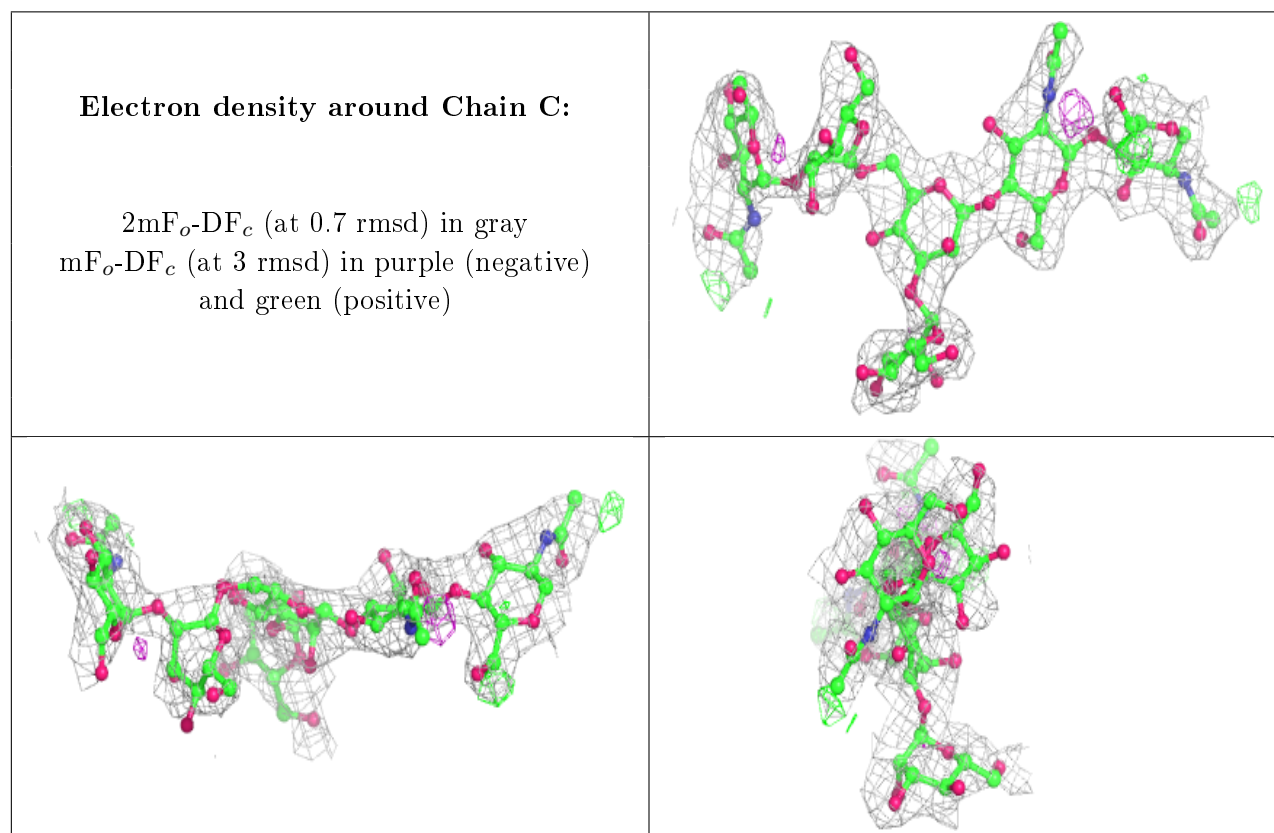
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	F	2	14/15	0.45	0.33	91,110,122,124	0

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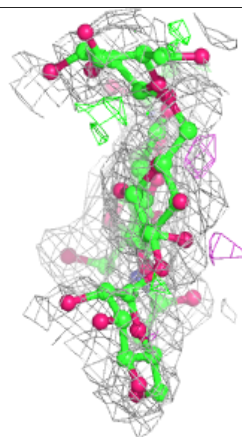
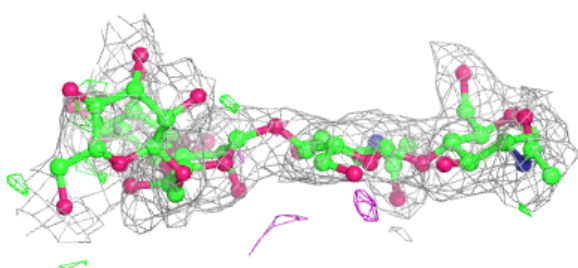
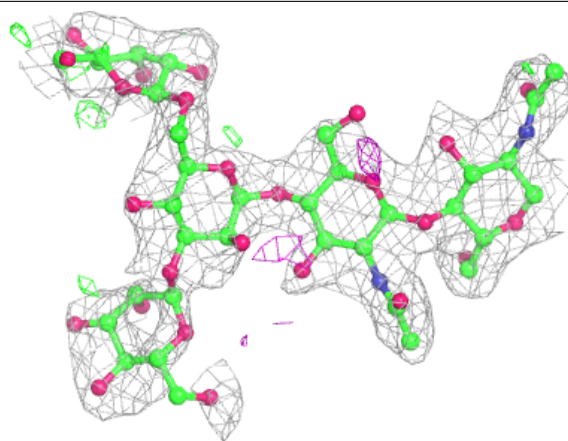
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	D	5	11/12	0.51	0.20	86,95,109,111	0
4	MAN	D	4	11/12	0.57	0.30	79,100,103,104	0
3	NAG	C	5	14/15	0.62	0.23	66,78,89,95	0
3	MAN	C	6	11/12	0.65	0.24	84,96,108,109	0
6	NAG	F	1	14/15	0.66	0.32	55,92,110,114	0
5	BMA	E	3	11/12	0.76	0.22	99,102,111,112	0
3	NAG	C	2	14/15	0.78	0.22	56,64,78,80	0
4	BMA	D	3	11/12	0.78	0.21	67,83,92,95	0
5	NAG	E	2	14/15	0.81	0.24	56,75,100,105	0
3	MAN	C	4	11/12	0.83	0.19	82,89,96,100	0
3	BMA	C	3	11/12	0.87	0.21	84,90,100,101	0
3	NAG	C	1	14/15	0.89	0.15	38,49,56,59	0
5	NAG	E	1	14/15	0.91	0.12	28,40,49,71	0
4	NAG	D	2	14/15	0.91	0.22	32,44,59,65	0
4	NAG	D	1	14/15	0.93	0.13	26,38,52,57	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.

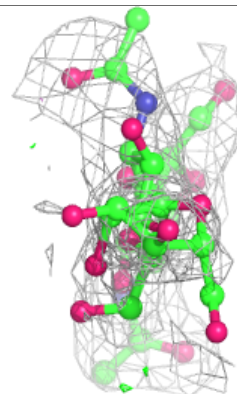
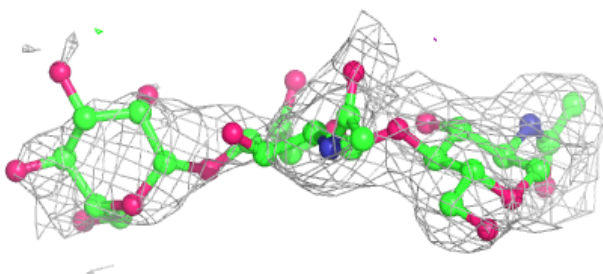
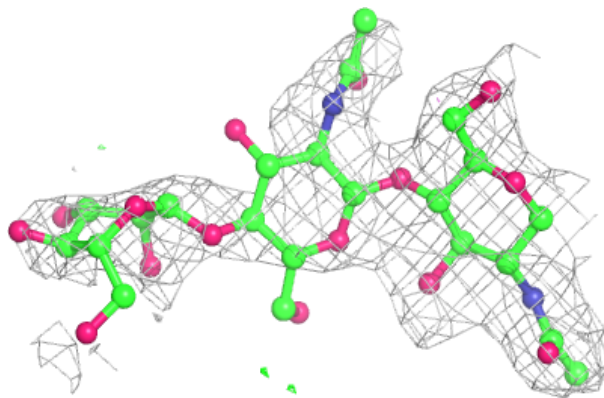


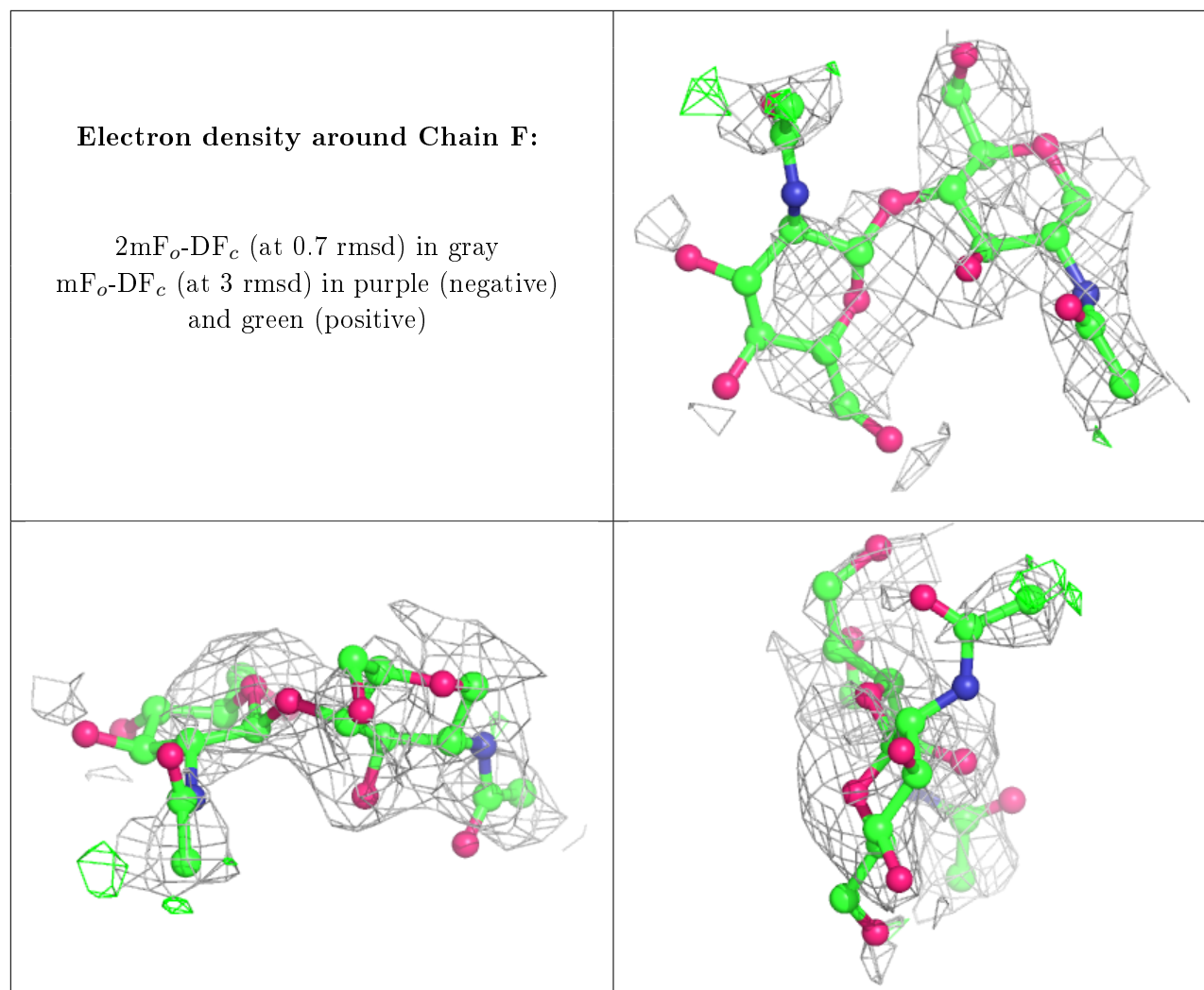
Electron density around Chain D:

$2mF_o-DF_c$ (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)





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.

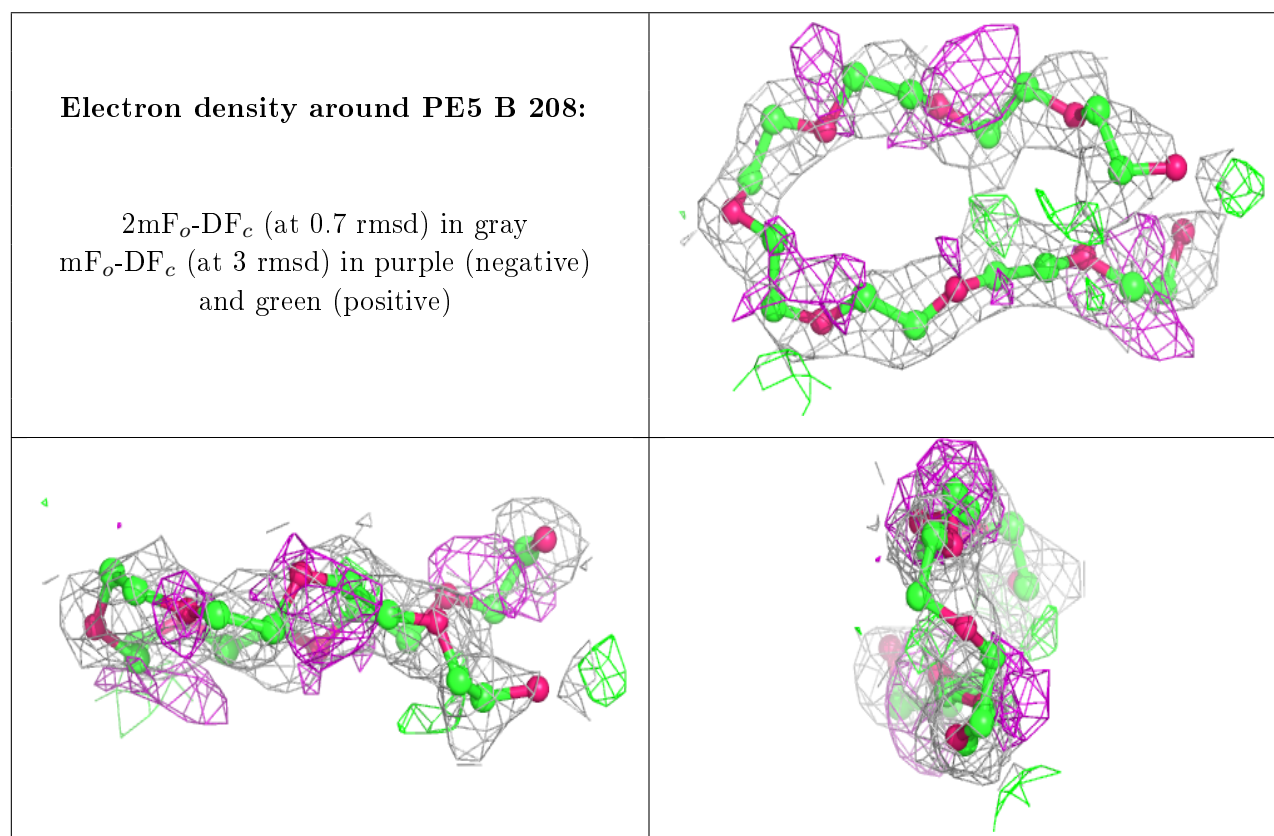
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	A	401	14/15	0.73	0.29	43,67,75,76	0
8	PEG	B	205	7/7	0.81	0.23	24,33,42,50	0
7	NAG	A	416	14/15	0.83	0.14	41,60,71,75	0
8	PEG	B	203	7/7	0.86	0.22	29,37,41,46	0
8	PEG	A	417	7/7	0.86	0.28	19,26,38,41	0
9	PE5	B	208	25/27	0.88	0.24	8,31,48,56	0
8	PEG	A	418	7/7	0.89	0.28	19,25,37,40	0
8	PEG	B	204	7/7	0.89	0.25	18,24,37,40	0
8	PEG	B	207	7/7	0.91	0.13	46,51,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	B	206	7/7	0.94	0.24	21,29,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.