



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:27 PM BST

PDB ID : 5CD5  
Title : Crystal structure of an immature VRC01-class antibody DRVIA7 from a Chinese donor bound to clade A/E HIV-1 gp120 core  
Authors : Kong, L.; Wilson, I.A.  
Deposited on : 2015-07-03  
Resolution : 3.40 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.

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

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

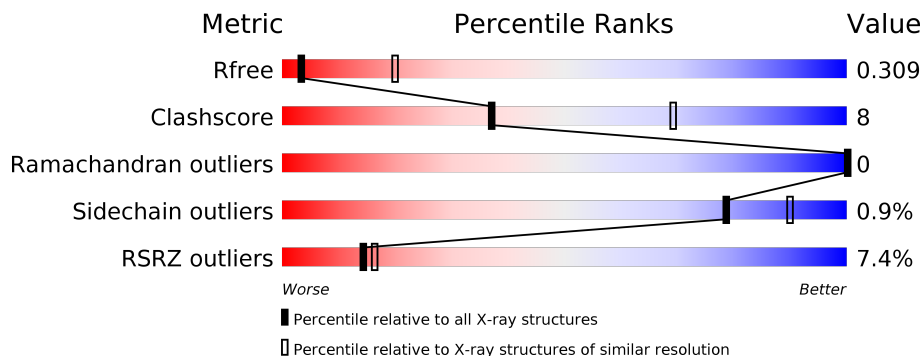
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



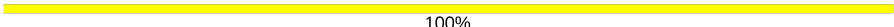
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	353	
2	C	220	
3	D	210	
4	B	2	
4	G	2	
5	E	4	

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Mol	Chain	Length	Quality of chain
6	F	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	1	-	-	-	X
4	NAG	G	2	-	-	-	X
5	MAN	E	4	-	-	-	X
6	NAG	F	1	-	-	-	X
6	NAG	F	2	-	-	-	X
6	BMA	F	3	-	-	-	X
7	NAG	A	505	-	-	-	X
7	NAG	A	506	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6215 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 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2685	1685	467	510	23	0	0	0

- Molecule 2 is a protein called DRVIA7 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	220	1690	1066	291	324	9	0	0	0

- Molecule 3 is a protein called DRVIA7 Fab Light Chain.

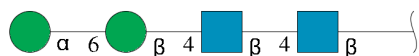
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	207	1611	1009	275	322	5	0	0	0

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



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

- Molecule 5 is an oligosaccharide called 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.



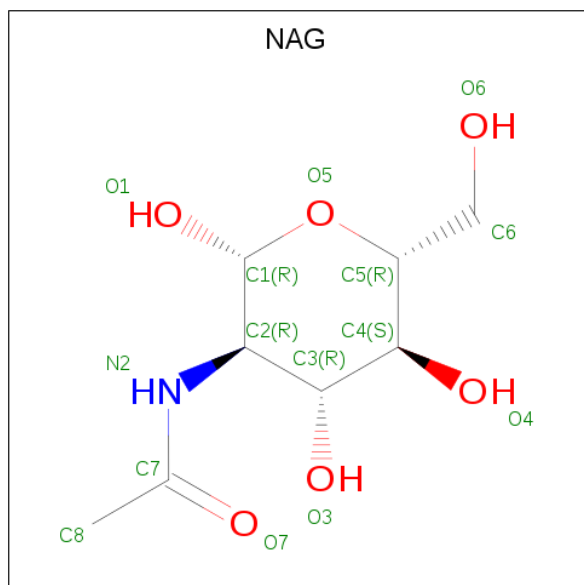
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
5	E	4	50	28	2	20	0	0	0

- Molecule 6 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
6	F	3	39	22	2	15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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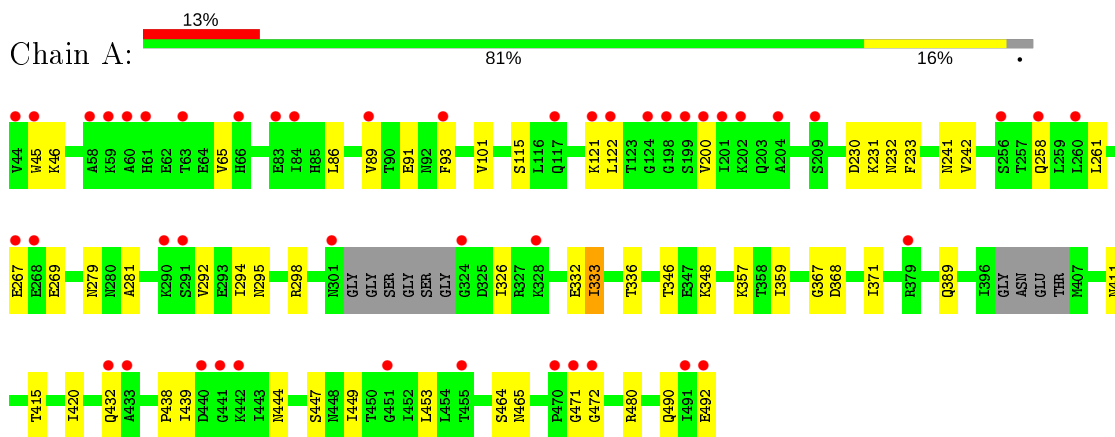
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

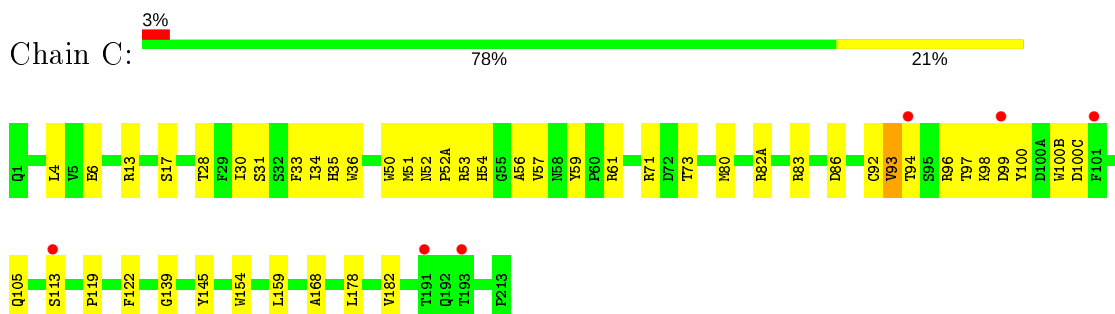
### 3 Residue-property plots [i](#)

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.

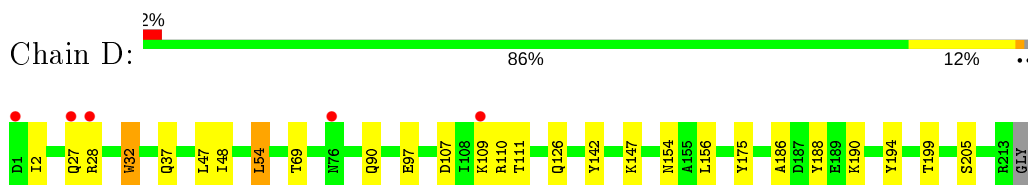
- Molecule 1: 93TH057 HIV-1 gp120 core



- Molecule 2: DRVIA7 Fab Heavy Chain



- Molecule 3: DRVIA7 Fab Light Chain




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



MAG1  
MAG2

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

Chain G:  100%MAG1  
MAG2

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

Chain E:  50%MAG1  
MAG2  
BMA3  
MAMA

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

Chain F:  100%MAG1  
MAG2  
BMA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.33Å 72.33Å 338.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.97 – 3.40 28.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.97-3.40) 88.5 (28.97-3.39)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 3.39Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.253 , 0.306 0.268 , 0.309	Depositor DCC
$R_{free}$ test set	654 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	105.2	Xtrriage
Anisotropy	0.403	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 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	0.23	0/2741	0.44	0/3719
2	C	0.25	0/1735	0.50	0/2363
3	D	0.23	0/1644	0.42	0/2231
All	All	0.23	0/6120	0.45	0/8313

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2621	47	0
2	C	1690	0	1643	34	1
3	D	1611	0	1580	18	1
4	B	28	0	25	0	0
4	G	28	0	25	0	0
5	E	50	0	43	1	0
6	F	39	0	32	0	0
7	A	84	0	78	5	0
All	All	6215	0	6047	95	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 8.

All (95) 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:357:LYS:CE	1:A:464:SER:O	1.82	1.26
1:A:357:LYS:HE2	1:A:464:SER:O	1.38	1.19
1:A:357:LYS:HE3	1:A:464:SER:O	1.55	1.03
3:D:2:ILE:HG12	3:D:27:GLN:HB2	1.49	0.94
2:C:6:GLU:OE2	2:C:92:CYS:N	2.08	0.86
1:A:357:LYS:HE3	1:A:464:SER:C	1.97	0.83
1:A:357:LYS:CE	1:A:464:SER:C	2.51	0.76
1:A:357:LYS:HE3	1:A:464:SER:CA	2.18	0.73
3:D:2:ILE:HG12	3:D:27:GLN:CB	2.21	0.71
3:D:32:TRP:O	3:D:90:GLN:NE2	2.23	0.70
2:C:28:THR:O	2:C:31:SER:OG	2.11	0.68
1:A:368:ASP:OD2	2:C:71:ARG:NH1	2.28	0.66
3:D:2:ILE:O	3:D:97:GLU:HG3	1.97	0.64
1:A:230:ASP:HB2	1:A:233:PHE:HB2	1.80	0.64
1:A:346:THR:HG23	1:A:359:ILE:HB	1.80	0.63
2:C:34:ILE:HG12	2:C:94:THR:HG22	1.81	0.63
2:C:4:LEU:HD11	2:C:94:THR:HG23	1.81	0.62
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.81	0.62
1:A:357:LYS:HE3	1:A:464:SER:HA	1.81	0.61
1:A:101:VAL:HG21	1:A:480:ARG:HG3	1.83	0.60
1:A:46:LYS:HE3	1:A:492:GLU:OE2	2.01	0.60
2:C:30:ILE:HG23	2:C:53:ARG:HG2	1.82	0.60
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.85	0.59
1:A:447:SER:OG	7:A:503:NAG:N2	2.33	0.58
2:C:54:HIS:CD2	2:C:56:ALA:HB2	2.38	0.58
1:A:447:SER:HG	7:A:503:NAG:HN2	1.48	0.58
2:C:168:ALA:HA	2:C:178:LEU:HB3	1.85	0.58
1:A:298:ARG:NH2	1:A:439:ILE:O	2.36	0.58
1:A:465:ASN:HB2	2:C:61:ARG:NH2	2.18	0.58
3:D:28:ARG:HA	3:D:69:THR:HG22	1.86	0.57
3:D:110:ARG:HG2	3:D:111:THR:N	2.20	0.56
1:A:357:LYS:HB3	1:A:464:SER:O	2.05	0.56
2:C:71:ARG:NH2	2:C:73:THR:OG1	2.39	0.56
1:A:279:ASN:ND2	2:C:100(B):TRP:HE1	2.03	0.56
1:A:122:LEU:HD12	1:A:432:GLN:HB2	1.89	0.54
1:A:389:GLN:HG2	7:A:506:NAG:H81	1.90	0.54
1:A:294:ILE:N	1:A:447:SER:O	2.30	0.54
1:A:46:LYS:O	1:A:490:GLN:N	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.90	0.53
1:A:294:ILE:HG12	1:A:333:ILE:HD11	1.91	0.52
1:A:298:ARG:NH1	1:A:326:ILE:O	2.38	0.52
2:C:35:HIS:HB2	2:C:93:VAL:HG12	1.92	0.52
3:D:107:ASP:OD1	3:D:175:TYR:OH	2.22	0.52
2:C:17:SER:HB2	2:C:82(A):ARG:HG2	1.91	0.51
1:A:453:LEU:HD13	1:A:472:GLY:HA3	1.91	0.51
2:C:168:ALA:HB2	2:C:178:LEU:HD23	1.93	0.50
1:A:261:LEU:HD21	1:A:294:ILE:HD12	1.93	0.50
5:E:1:NAG:H61	5:E:2:NAG:HN2	1.76	0.50
2:C:36:TRP:CE2	2:C:80:MET:HB2	2.47	0.49
2:C:35:HIS:ND1	2:C:50:TRP:HB3	2.28	0.49
2:C:97:THR:HG21	2:C:100(C):ASP:OD2	2.14	0.48
3:D:110:ARG:NH1	3:D:111:THR:O	2.45	0.48
2:C:13:ARG:HG2	2:C:113:SER:HA	1.95	0.48
1:A:279:ASN:OD1	1:A:281:ALA:N	2.46	0.47
1:A:295:ASN:OD1	1:A:444:ASN:ND2	2.47	0.47
1:A:292:VAL:O	1:A:449:ILE:N	2.46	0.46
1:A:332:GLU:O	1:A:333:ILE:HD12	2.15	0.46
2:C:51:MET:SD	2:C:71:ARG:HB3	2.57	0.45
1:A:258:GLN:HG2	1:A:471:GLY:HA2	1.97	0.45
3:D:147:LYS:HB3	3:D:199:THR:HB	1.99	0.45
1:A:45:TRP:HZ2	1:A:89:VAL:HG11	1.80	0.45
2:C:139:GLY:HA2	2:C:154:TRP:CH2	2.52	0.45
1:A:91:GLU:HB2	1:A:242:VAL:HG21	1.98	0.45
1:A:367:GLY:HA3	1:A:371:ILE:HD11	1.98	0.45
2:C:83:ARG:N	2:C:86:ASP:OD2	2.43	0.45
3:D:2:ILE:HG12	3:D:27:GLN:CG	2.46	0.45
3:D:48:ILE:HD13	3:D:54:LEU:HA	1.98	0.44
1:A:45:TRP:CH2	1:A:86:LEU:HD13	2.51	0.44
1:A:389:GLN:NE2	1:A:415:THR:O	2.41	0.44
2:C:30:ILE:HG23	2:C:53:ARG:CG	2.48	0.44
3:D:188:TYR:O	3:D:194:TYR:OH	2.30	0.44
2:C:36:TRP:CH2	2:C:92:CYS:HB3	2.52	0.44
1:A:281:ALA:HB1	2:C:33:PHE:HE2	1.82	0.43
1:A:232:ASN:OD1	1:A:269:GLU:HB2	2.19	0.43
2:C:97:THR:OG1	2:C:100:TYR:HB3	2.18	0.43
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.54	0.43
3:D:109:LYS:HA	3:D:142:TYR:OH	2.19	0.43
2:C:122:PHE:CE2	3:D:126:GLN:HG3	2.53	0.43
1:A:420:ILE:HG21	1:A:438:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:HD21	7:A:502:NAG:C1	2.32	0.42
3:D:186:ALA:O	3:D:190:LYS:HG3	2.20	0.42
1:A:336:THR:OG1	1:A:411:ASN:HB3	2.20	0.42
2:C:54:HIS:HD2	2:C:56:ALA:HB2	1.80	0.42
1:A:231:LYS:HG2	1:A:267:GLU:OE1	2.21	0.41
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.88	0.41
1:A:65:VAL:HB	1:A:115:SER:HB3	2.01	0.41
3:D:2:ILE:CG1	3:D:27:GLN:HB2	2.36	0.41
2:C:96:ARG:HG3	2:C:97:THR:N	2.35	0.41
2:C:30:ILE:HG22	2:C:53:ARG:HE	1.86	0.41
2:C:57:VAL:HG11	2:C:59:TYR:CZ	2.56	0.41
1:A:389:GLN:HA	7:A:506:NAG:H81	2.02	0.41
2:C:98:LYS:O	2:C:99:ASP:HB2	2.20	0.41
3:D:110:ARG:HH11	3:D:110:ARG:HG2	1.85	0.40
1:A:121:LYS:O	1:A:200:VAL:HA	2.21	0.40
2:C:52:ASN:HA	2:C:52(A):PRO:HD3	1.90	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:C:105:GLN:O	3:D:205:SER:OG[5_755]	2.10	0.10

## 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	337/353 (96%)	327 (97%)	10 (3%)	0	100	100
2	C	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
3	D	205/210 (98%)	200 (98%)	5 (2%)	0	100	100
All	All	760/783 (97%)	742 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	306/311 (98%)	305 (100%)	1 (0%)	92	97
2	C	190/190 (100%)	189 (100%)	1 (0%)	88	94
3	D	183/185 (99%)	179 (98%)	4 (2%)	52	75
All	All	679/686 (99%)	673 (99%)	6 (1%)	78	90

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

Mol	Chain	Res	Type
1	A	333	ILE
2	C	93	VAL
3	D	32	TRP
3	D	54	LEU
3	D	154	ASN
3	D	156	LEU

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

Mol	Chain	Res	Type
2	C	54	HIS

### 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

11 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
4	NAG	B	1	1,4	14,14,15	1.09	2 (14%)	17,19,21	1.84	4 (23%)
4	NAG	B	2	4	14,14,15	1.35	2 (14%)	17,19,21	3.20	5 (29%)
5	NAG	E	1	1,5	14,14,15	1.09	2 (14%)	17,19,21	1.84	4 (23%)
5	NAG	E	2	5	14,14,15	1.35	2 (14%)	17,19,21	3.20	6 (35%)
5	BMA	E	3	5	11,11,12	1.48	2 (18%)	15,15,17	3.36	10 (66%)
5	MAN	E	4	5	11,11,12	1.43	2 (18%)	15,15,17	1.00	2 (13%)
6	NAG	F	1	1,6	14,14,15	1.09	2 (14%)	17,19,21	1.85	4 (23%)
6	NAG	F	2	6	14,14,15	1.35	2 (14%)	17,19,21	3.20	5 (29%)
6	BMA	F	3	6	11,11,12	1.49	2 (18%)	15,15,17	3.36	10 (66%)
4	NAG	G	1	1,4	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
4	NAG	G	2	4	14,14,15	1.38	3 (21%)	17,19,21	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	3/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1

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

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	4	MAN	C2-C3	-3.15	1.47	1.52
5	E	3	BMA	O5-C5	-3.07	1.37	1.43
6	F	3	BMA	O5-C5	-3.05	1.37	1.43
4	B	2	NAG	C4-C5	-3.01	1.46	1.53
5	E	2	NAG	C4-C5	-3.00	1.46	1.53
6	F	2	NAG	C4-C5	-2.96	1.46	1.53
5	E	4	MAN	O5-C1	2.65	1.47	1.43
4	G	2	NAG	C7-N2	2.38	1.42	1.34
6	F	2	NAG	O4-C4	-2.33	1.37	1.43
4	B	2	NAG	O4-C4	-2.29	1.37	1.43
5	E	2	NAG	O4-C4	-2.25	1.37	1.43
4	G	2	NAG	O7-C7	2.16	1.28	1.23
5	E	1	NAG	O4-C4	2.15	1.48	1.43
4	B	1	NAG	O4-C4	2.14	1.48	1.43
6	F	1	NAG	O4-C4	2.11	1.48	1.43
6	F	1	NAG	O5-C1	-2.08	1.40	1.43
5	E	1	NAG	O5-C1	-2.07	1.40	1.43
4	G	2	NAG	O5-C1	2.06	1.47	1.43
4	B	1	NAG	O5-C1	-2.03	1.40	1.43
5	E	3	BMA	O5-C1	-2.01	1.40	1.43
6	F	3	BMA	O5-C1	-2.01	1.40	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2	NAG	O5-C5-C6	7.97	119.71	107.20
5	E	2	NAG	O5-C5-C6	7.95	119.67	107.20
4	B	2	NAG	O5-C5-C6	7.94	119.65	107.20
4	B	2	NAG	C2-N2-C7	-7.85	111.73	122.90
5	E	2	NAG	C2-N2-C7	-7.81	111.78	122.90
6	F	2	NAG	C2-N2-C7	-7.81	111.79	122.90
6	F	3	BMA	C1-O5-C5	-6.86	102.89	112.19
5	E	3	BMA	C1-O5-C5	-6.86	102.89	112.19
6	F	3	BMA	C2-C3-C4	-5.35	101.64	110.89
5	E	3	BMA	C2-C3-C4	-5.33	101.67	110.89
6	F	3	BMA	O2-C2-C3	5.18	120.51	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	O2-C2-C3	5.14	120.44	110.14
5	E	1	NAG	C4-C3-C2	-4.57	104.32	111.02
4	B	1	NAG	C4-C3-C2	-4.54	104.36	111.02
6	F	1	NAG	C4-C3-C2	-4.53	104.37	111.02
6	F	1	NAG	O5-C1-C2	-3.63	105.56	111.29
4	B	1	NAG	O5-C1-C2	-3.61	105.58	111.29
5	E	1	NAG	O5-C1-C2	-3.59	105.62	111.29
5	E	3	BMA	O5-C1-C2	3.50	116.17	110.77
6	F	3	BMA	O5-C1-C2	3.49	116.16	110.77
5	E	2	NAG	O4-C4-C5	-3.44	100.76	109.30
4	B	2	NAG	O4-C4-C5	-3.44	100.76	109.30
6	F	2	NAG	O4-C4-C5	-3.43	100.78	109.30
5	E	3	BMA	O3-C3-C4	-3.17	103.02	110.35
6	F	2	NAG	O6-C6-C5	-3.15	100.49	111.29
4	B	2	NAG	O6-C6-C5	-3.14	100.50	111.29
6	F	3	BMA	O3-C3-C4	-3.14	103.08	110.35
4	G	1	NAG	O5-C5-C6	3.14	112.13	107.20
5	E	3	BMA	O3-C3-C2	3.14	116.01	109.99
5	E	2	NAG	O6-C6-C5	-3.13	100.57	111.29
6	F	3	BMA	O3-C3-C2	3.10	115.93	109.99
5	E	3	BMA	O2-C2-C1	-2.86	103.31	109.15
6	F	3	BMA	O2-C2-C1	-2.84	103.35	109.15
6	F	1	NAG	C2-N2-C7	-2.82	118.88	122.90
5	E	1	NAG	C2-N2-C7	-2.79	118.93	122.90
4	B	1	NAG	C2-N2-C7	-2.79	118.94	122.90
6	F	1	NAG	C1-O5-C5	2.74	115.91	112.19
4	B	1	NAG	C1-O5-C5	2.69	115.84	112.19
5	E	1	NAG	C1-O5-C5	2.67	115.81	112.19
6	F	3	BMA	O6-C6-C5	-2.60	102.37	111.29
5	E	3	BMA	O6-C6-C5	-2.59	102.42	111.29
6	F	3	BMA	C3-C4-C5	2.36	114.45	110.24
5	E	3	BMA	C3-C4-C5	2.35	114.43	110.24
5	E	3	BMA	C1-C2-C3	-2.33	106.80	109.67
6	F	3	BMA	C1-C2-C3	-2.32	106.81	109.67
5	E	2	NAG	O4-C4-C3	-2.27	105.10	110.35
4	B	2	NAG	O4-C4-C3	-2.25	105.15	110.35
6	F	2	NAG	O4-C4-C3	-2.23	105.19	110.35
5	E	4	MAN	O3-C3-C2	-2.17	105.83	109.99
5	E	4	MAN	C1-C2-C3	2.14	112.30	109.67
5	E	2	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

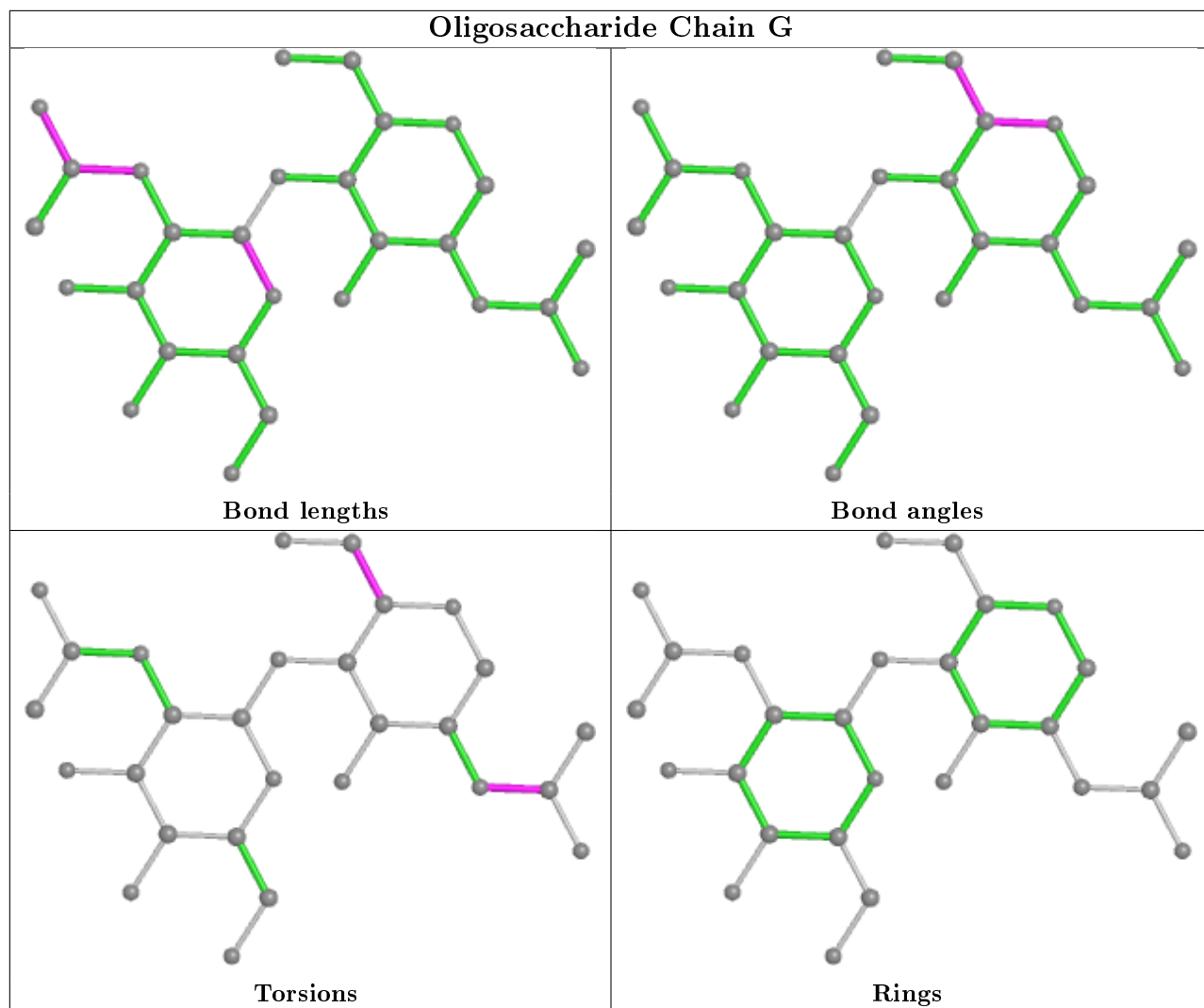
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
6	F	2	NAG	C8-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2

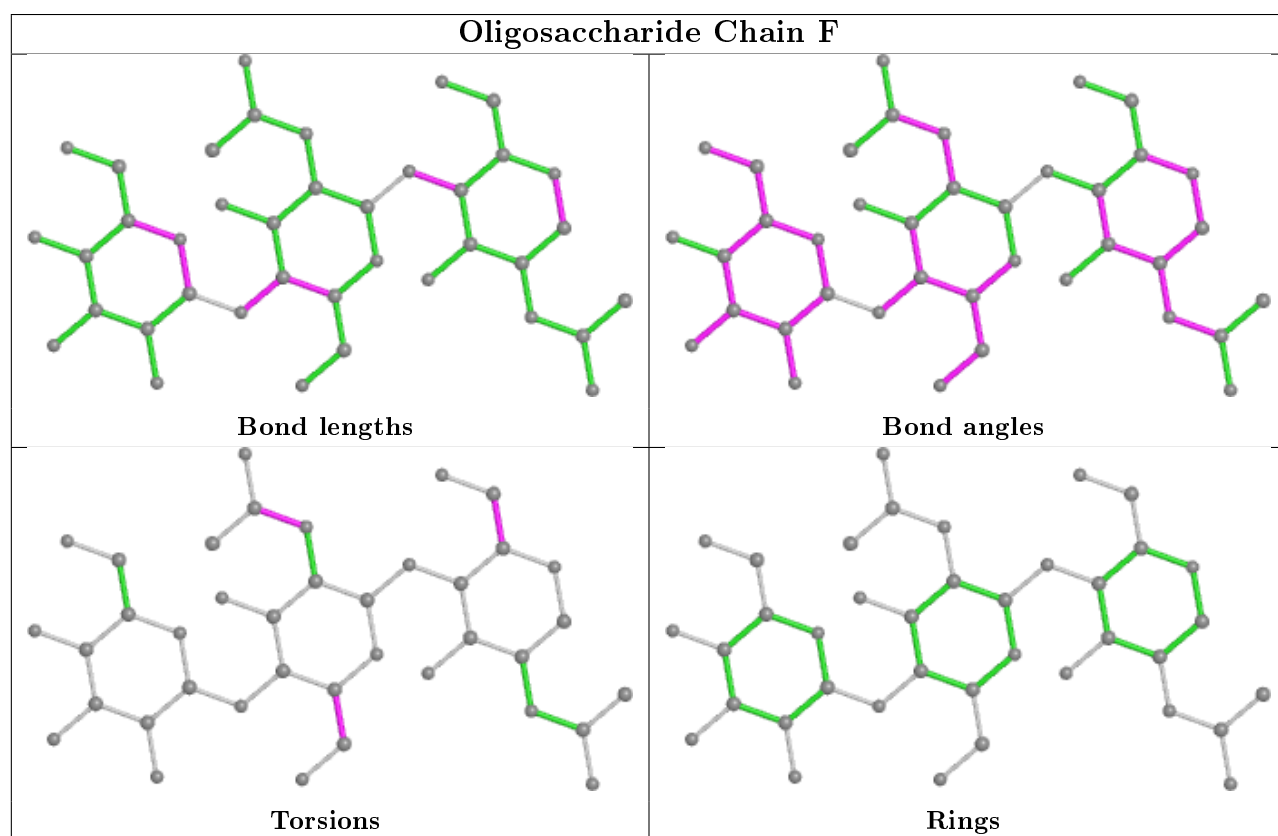
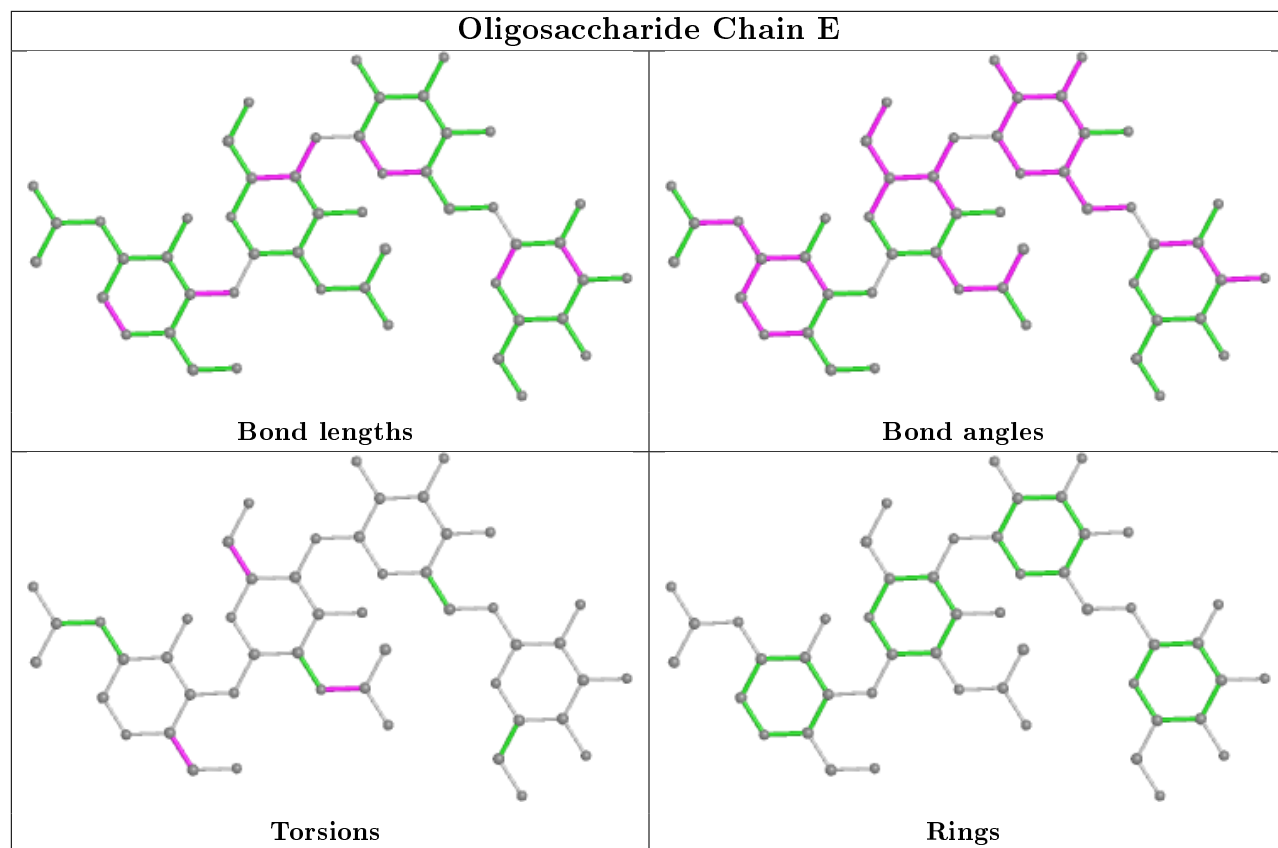
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	1	0
5	E	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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	506	1	14,14,15	0.46	0	17,19,21	1.73	4 (23%)
7	NAG	A	502	-	14,14,15	0.29	0	17,19,21	0.61	0
7	NAG	A	505	1	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
7	NAG	A	503	1	14,14,15	0.51	0	17,19,21	1.20	1 (5%)
7	NAG	A	504	1	14,14,15	1.17	0	17,19,21	1.25	2 (11%)
7	NAG	A	501	1	14,14,15	1.17	0	17,19,21	1.25	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
7	NAG	A	506	1	-	4/6/23/26	0/1/1/1
7	NAG	A	502	-	-	2/6/23/26	0/1/1/1
7	NAG	A	505	1	-	4/6/23/26	0/1/1/1
7	NAG	A	503	1	-	0/6/23/26	0/1/1/1
7	NAG	A	504	1	-	0/6/23/26	0/1/1/1
7	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	506	NAG	O5-C1-C2	-4.28	104.53	111.29
7	A	503	NAG	O5-C1-C2	-3.83	105.25	111.29
7	A	504	NAG	C4-C3-C2	-3.19	106.34	111.02
7	A	501	NAG	C4-C3-C2	-3.18	106.36	111.02
7	A	506	NAG	C2-N2-C7	-2.97	118.68	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	506	NAG	C1-O5-C5	2.85	116.06	112.19
7	A	504	NAG	C2-N2-C7	-2.69	119.07	122.90
7	A	501	NAG	C2-N2-C7	-2.66	119.11	122.90
7	A	506	NAG	C3-C4-C5	2.55	114.79	110.24
7	A	505	NAG	C4-C3-C2	2.04	114.01	111.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	505	NAG	C8-C7-N2-C2
7	A	506	NAG	O5-C5-C6-O6
7	A	501	NAG	O5-C5-C6-O6
7	A	502	NAG	C8-C7-N2-C2
7	A	505	NAG	O7-C7-N2-C2
7	A	506	NAG	C4-C5-C6-O6
7	A	506	NAG	C8-C7-N2-C2
7	A	506	NAG	O7-C7-N2-C2
7	A	502	NAG	O7-C7-N2-C2
7	A	501	NAG	C4-C5-C6-O6
7	A	505	NAG	C4-C5-C6-O6
7	A	505	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	506	NAG	2	0
7	A	502	NAG	1	0
7	A	503	NAG	2	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, 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	343/353 (97%)	0.78	46 (13%) <b>3</b> <b>4</b>	104, 166, 216, 276	0
2	C	220/220 (100%)	0.18	6 (2%) 54 53	78, 120, 156, 178	0
3	D	207/210 (98%)	0.20	5 (2%) 59 57	70, 117, 165, 198	0
All	All	770/783 (98%)	0.45	57 (7%) <b>14</b> <b>16</b>	70, 135, 203, 276	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	7.4
1	A	44	VAL	5.4
1	A	200	VAL	4.9
1	A	63	THR	4.8
1	A	324	GLY	4.7
3	D	27	GLN	4.7
3	D	1	ASP	4.5
1	A	440	ASP	4.5
1	A	45	TRP	4.3
1	A	59	LYS	4.3
1	A	89	VAL	4.2
1	A	60	ALA	4.2
1	A	199	SER	3.9
1	A	267	GLU	3.7
1	A	83	GLU	3.6
1	A	58	ALA	3.5
3	D	28	ARG	3.4
1	A	472	GLY	3.4
3	D	76	ASN	3.2
1	A	256	SER	3.2
1	A	202	LYS	3.2
1	A	117	GLN	3.2
1	A	492	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	290	LYS	3.1
1	A	61	HIS	3.1
1	A	433	ALA	3.0
1	A	124	GLY	3.0
1	A	432	GLN	3.0
1	A	301	ASN	3.0
1	A	491	ILE	2.9
1	A	258	GLN	2.9
1	A	451	GLY	2.7
1	A	204	ALA	2.6
1	A	471	GLY	2.6
1	A	291	SER	2.5
1	A	121	LYS	2.5
1	A	455	THR	2.4
1	A	84	ILE	2.4
1	A	442	LYS	2.4
1	A	122	LEU	2.4
1	A	260	LEU	2.3
1	A	93	PHE	2.3
1	A	441	GLY	2.3
1	A	201	ILE	2.2
2	C	193	THR	2.2
2	C	113	SER	2.2
3	D	109	LYS	2.1
1	A	209	SER	2.1
2	C	99	ASP	2.1
1	A	470	PRO	2.1
2	C	101	PHE	2.1
2	C	94	THR	2.0
2	C	191	THR	2.0
1	A	66	HIS	2.0
1	A	268	GLU	2.0
1	A	328	LYS	2.0
1	A	379	ARG	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.

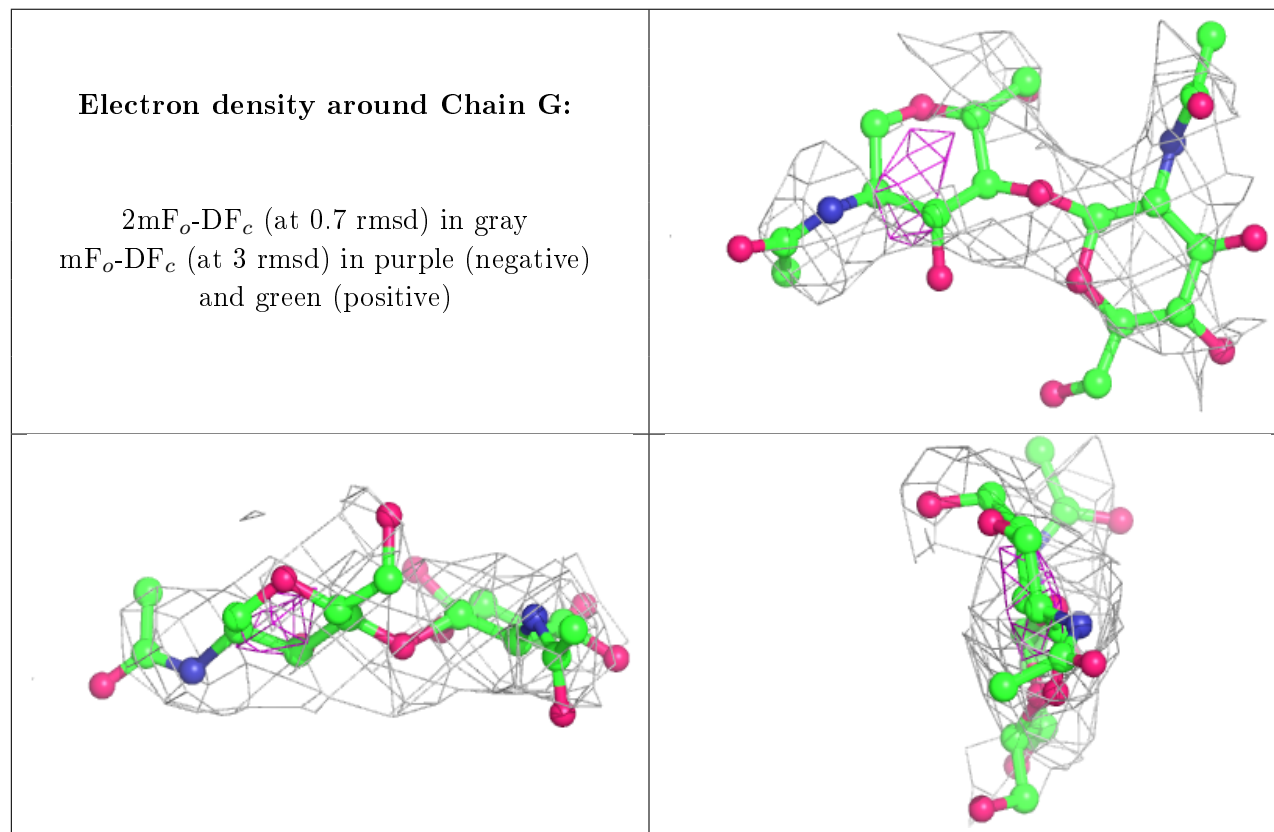


### 6.3 Carbohydrates i

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.

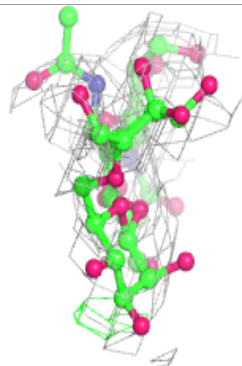
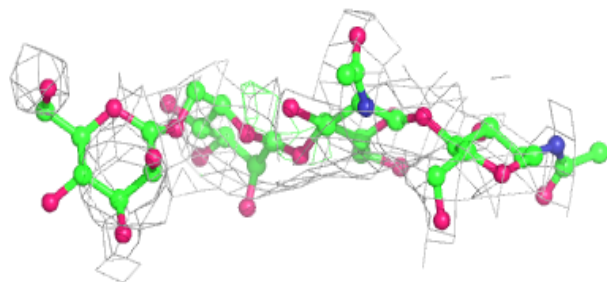
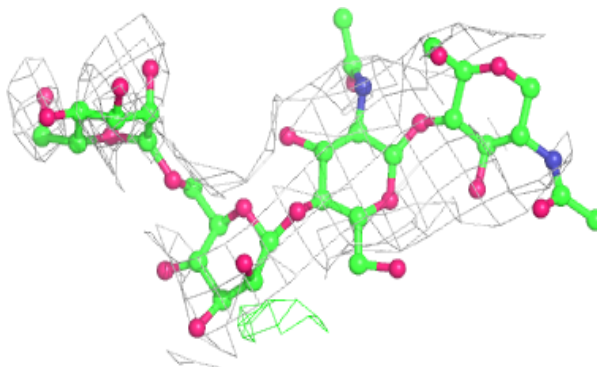
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	E	4	11/12	0.44	0.50	189,190,190,190	0
6	NAG	F	1	14/15	0.56	0.43	141,147,155,162	0
5	BMA	E	3	11/12	0.59	0.36	177,181,185,186	0
4	NAG	G	2	14/15	0.68	0.57	196,199,199,199	0
4	NAG	B	2	14/15	0.72	0.34	141,148,150,150	0
4	NAG	G	1	14/15	0.74	0.44	125,134,138,139	0
6	NAG	F	2	14/15	0.75	0.65	169,175,176,178	0
6	BMA	F	3	11/12	0.78	0.49	179,181,181,181	0
5	NAG	E	1	14/15	0.81	0.31	116,129,134,143	0
4	NAG	B	1	14/15	0.88	0.32	109,120,123,132	0
5	NAG	E	2	14/15	0.92	0.38	153,160,165,172	0

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

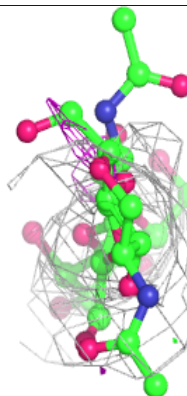
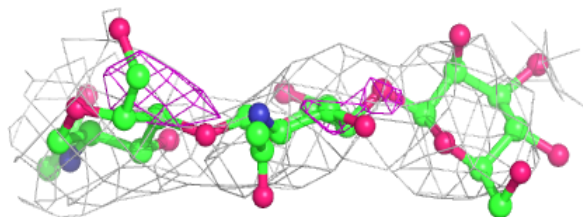
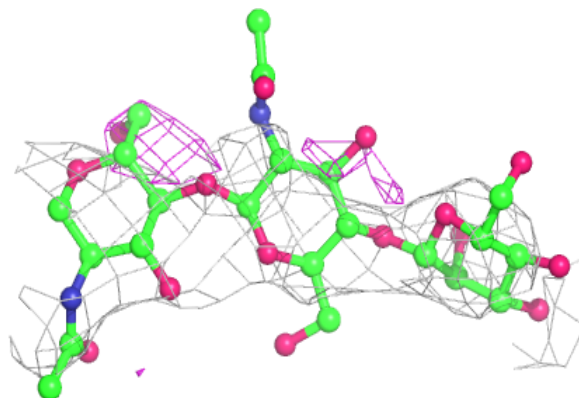


**Electron density around Chain E:**

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

**Electron density around Chain F:**

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



## 6.4 Ligands [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
7	NAG	A	505	14/15	0.49	0.56	140,146,154,154	0
7	NAG	A	506	14/15	0.75	0.43	130,136,137,138	0
7	NAG	A	504	14/15	0.76	0.34	109,119,121,122	0
7	NAG	A	502	14/15	0.78	0.35	172,173,174,175	0
7	NAG	A	503	14/15	0.81	0.34	105,109,112,113	0
7	NAG	A	501	14/15	0.84	0.25	107,117,120,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.