



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 PM UTC

PDB ID : 7DEB / pdb\_00007deb  
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus  
A/duck/Eastern China/L0230/2010 (H5N2)  
Authors : Sun, H.; Sun, H.; Song, J.; Zhang, W.; Qi, J.; Gao, G.F.; Liu, J.  
Deposited on : 2020-11-03  
Resolution : 2.60 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](mailto: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>.

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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

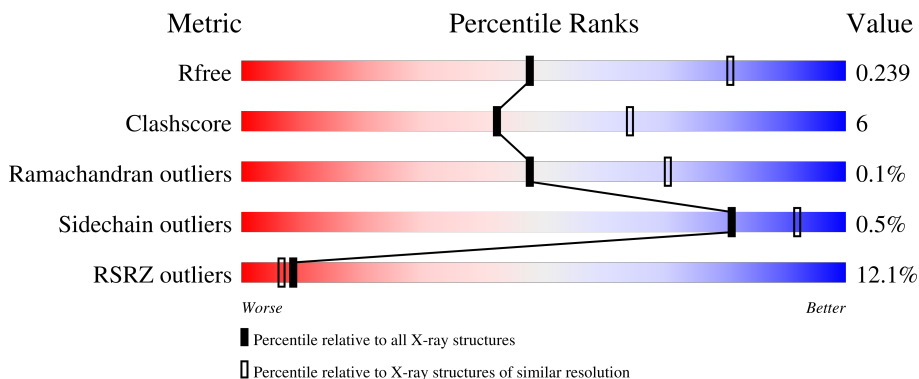
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



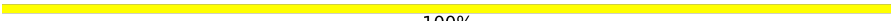
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	505	 13% 84% 13%
1	B	505	 5% 86% 11%
1	C	505	 17% 82% 15%
2	D	3	 67% 33%
3	E	2	 100%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

## 2 Entry composition [i](#)

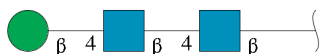
There are 5 unique types of molecules in this entry. The entry contains 12488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	494	Total 3946	C 2480	N 686	O 758	S 22	0	0	0
1	B	494	Total 3946	C 2480	N 686	O 758	S 22	0	0	0
1	C	494	Total 3946	C 2480	N 686	O 758	S 22	0	0	0

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

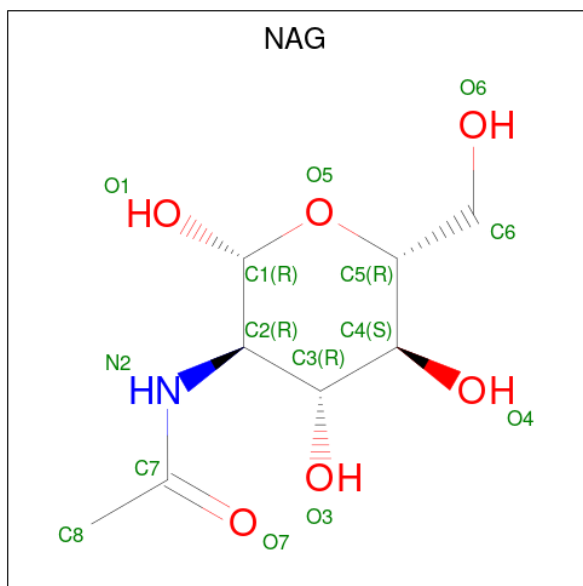
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	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		

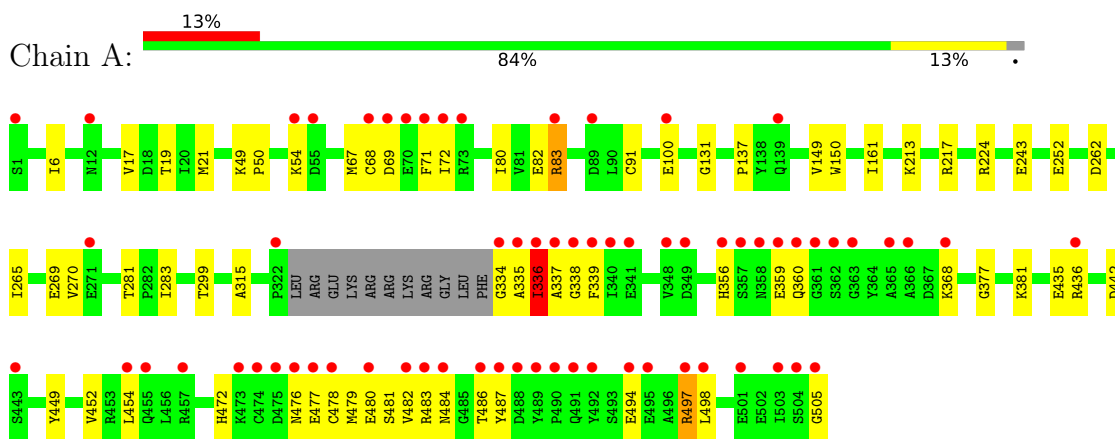
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	181	Total	O	0	0
			181	181		
5	C	160	Total	O	0	0
			160	160		

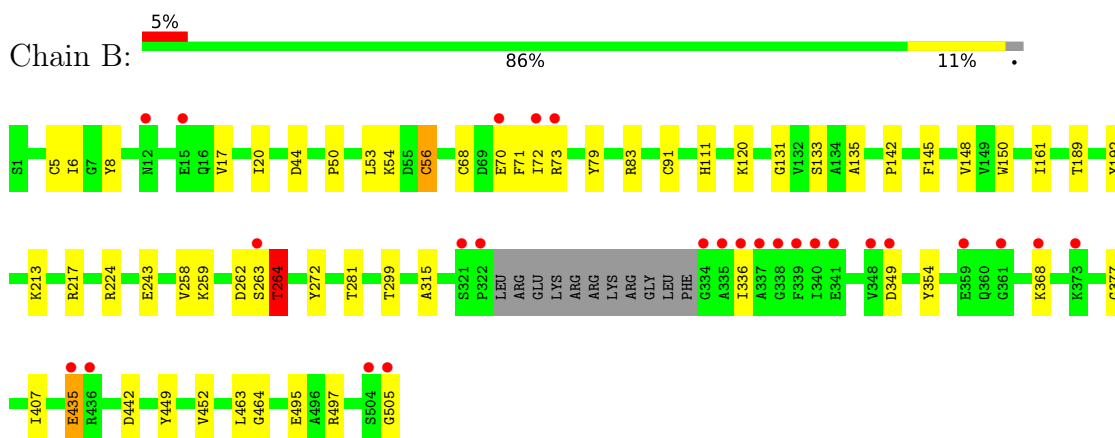
### 3 Residue-property plots [i](#)

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.

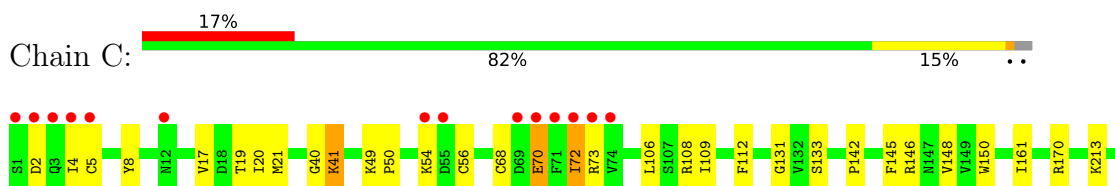
- Molecule 1: Hemagglutinin

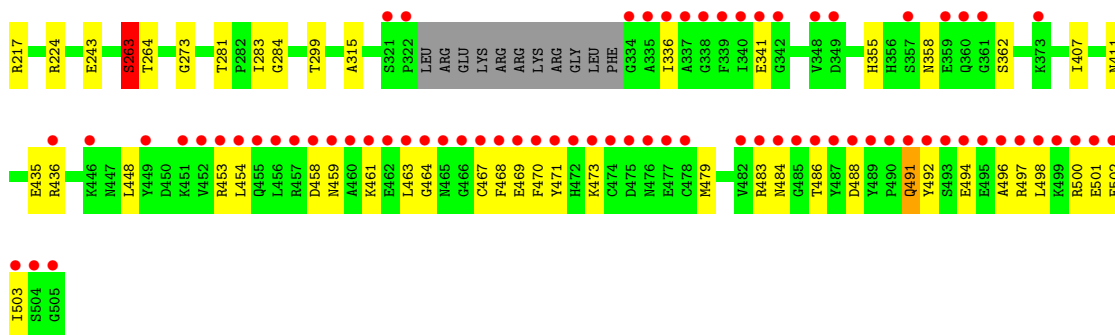


- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin





- 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: 67% 33%

MAG1  
MAG2  
BMA3

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

Chain E: 100%

MAG1  
MAG2

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

Chain F: 100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.96Å 164.86Å 230.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.58 – 2.60 46.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.58-2.60) 99.6 (46.58-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 7.0.053	Depositor
R, $R_{free}$	0.206 , 0.238 0.207 , 0.239	Depositor DCC
$R_{free}$ test set	5581 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, BMA

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	0.32	4/4036 (0.1%)	0.58	10/5468 (0.2%)
1	B	0.35	2/4036 (0.0%)	0.51	5/5468 (0.1%)
1	C	0.31	3/4036 (0.1%)	0.56	5/5468 (0.1%)
All	All	0.33	9/12108 (0.1%)	0.55	20/16404 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	SER	C-O	-6.78	1.15	1.24
1	A	262	ASP	C-N	6.55	1.39	1.33
1	B	56	CYS	C-O	-5.97	1.16	1.23
1	A	497	ARG	CZ-NH2	5.79	1.41	1.33
1	A	497	ARG	NE-CZ	-5.72	1.26	1.33
1	C	263	SER	CA-CB	-5.68	1.49	1.54
1	B	264	THR	C-O	-5.56	1.16	1.24
1	A	497	ARG	CB-CG	5.40	1.68	1.52
1	C	170	ARG	CB-CG	-5.24	1.36	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ARG	CG-CD-NE	-10.98	87.84	112.00
1	B	349	ASP	CB-CA-C	-8.68	96.48	111.23
1	C	491	GLN	CB-CA-C	-8.43	97.88	110.95
1	A	359	GLU	CA-CB-CG	-8.25	97.61	114.10
1	B	435	GLU	CB-CA-C	-7.97	98.37	110.88
1	A	82	GLU	CA-C-N	-7.87	109.05	122.67
1	A	82	GLU	C-N-CA	-7.87	109.05	122.67
1	A	359	GLU	CB-CA-C	7.07	122.81	110.64
1	B	368	LYS	CD-CE-NZ	-6.88	89.88	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ALA	N-CA-C	6.18	117.85	110.19
1	C	41	LYS	CG-CD-CE	-6.12	97.22	111.30
1	A	497	ARG	CG-CD-NE	5.97	125.14	112.00
1	A	83	ARG	CB-CA-C	5.72	120.35	110.45
1	A	359	GLU	N-CA-CB	-5.68	101.61	110.98
1	C	263	SER	O-C-N	-5.55	118.95	123.11
1	A	497	ARG	CA-CB-CG	5.22	124.55	114.10
1	A	69	ASP	N-CA-C	5.21	118.10	111.69
1	B	53	LEU	N-CA-C	-5.17	101.55	109.76
1	C	41	LYS	CD-CE-NZ	5.16	128.42	111.90
1	B	349	ASP	N-CA-CB	5.02	118.58	111.25

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	3946	0	3803	54	0
1	B	3946	0	3805	42	0
1	C	3946	0	3803	65	0
2	D	39	0	34	1	1
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
5	A	172	0	0	2	0
5	B	181	0	0	3	1
5	C	160	0	0	3	0
All	All	12488	0	11534	149	1

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 6.

All (149) 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:B:56:CYS:SG	1:B:68:CYS:SG	1.47	1.35
1:A:334:GLY:O	1:A:338:GLY:HA3	1.50	1.12
1:B:259:LYS:NZ	1:B:262:ASP:OD1	1.86	1.07
1:A:480:GLU:HA	1:A:483:ARG:HD2	1.46	0.96
1:A:54:LYS:HE3	1:A:83:ARG:HD2	1.48	0.96
1:A:83:ARG:NE	1:A:269:GLU:OE1	2.05	0.90
1:A:497:ARG:HE	1:A:498:LEU:HD21	1.33	0.90
1:C:494:GLU:HA	1:C:497:ARG:HG2	1.57	0.87
1:B:56:CYS:SG	1:B:68:CYS:CB	2.61	0.87
1:A:497:ARG:HE	1:A:498:LEU:CD2	1.88	0.85
1:A:213:LYS:O	1:A:217:ARG:NH2	2.13	0.81
1:B:263:SER:OG	1:B:264:THR:N	2.13	0.80
1:A:334:GLY:O	1:A:338:GLY:CA	2.30	0.78
1:B:407:ILE:CD1	1:C:407:ILE:HG21	2.12	0.77
1:C:411:ASN:ND2	5:C:701:HOH:O	2.14	0.77
1:A:54:LYS:CE	1:A:83:ARG:HD2	2.13	0.77
1:C:213:LYS:O	1:C:217:ARG:NH2	2.18	0.77
1:B:407:ILE:HD11	1:C:407:ILE:HG21	1.65	0.76
1:C:496:ALA:O	1:C:500:ARG:HB2	1.89	0.73
1:B:213:LYS:O	1:B:217:ARG:NH2	2.22	0.73
1:A:68:CYS:HB2	1:A:71:PHE:HZ	1.53	0.73
1:A:472:HIS:NE2	1:A:487:TYR:OH	2.21	0.71
1:B:495:GLU:OE1	5:B:701:HOH:O	2.09	0.69
1:B:20:ILE:HG22	1:B:435:GLU:OE1	1.94	0.67
1:A:497:ARG:NE	1:A:498:LEU:HD21	2.08	0.65
1:B:259:LYS:CE	1:B:262:ASP:OD1	2.45	0.64
1:A:368:LYS:H	1:A:368:LYS:HE2	1.63	0.63
1:C:491:GLN:NE2	1:C:492:TYR:CZ	2.67	0.62
1:A:100:GLU:H	1:A:100:GLU:CD	2.10	0.60
1:B:131:GLY:HA3	1:B:150:TRP:HB3	1.84	0.60
1:C:358:ASN:ND2	5:C:703:HOH:O	2.34	0.59
1:C:224:ARG:NH1	5:C:706:HOH:O	2.34	0.59
1:A:478:CYS:O	1:A:482:VAL:HG23	2.02	0.59
1:C:131:GLY:HA3	1:C:150:TRP:HB3	1.86	0.57
1:C:355:HIS:HE1	1:C:362:SER:HB2	1.70	0.57
1:B:70:GLU:HB3	1:B:72:ILE:HG23	1.87	0.57
1:A:484:ASN:OD1	1:A:486:THR:OG1	2.20	0.56
1:C:72:ILE:HG23	1:C:72:ILE:O	2.03	0.56
1:A:336:ILE:O	1:A:337:ALA:HB3	2.06	0.56
1:B:6:ILE:HD11	1:B:452:VAL:HG21	1.88	0.56
1:A:505:GLY:HA2	1:B:497:ARG:HH22	1.70	0.56
1:C:68:CYS:O	1:C:146:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLU:HB2	1:A:483:ARG:HH11	1.70	0.56
1:A:54:LYS:HE3	1:A:83:ARG:CD	2.31	0.55
1:C:494:GLU:CA	1:C:497:ARG:HG2	2.34	0.55
1:C:70:GLU:HB3	1:C:146:ARG:CZ	2.37	0.55
1:C:463:LEU:HD21	1:C:469:GLU:HB2	1.88	0.54
1:A:161:ILE:O	1:A:243:GLU:HA	2.07	0.54
1:B:145:PHE:HB2	1:B:148:VAL:HG12	1.90	0.54
1:C:70:GLU:H	1:C:70:GLU:CD	2.13	0.54
1:C:488:ASP:HB3	1:C:491:GLN:HB2	1.90	0.53
1:B:120:LYS:NZ	5:B:705:HOH:O	2.38	0.53
1:C:497:ARG:HG3	1:C:498:LEU:N	2.22	0.53
1:C:4:ILE:HB	1:C:470:PHE:CZ	2.44	0.53
1:C:54:LYS:O	1:C:56:CYS:N	2.42	0.52
1:B:8:TYR:CZ	1:B:336:ILE:HG12	2.45	0.52
1:B:495:GLU:OE2	5:B:702:HOH:O	2.19	0.52
1:C:161:ILE:O	1:C:243:GLU:HA	2.10	0.52
1:A:67:MET:HE2	1:A:91:CYS:HB3	1.92	0.52
1:C:263:SER:OG	1:C:264:THR:N	2.41	0.51
1:A:72:ILE:O	1:A:72:ILE:HG23	2.11	0.51
1:B:8:TYR:CE1	1:B:336:ILE:HG12	2.46	0.51
1:A:334:GLY:O	1:A:339:PHE:N	2.43	0.51
1:C:453:ARG:HH21	1:C:454:LEU:HD21	1.76	0.51
1:A:436:ARG:NH1	1:C:436:ARG:HG2	2.26	0.50
1:C:5:CYS:HA	1:C:467:CYS:HA	1.94	0.50
1:C:49:LYS:HG2	1:C:50:PRO:HD2	1.93	0.50
1:C:2:ASP:OD2	1:C:473:LYS:HD2	2.12	0.50
1:A:68:CYS:HB2	1:A:71:PHE:CZ	2.40	0.49
1:A:454:LEU:HD22	1:C:464:GLY:HA2	1.95	0.49
1:C:458:ASP:O	1:C:500:ARG:NH1	2.45	0.49
1:C:494:GLU:OE2	1:C:497:ARG:NH2	2.34	0.48
1:A:149:VAL:HG23	1:A:252:GLU:HB2	1.96	0.48
1:A:19:THR:HB	1:A:435:GLU:HB2	1.96	0.47
1:A:68:CYS:CB	1:A:71:PHE:HZ	2.24	0.47
1:C:145:PHE:HB2	1:C:148:VAL:HG12	1.97	0.47
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.73	0.47
1:C:484:ASN:OD1	1:C:486:THR:OG1	2.24	0.47
1:C:463:LEU:HB2	1:C:467:CYS:O	2.16	0.46
1:A:49:LYS:HG2	1:A:50:PRO:HD2	1.97	0.46
2:D:2:NAG:H4	2:D:3:BMA:O2	2.14	0.46
1:A:67:MET:SD	1:A:137:PRO:HD2	2.56	0.46
1:A:270:VAL:HG21	1:A:283:ILE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HB	1:C:470:PHE:HZ	1.80	0.46
1:C:106:LEU:HA	1:C:109:ILE:CD1	2.46	0.46
1:B:5:CYS:O	1:B:354:TYR:HA	2.16	0.45
1:C:109:ILE:HG21	1:C:112:PHE:HB2	1.97	0.45
1:B:161:ILE:O	1:B:243:GLU:HA	2.16	0.45
1:B:464:GLY:HA2	1:C:454:LEU:HD22	1.99	0.45
1:B:44:ASP:OD1	1:B:272:TYR:OH	2.31	0.45
1:B:281:THR:HG22	1:B:299:THR:HG22	1.98	0.45
1:B:8:TYR:OH	1:B:336:ILE:HG23	2.17	0.44
1:A:381:LYS:HE3	1:C:21:MET:HE3	2.00	0.44
1:C:8:TYR:CZ	1:C:336:ILE:HG23	2.53	0.44
1:C:501:GLU:HG2	1:C:501:GLU:O	2.18	0.44
1:A:377:GLY:C	1:C:21:MET:HE2	2.43	0.44
1:C:491:GLN:NE2	1:C:492:TYR:OH	2.51	0.44
1:B:6:ILE:HG13	1:B:449:TYR:HA	1.99	0.44
1:C:470:PHE:CZ	1:C:479:MET:HE1	2.53	0.44
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.99	0.43
1:A:481:SER:HB2	1:A:486:THR:O	2.18	0.43
1:A:494:GLU:HA	1:A:497:ARG:CB	2.48	0.43
1:B:54:LYS:O	1:B:83:ARG:HD2	2.18	0.43
1:C:41:LYS:H	1:C:284:GLY:HA2	1.82	0.43
1:B:505:GLY:HA3	1:C:497:ARG:NH1	2.33	0.43
1:A:6:ILE:HG13	1:A:449:TYR:HA	2.00	0.43
1:A:21:MET:HE2	1:B:377:GLY:C	2.44	0.43
1:C:108:ARG:O	1:C:109:ILE:HD12	2.19	0.43
1:A:6:ILE:HD11	1:A:452:VAL:HG21	2.01	0.43
1:C:4:ILE:CG2	1:C:468:PHE:HB2	2.48	0.43
1:B:50:PRO:HB3	1:B:79:TYR:CE1	2.54	0.43
1:C:19:THR:HB	1:C:435:GLU:HB2	1.99	0.43
1:A:477:GLU:O	1:A:481:SER:HB3	2.19	0.43
1:B:336:ILE:HB	1:B:442:ASP:OD1	2.18	0.43
1:B:407:ILE:CD1	1:C:407:ILE:CG2	2.90	0.43
1:C:41:LYS:HD2	1:C:273:GLY:HA3	2.01	0.43
1:C:473:LYS:HA	1:C:473:LYS:HD3	1.64	0.43
1:C:40:GLY:HA2	1:C:283:ILE:O	2.19	0.43
1:C:479:MET:HB3	1:C:483:ARG:NH2	2.34	0.43
1:A:494:GLU:HA	1:A:497:ARG:HB3	2.01	0.42
1:C:133:SER:C	1:C:142:PRO:HB3	2.44	0.42
1:C:281:THR:HG22	1:C:299:THR:HG22	2.01	0.42
1:A:224:ARG:NH1	5:A:711:HOH:O	2.51	0.42
1:A:281:THR:HG22	1:A:299:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:HIS:HB2	1:A:479:MET:HE3	2.01	0.42
1:C:17:VAL:HG21	1:C:315:ALA:HB2	2.00	0.42
1:A:224:ARG:NH2	5:A:716:HOH:O	2.53	0.42
1:C:500:ARG:C	1:C:502:GLU:H	2.27	0.42
1:B:495:GLU:OE2	1:B:495:GLU:N	2.27	0.42
1:C:341:GLU:H	1:C:341:GLU:HG3	1.59	0.42
1:A:336:ILE:HG13	1:A:442:ASP:HA	2.02	0.42
1:A:381:LYS:HG3	1:C:20:ILE:HG12	2.01	0.42
1:B:17:VAL:HG21	1:B:315:ALA:HB2	2.02	0.42
1:B:91:CYS:HB2	1:B:135:ALA:O	2.19	0.41
1:A:17:VAL:HG21	1:A:315:ALA:HB2	2.01	0.41
1:B:189:THR:HA	1:B:192:TYR:O	2.20	0.41
1:B:71:PHE:HA	1:B:73:ARG:NH1	2.36	0.41
1:A:80:ILE:HB	1:A:265:ILE:HG13	2.02	0.41
1:A:360:GLN:OE1	1:A:476:ASN:CG	2.64	0.41
1:A:497:ARG:HH21	1:A:498:LEU:HD21	1.86	0.41
1:C:72:ILE:O	1:C:72:ILE:CG2	2.69	0.41
1:C:448:LEU:HD12	1:C:448:LEU:HA	1.83	0.41
1:C:459:ASN:O	1:C:471:TYR:HB2	2.21	0.40
1:B:111:HIS:HB3	1:B:258:VAL:HB	2.02	0.40
1:B:217:ARG:O	1:B:224:ARG:HD3	2.22	0.40
1:B:133:SER:C	1:B:142:PRO:HB3	2.46	0.40
1:C:461:LYS:NZ	1:C:503:ILE:HD13	2.36	0.40
1:A:505:GLY:HA2	1:B:497:ARG:NH2	2.36	0.40
1:B:463:LEU:HD12	1:B:463:LEU:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:BMA:O6	5:B:879:HOH:O[4_545]	2.14	0.06

## 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	490/505 (97%)	472 (96%)	17 (4%)	1 (0%)	43	66
1	B	490/505 (97%)	473 (96%)	17 (4%)	0	100	100
1	C	490/505 (97%)	470 (96%)	20 (4%)	0	100	100
All	All	1470/1515 (97%)	1415 (96%)	54 (4%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	ILE

### 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	435/445 (98%)	434 (100%)	1 (0%)	87	95
1	B	435/445 (98%)	434 (100%)	1 (0%)	87	95
1	C	435/445 (98%)	431 (99%)	4 (1%)	70	87
All	All	1305/1335 (98%)	1299 (100%)	6 (0%)	81	92

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

Mol	Chain	Res	Type
1	A	336	ILE
1	B	264	THR
1	C	70	GLU
1	C	72	ILE
1	C	73	ARG
1	C	263	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	169	ASN
1	A	455	GLN
1	A	459	ASN
1	B	16	GLN
1	B	360	GLN
1	C	16	GLN
1	C	46	ASN
1	C	241	HIS
1	C	390	ASN
1	C	491	GLN

### 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](#)

7 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	0.25	0	17,19,21	1.05	1 (5%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	0.72	0
2	BMA	D	3	2	11,11,12	1.04	1 (9%)	15,15,17	1.53	3 (20%)
3	NAG	E	1	3,1	14,14,15	0.27	0	17,19,21	0.76	1 (5%)
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.74	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.22	0	17,19,21	0.86	1 (5%)
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.73	1 (5%)

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	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C1-C2	2.76	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.66	117.09	112.19
2	D	3	BMA	O2-C2-C3	-3.27	103.38	110.15
2	D	3	BMA	C1-O5-C5	3.26	116.56	112.19
3	F	1	NAG	C1-O5-C5	3.09	116.32	112.19
3	F	2	NAG	C1-O5-C5	2.71	115.81	112.19
3	E	1	NAG	C1-O5-C5	2.65	115.74	112.19
3	E	2	NAG	C1-O5-C5	2.52	115.57	112.19
2	D	3	BMA	C1-C2-C3	-2.23	106.39	109.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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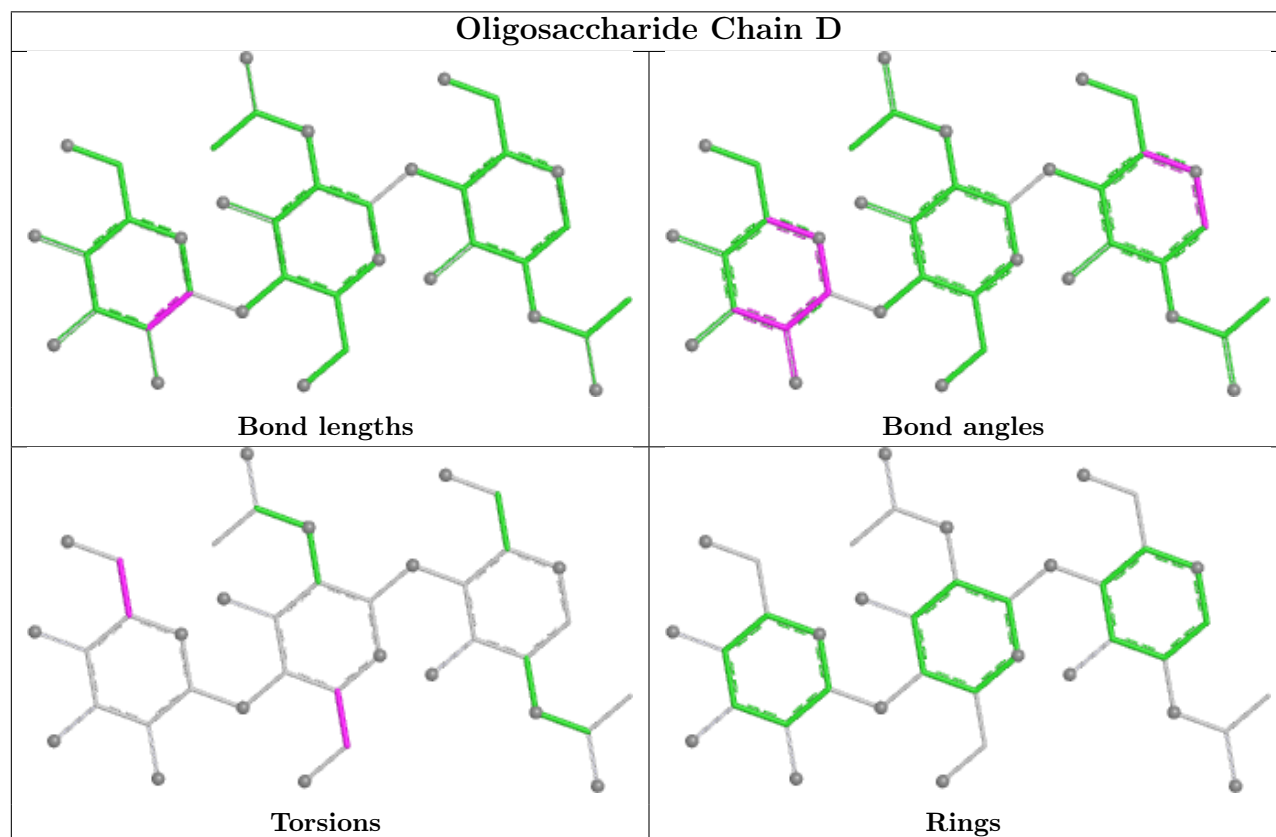
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

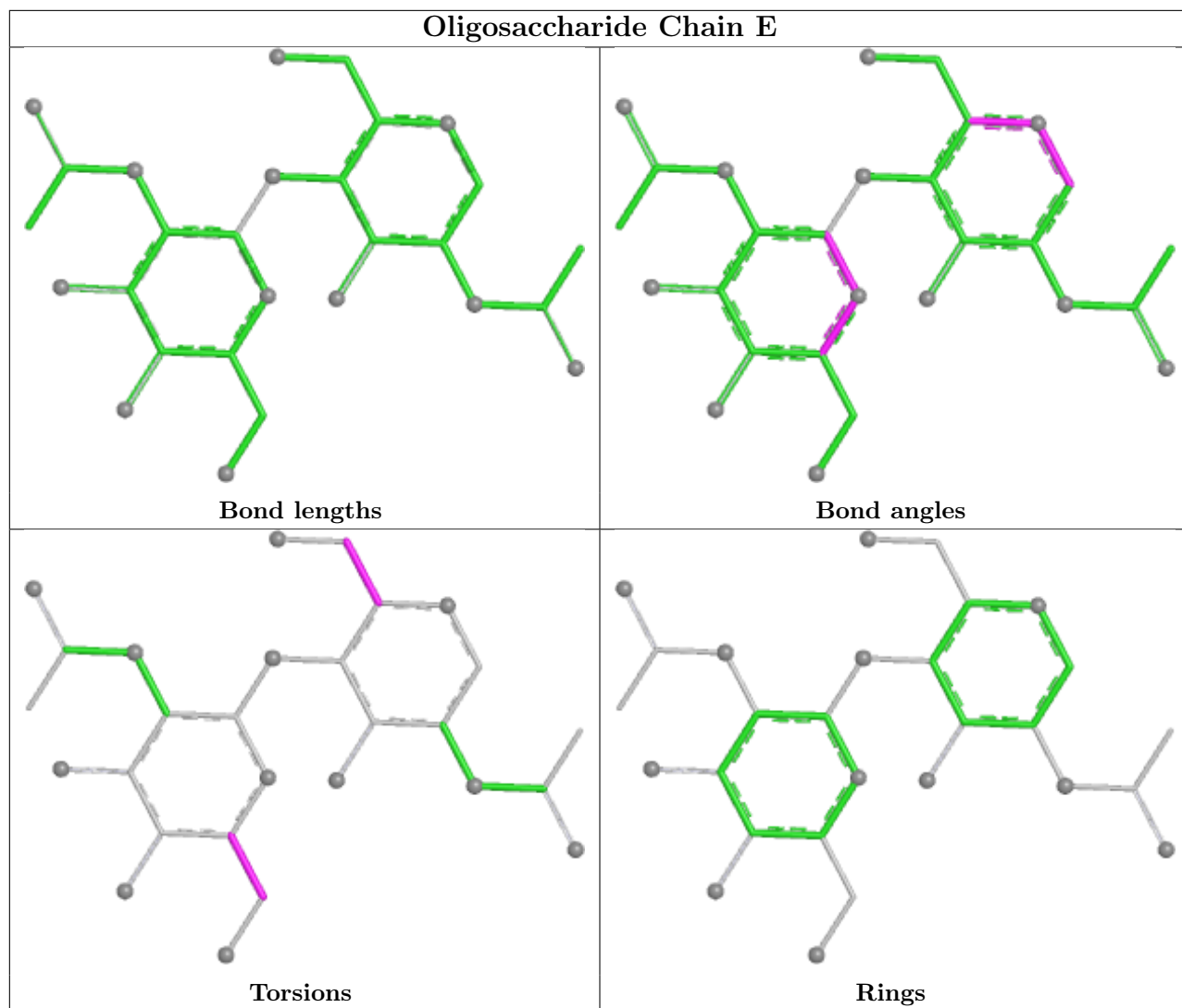
There are no ring outliers.

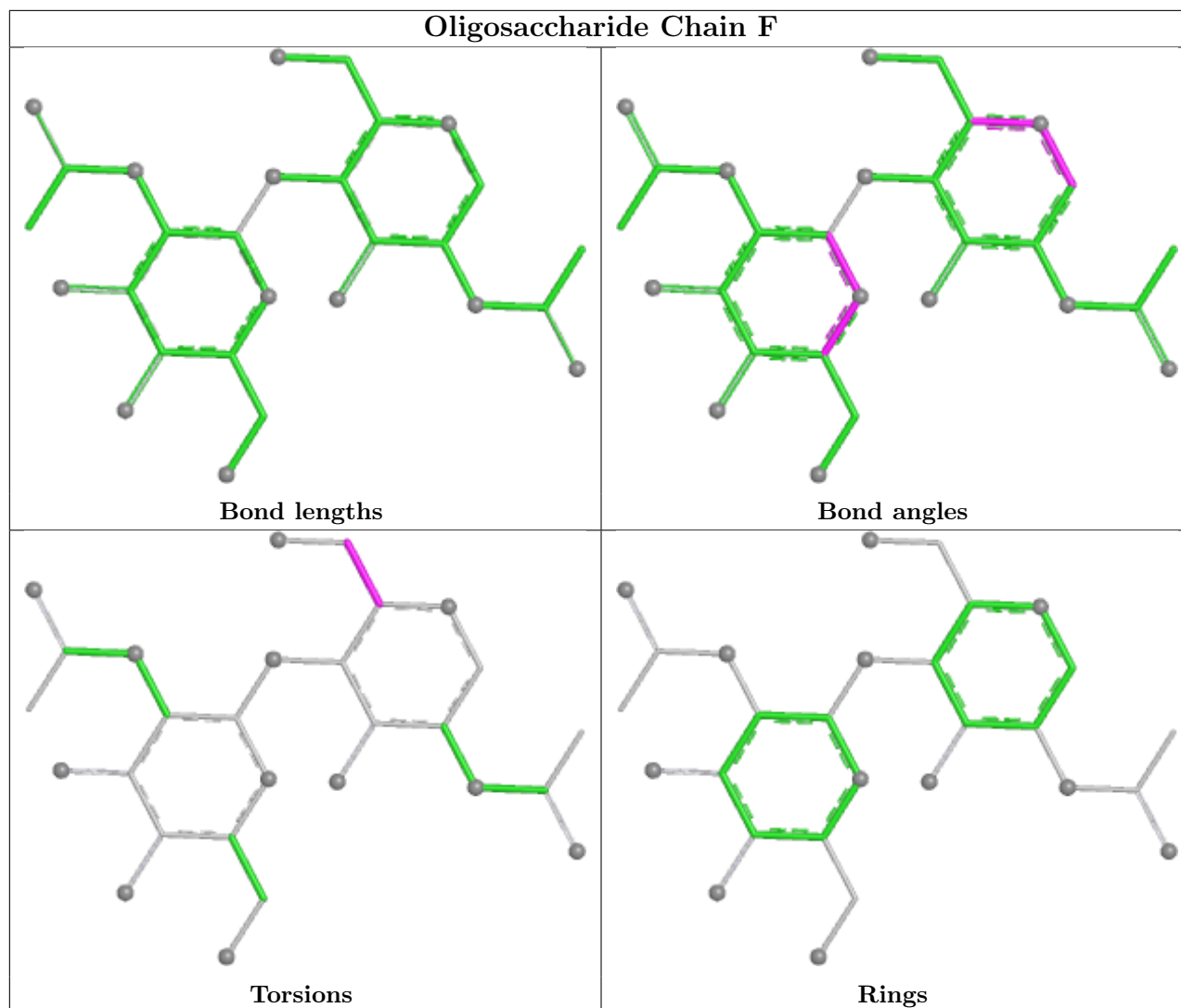
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	BMA	1	1
2	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](#)

3 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	$\# Z  > 2$
4	NAG	B	601	1	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
4	NAG	C	601	1	14,14,15	0.56	0	17,19,21	0.79	1 (5%)
4	NAG	A	601	1	14,14,15	0.49	0	17,19,21	0.82	1 (5%)

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	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	3.02	116.24	112.19
4	C	601	NAG	C1-O5-C5	2.89	116.06	112.19
4	B	601	NAG	C1-O5-C5	2.82	115.96	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/505 (97%)	0.38	67 (13%) <b>7</b> <b>5</b>	25, 43, 98, 133	0
1	B	494/505 (97%)	0.02	26 (5%) <b>32</b> <b>26</b>	25, 41, 69, 111	0
1	C	494/505 (97%)	0.63	87 (17%) <b>4</b> <b>3</b>	25, 44, 104, 126	0
All	All	1482/1515 (97%)	0.35	180 (12%) <b>8</b> <b>6</b>	25, 43, 96, 133	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	470	PHE	10.9
1	C	468	PHE	9.6
1	C	505	GLY	8.6
1	C	72	ILE	8.6
1	C	71	PHE	8.1
1	C	460	ALA	8.1
1	B	334	GLY	7.6
1	C	503	ILE	7.6
1	C	469	GLU	6.8
1	C	322	PRO	6.6
1	C	462	GLU	6.5
1	C	501	GLU	6.5
1	B	322	PRO	6.2
1	C	461	LYS	6.1
1	A	71	PHE	6.0
1	C	471	TYR	5.9
1	C	467	CYS	5.9
1	A	488	ASP	5.8
1	A	54	LYS	5.8
1	A	72	ILE	5.7
1	C	336	ILE	5.7
1	C	463	LEU	5.7
1	C	456	LEU	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	334	GLY	5.6
1	C	495	GLU	5.5
1	C	473	LYS	5.5
1	A	359	GLU	5.4
1	C	337	ALA	5.4
1	C	472	HIS	5.3
1	A	360	GLN	5.2
1	C	484	ASN	5.2
1	C	1	SER	5.1
1	A	69	ASP	5.1
1	A	334	GLY	5.1
1	B	337	ALA	5.0
1	C	464	GLY	5.0
1	C	492	TYR	5.0
1	C	455	GLN	4.9
1	C	476	ASN	4.8
1	C	478	CYS	4.8
1	B	338	GLY	4.8
1	A	490	PRO	4.7
1	C	454	LEU	4.5
1	A	497	ARG	4.5
1	B	336	ILE	4.5
1	C	465	ASN	4.4
1	A	335	ALA	4.4
1	B	339	PHE	4.4
1	A	494	GLU	4.4
1	C	339	PHE	4.4
1	C	491	GLN	4.3
1	A	362	SER	4.2
1	C	474	CYS	4.2
1	A	339	PHE	4.2
1	A	73	ARG	4.2
1	A	322	PRO	4.2
1	A	337	ALA	4.2
1	C	500	ARG	4.2
1	C	490	PRO	4.2
1	C	453	ARG	4.1
1	C	70	GLU	4.1
1	C	482	VAL	4.1
1	C	486	THR	4.1
1	C	487	TYR	4.0
1	C	73	ARG	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	335	ALA	4.0
1	A	492	TYR	3.9
1	C	483	ARG	3.9
1	C	452	VAL	3.9
1	A	349	ASP	3.8
1	A	336	ILE	3.8
1	A	361	GLY	3.8
1	A	363	GLY	3.8
1	A	457	ARG	3.8
1	C	54	LYS	3.8
1	B	341	GLU	3.7
1	A	487	TYR	3.7
1	C	485	GLY	3.7
1	C	341	GLU	3.7
1	A	368	LYS	3.7
1	A	484	ASN	3.6
1	A	504	SER	3.6
1	A	501	GLU	3.6
1	C	457	ARG	3.6
1	B	505	GLY	3.6
1	C	449	TYR	3.6
1	B	359	GLU	3.6
1	C	477	GLU	3.6
1	C	459	ASN	3.5
1	C	349	ASP	3.5
1	C	458	ASP	3.5
1	C	357	SER	3.4
1	A	341	GLU	3.4
1	C	498	LEU	3.4
1	C	504	SER	3.3
1	C	69	ASP	3.3
1	C	451	LYS	3.3
1	A	1	SER	3.3
1	A	83	ARG	3.3
1	C	436	ARG	3.3
1	C	494	GLU	3.2
1	B	263	SER	3.2
1	A	489	TYR	3.2
1	B	72	ILE	3.2
1	B	373	LYS	3.1
1	A	486	THR	3.1
1	A	338	GLY	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	338	GLY	3.1
1	A	503	ILE	3.1
1	A	70	GLU	3.1
1	C	488	ASP	3.1
1	A	473	LYS	3.0
1	A	491	GLN	3.0
1	A	482	VAL	3.0
1	B	12	ASN	3.0
1	B	73	ARG	3.0
1	A	474	CYS	2.9
1	C	3	GLN	2.9
1	C	361	GLY	2.9
1	C	466	GLY	2.9
1	A	348	VAL	2.9
1	C	502	GLU	2.8
1	A	475	ASP	2.8
1	C	496	ALA	2.8
1	C	321	SER	2.8
1	C	489	TYR	2.8
1	C	5	CYS	2.8
1	A	478	CYS	2.7
1	A	356	HIS	2.7
1	A	455	GLN	2.7
1	C	55	ASP	2.7
1	C	340	ILE	2.7
1	C	497	ARG	2.7
1	C	359	GLU	2.7
1	A	483	ARG	2.6
1	A	139	GLN	2.6
1	C	2	ASP	2.6
1	C	74	VAL	2.6
1	C	348	VAL	2.6
1	C	360	GLN	2.6
1	B	435	GLU	2.6
1	B	349	ASP	2.5
1	A	498	LEU	2.5
1	A	480	GLU	2.5
1	C	499	LYS	2.4
1	B	321	SER	2.4
1	C	475	ASP	2.4
1	A	495	GLU	2.4
1	A	365	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	477	GLU	2.4
1	A	436	ARG	2.4
1	B	504	SER	2.4
1	B	340	ILE	2.3
1	A	357	SER	2.3
1	B	348	VAL	2.3
1	B	15	GLU	2.3
1	B	368	LYS	2.3
1	A	271	GLU	2.3
1	A	366	ALA	2.2
1	C	335	ALA	2.2
1	A	100	GLU	2.2
1	A	358	ASN	2.2
1	A	55	ASP	2.2
1	B	436	ARG	2.1
1	C	12	ASN	2.1
1	A	89	ASP	2.1
1	A	443	SER	2.1
1	C	493	SER	2.1
1	A	476	ASN	2.1
1	A	505	GLY	2.1
1	B	361	GLY	2.1
1	C	342	GLY	2.1
1	A	454	LEU	2.1
1	A	340	ILE	2.1
1	B	70	GLU	2.0
1	A	68	CYS	2.0
1	C	373	LYS	2.0
1	C	446	LYS	2.0
1	A	12	ASN	2.0
1	C	4	ILE	2.0

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

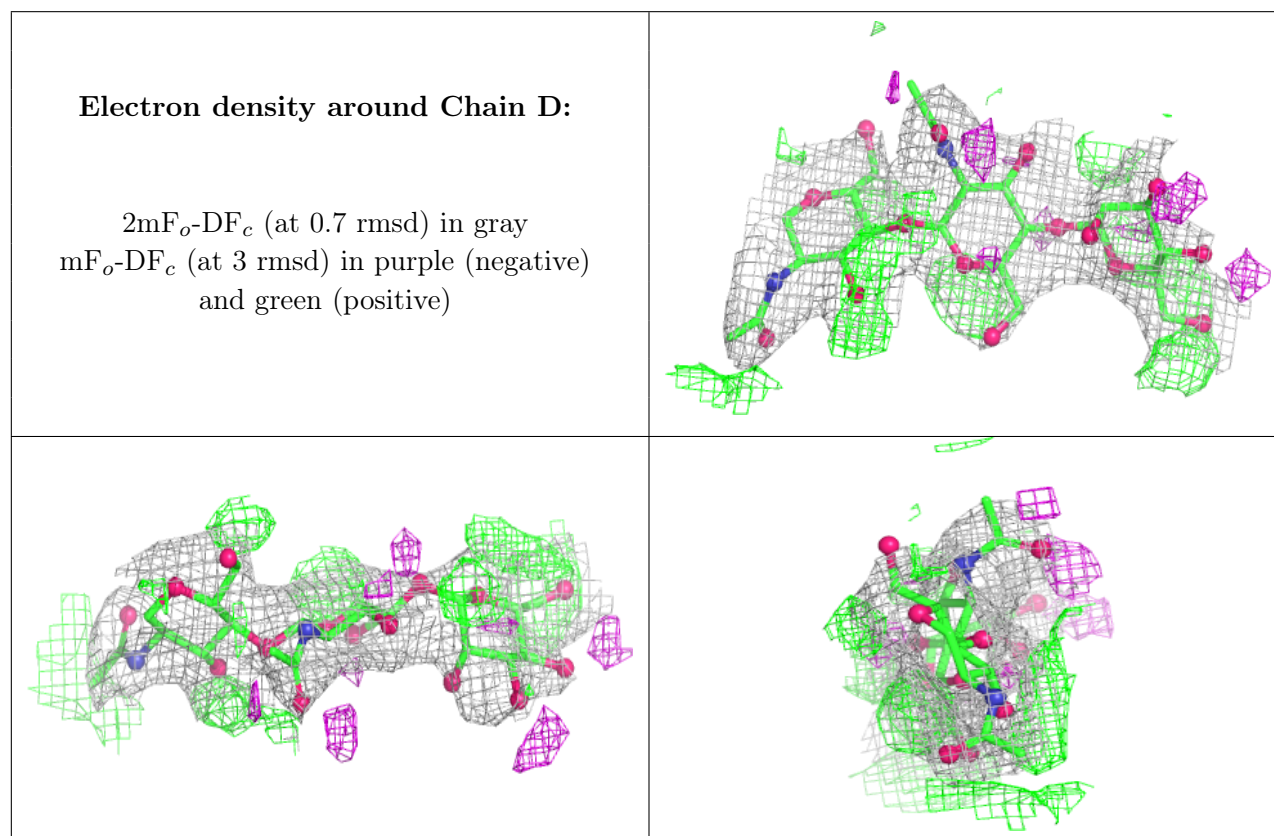
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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.

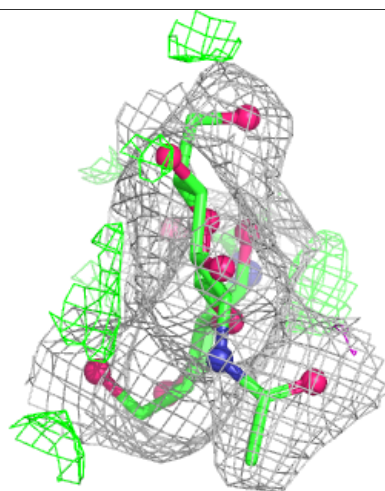
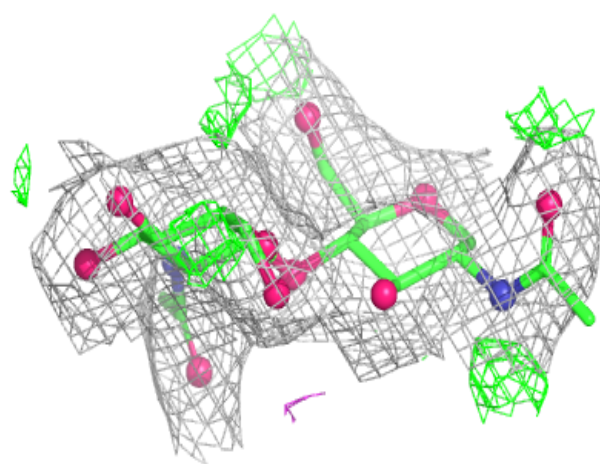
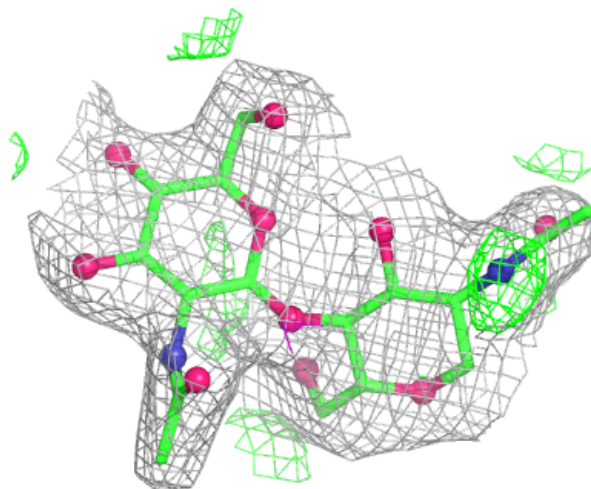
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	2	14/15	0.58	0.23	81,109,124,125	0
2	BMA	D	3	11/12	0.75	0.22	37,82,93,95	0
3	NAG	E	2	14/15	0.81	0.17	46,81,90,98	0
2	NAG	D	1	14/15	0.85	0.15	43,58,76,79	0
3	NAG	F	1	14/15	0.87	0.13	44,75,94,117	0
2	NAG	D	2	14/15	0.87	0.17	46,66,81,88	0
3	NAG	E	1	14/15	0.91	0.11	51,57,68,70	0

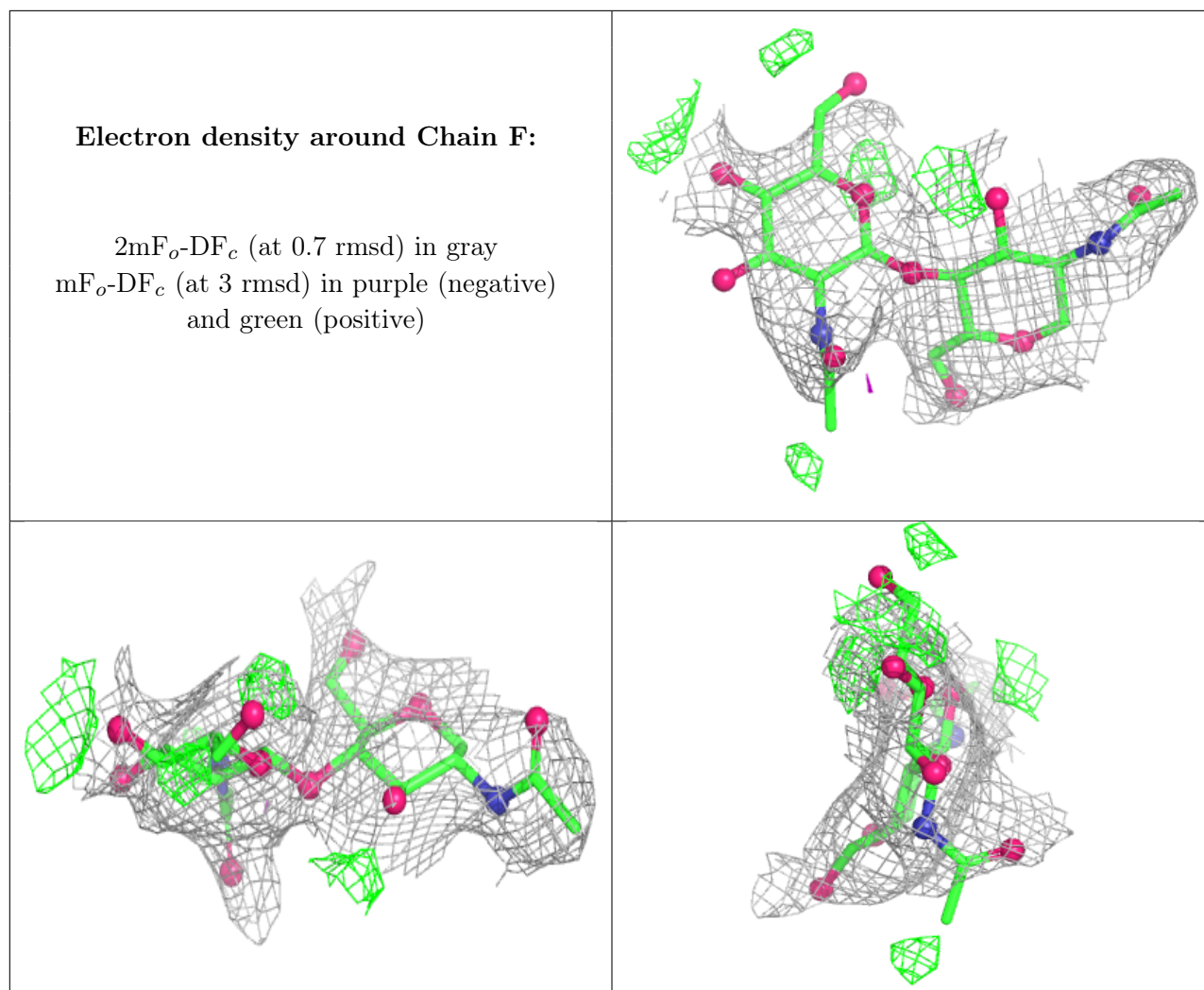
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	601	14/15	0.60	0.20	62,87,105,106	0
4	NAG	A	601	14/15	0.64	0.20	61,93,100,106	0
4	NAG	C	601	14/15	0.71	0.21	73,94,108,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.