



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:30 AM BST

PDB ID : 5YDI  
Title : Crystal structure of acetylcholinesterase catalytic subunits of the malaria vector *Anopheles gambiae*, new crystal packing  
Authors : Han, Q.; Guan, H.; Ding, H.; Liao, C.; Robinson, H.; Li, J.  
Deposited on : 2017-09-13  
Resolution : 3.45 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

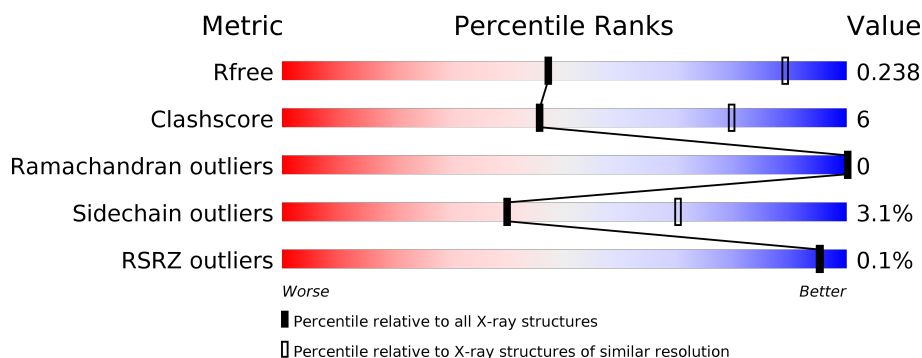
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	553	<div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	B	553	<div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	C	553	<div> <div>82%</div> <div>14%</div> <div>..</div> </div>
2	D	3	<div> <div>100%</div> </div>
2	F	3	<div> <div>100%</div> </div>
3	E	6	<div> <div>100%</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
2	NAG	D	1	-	-	-	X
2	NAG	D	2	-	-	-	X
2	BMA	D	3	-	-	-	X
2	NAG	F	1	-	-	X	-
2	NAG	F	2	-	-	X	X
2	BMA	F	3	-	-	-	X
3	NAG	E	2	-	-	-	X
3	BMA	E	3	-	-	-	X
3	MAN	E	4	-	-	-	X
3	MAN	E	5	-	-	-	X
3	MAN	E	6	-	-	-	X
4	NAG	A	801	-	-	-	X

## 2 Entry composition [i](#)

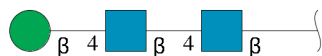
There are 7 unique types of molecules in this entry. The entry contains 12977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

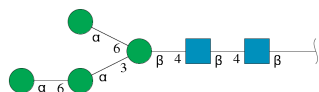
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			
1	B	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			
1	C	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			

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



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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



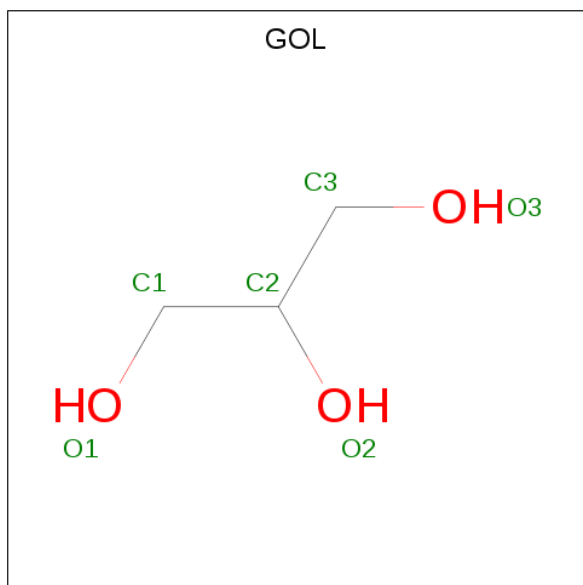
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

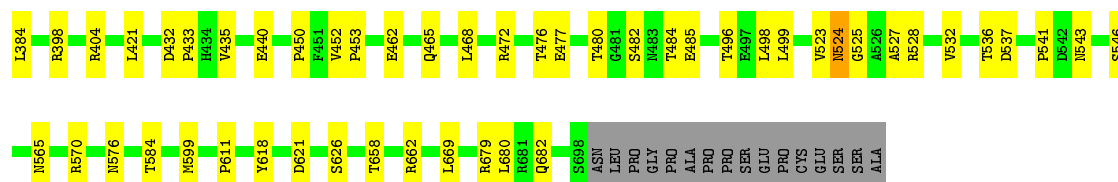
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Na 2 2	0	0
6	A	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	1	Total O 1 1	0	0
7	C	6	Total O 6 6	0	0





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

Chain D:  100%


NAG1  
NAG2  
BMA3

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

Chain F:  100%

NAG1  
NAG2  
BMA3

- Molecule 3: alpha-D-mannopyranose-(1-6)-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

Chain E:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.44Å 235.91Å 167.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.72 – 3.45 63.72 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.72-3.45) 99.8 (63.72-3.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.200 , 0.242 0.197 , 0.238	Depositor DCC
$R_{free}$ test set	1697 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: MAN, GOL, BMA, NAG, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/4373	0.49	0/5968
1	B	0.29	0/4373	0.48	0/5968
1	C	0.29	0/4373	0.48	0/5968
All	All	0.29	0/13119	0.48	0/17904

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	4249	0	4098	56	0
1	B	4249	0	4099	52	0
1	C	4249	0	4099	46	0
2	D	39	0	34	0	0
2	F	39	0	34	13	0
3	E	72	0	61	0	0
4	A	28	0	26	0	0
4	C	14	0	13	1	0
5	A	12	0	16	2	0
5	B	6	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	8	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	6	0	0	0	0
All	All	12977	0	12495	164	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 6.

All (164) 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)
2:F:2:NAG:H83	2:F:2:NAG:H5	1.24	1.09
2:F:1:NAG:H3	2:F:2:NAG:N2	1.71	1.05
2:F:1:NAG:H3	2:F:2:NAG:HN2	1.24	0.99
2:F:2:NAG:C5	2:F:2:NAG:H83	1.97	0.94
1:A:529:GLN:HA	1:A:532:VAL:HG22	1.53	0.90
2:F:2:NAG:C8	2:F:2:NAG:H5	2.02	0.89
1:C:282:TYR:OH	5:C:805:GOL:H32	1.72	0.88
1:A:174:ARG:HD2	1:A:218:VAL:HG22	1.55	0.86
1:A:359:GLU:HG2	1:A:604:ILE:HD11	1.55	0.86
1:C:611:PRO:HA	1:C:618:TYR:HD2	1.41	0.85
1:A:239:PHE:HD1	1:A:240:PRO:HD2	1.45	0.81
1:C:611:PRO:HA	1:C:618:TYR:CD2	2.16	0.81
1:A:282:TYR:OH	5:A:803:GOL:H32	1.80	0.80
1:A:164:ASP:HB3	1:A:167:VAL:HG22	1.64	0.79
2:F:1:NAG:H3	2:F:2:NAG:C2	2.06	0.78
2:F:2:NAG:H62	2:F:3:BMA:O5	1.84	0.77
2:F:1:NAG:C3	2:F:2:NAG:HN2	1.99	0.75
2:F:1:NAG:C3	2:F:2:NAG:C2	2.64	0.71
2:F:2:NAG:H62	2:F:3:BMA:C1	2.21	0.70
1:A:233:ASP:OD1	1:A:235:VAL:HG12	1.90	0.70
1:C:432:ASP:HB3	1:C:435:VAL:HG12	1.76	0.67
1:C:498:LEU:HD23	1:C:499:LEU:HB2	1.76	0.67
1:C:190:VAL:HG12	1:C:261:VAL:HG22	1.77	0.66
2:F:1:NAG:C3	2:F:2:NAG:N2	2.55	0.66
1:B:274:LEU:HD21	1:B:307:LEU:HD23	1.78	0.66
1:B:188:VAL:HG23	1:B:262:ALA:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:HA	1:A:476:THR:HG21	1.80	0.64
1:C:188:VAL:HG23	1:C:263:PRO:HA	1.82	0.62
1:B:166:LEU:HD21	1:B:178:ILE:HA	1.81	0.62
2:F:2:NAG:H83	2:F:2:NAG:C4	2.29	0.62
1:A:239:PHE:CD1	1:A:240:PRO:HD2	2.33	0.61
1:A:293:HIS:HD1	1:A:293:HIS:N	1.99	0.60
1:C:231:ILE:H	1:C:231:ILE:HD12	1.67	0.59
1:B:375:SER:HA	1:B:378:LEU:HD12	1.84	0.59
1:A:498:LEU:HD11	1:A:507:VAL:HG22	1.85	0.59
1:C:485:GLU:O	1:C:599:MET:HA	2.03	0.58
1:B:170:THR:HG22	1:B:172:LYS:H	1.70	0.57
1:B:203:PRO:O	1:B:207:ARG:NH1	2.38	0.56
1:C:525:GLY:HA2	1:C:528:ARG:HE	1.70	0.56
1:A:239:PHE:HD1	1:A:240:PRO:CD	2.18	0.56
1:B:539:THR:HA	1:C:680:LEU:HD13	1.87	0.56
1:A:644:PRO:O	1:A:648:SER:HB2	2.06	0.55
1:B:611:PRO:HA	1:B:618:TYR:CD2	2.41	0.55
1:B:473:PHE:CZ	1:B:574:GLU:HG3	2.42	0.55
1:B:476:THR:HG22	1:B:477:GLU:N	2.22	0.54
1:A:274:LEU:HD21	1:A:307:LEU:HD23	1.89	0.54
1:C:452:VAL:HB	1:C:453:PRO:HD2	1.90	0.53
1:A:322:PRO:HD3	1:C:398:ARG:NH1	2.23	0.53
1:A:282:TYR:OH	5:A:803:GOL:C3	2.56	0.53
1:A:239:PHE:CE2	1:A:501:LYS:HD2	2.43	0.53
1:C:229:VAL:HG11	1:C:433:PRO:HB2	1.91	0.53
1:A:527:ALA:HB1	1:A:690:LEU:HD11	1.92	0.52
1:B:498:LEU:HD11	1:B:507:VAL:HG22	1.92	0.52
1:C:468:LEU:O	1:C:570:ARG:NH2	2.43	0.51
4:C:804:NAG:O4	4:C:804:NAG:H82	2.10	0.51
1:A:380:GLN:HG2	1:A:381:ARG:HG3	1.92	0.51
1:C:319:LEU:HD23	1:C:421:LEU:HD22	1.92	0.51
1:B:229:VAL:HG11	1:B:433:PRO:HB2	1.93	0.51
1:C:524:ASN:HD22	1:C:524:ASN:H	1.59	0.50
1:B:307:LEU:HD22	1:B:336:ALA:HB3	1.93	0.50
1:A:350:ASP:HB3	1:A:353:ARG:HB2	1.94	0.50
1:A:525:GLY:HA2	1:A:528:ARG:HB2	1.94	0.50
1:B:312:ALA:HB1	1:B:440:GLU:OE1	2.11	0.50
1:A:571:TYR:O	1:A:576:ASN:HB2	2.12	0.49
1:B:404:ARG:NH1	1:B:450:PRO:O	2.45	0.49
1:C:537:ASP:O	1:C:541:PRO:HA	2.13	0.49
1:B:315:GLY:O	1:B:328:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HD2	1:B:314:LEU:HD22	1.95	0.49
1:B:388:SER:OG	1:B:390:THR:HG22	2.13	0.48
1:B:381:ARG:HA	1:B:476:THR:HG21	1.95	0.48
1:C:462:GLU:OE2	1:C:472:ARG:HD2	2.12	0.48
1:A:485:GLU:O	1:A:599:MET:HA	2.14	0.48
1:C:274:LEU:HD21	1:C:307:LEU:HD23	1.96	0.48
1:A:526:ALA:HA	1:A:529:GLN:HE22	1.79	0.48
1:C:532:VAL:O	1:C:536:THR:HG22	2.13	0.48
1:C:543:ASN:HB3	1:C:546:SER:HB2	1.95	0.48
1:A:229:VAL:HG11	1:A:433:PRO:HB2	1.96	0.47
1:C:525:GLY:HA2	1:C:528:ARG:NE	2.30	0.47
1:A:312:ALA:HB1	1:A:440:GLU:OE1	2.14	0.47
1:B:175:ILE:HA	1:B:219:LEU:O	2.14	0.47
1:B:569:GLN:O	1:B:573:GLU:HG2	2.15	0.47
1:B:693:LEU:O	1:B:697:THR:HG22	2.15	0.47
1:C:357:PHE:HB3	1:C:383:ILE:HB	1.97	0.47
1:A:238:ASP:OD1	1:A:238:ASP:N	2.48	0.46
1:C:523:VAL:HB	1:C:527:ALA:HB3	1.96	0.46
1:C:307:LEU:HD22	1:C:336:ALA:HB3	1.96	0.46
1:C:343:ASN:HA	1:C:346:ARG:HH11	1.80	0.46
1:B:371:LEU:HD23	1:B:473:PHE:HB3	1.96	0.46
1:C:611:PRO:HG2	1:C:626:SER:HB2	1.97	0.46
1:B:367:SER:HB2	1:B:389:PRO:HD3	1.98	0.46
1:B:396:VAL:O	1:B:454:VAL:HG23	2.16	0.46
1:C:476:THR:HG22	1:C:477:GLU:N	2.30	0.46
1:A:523:VAL:HB	1:A:527:ALA:HB3	1.98	0.45
1:C:239:PHE:HA	1:C:240:PRO:HD3	1.80	0.45
1:A:321:THR:OG1	1:A:322:PRO:HD2	2.17	0.45
1:A:585:HIS:ND1	1:A:669:LEU:HD11	2.31	0.45
1:B:658:THR:HG23	1:B:661:GLY:HA3	1.97	0.45
1:B:359:GLU:HA	1:B:385:GLN:O	2.17	0.45
1:B:473:PHE:HZ	1:B:574:GLU:HG3	1.81	0.45
1:B:485:GLU:O	1:B:599:MET:HA	2.17	0.45
1:C:381:ARG:HA	1:C:476:THR:HG21	1.98	0.45
1:C:484:THR:CG2	1:C:584:THR:HG22	2.46	0.45
1:C:662:ARG:HE	1:C:680:LEU:HD21	1.82	0.45
1:A:182:ALA:HA	1:A:294:ARG:HD2	1.99	0.45
1:A:452:VAL:HB	1:A:453:PRO:HD2	1.99	0.45
1:B:523:VAL:HB	1:B:527:ALA:HB3	1.99	0.45
1:A:562:CYS:HB3	1:A:687:LYS:HE2	1.99	0.45
2:F:1:NAG:H4	2:F:2:NAG:H2	1.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:OD1	1:A:350:ASP:HB2	2.16	0.44
1:A:535:TYR:HE1	1:A:553:LYS:HB3	1.81	0.44
1:A:585:HIS:HD1	1:A:669:LEU:HD11	1.83	0.44
1:B:175:ILE:HD11	1:B:347:PHE:HZ	1.82	0.44
1:C:462:GLU:OE2	1:C:472:ARG:NH1	2.48	0.44
1:C:380:GLN:O	1:C:476:THR:HG21	2.18	0.44
1:B:196:TYR:CD1	1:B:258:ILE:HG13	2.53	0.44
1:A:234:THR:O	1:A:236:PHE:N	2.51	0.44
1:A:646:THR:O	1:A:647:ALA:HB3	2.18	0.44
1:C:272:VAL:HB	1:C:354:VAL:HA	1.99	0.44
1:C:565:ASN:HB3	1:C:662:ARG:HH22	1.83	0.44
1:A:192:LEU:HD23	1:A:224:PRO:HD3	2.00	0.43
1:B:170:THR:HB	1:B:173:GLY:O	2.18	0.43
1:A:293:HIS:ND1	1:A:293:HIS:N	2.58	0.43
1:C:679:ARG:HH21	1:C:682:GLN:HG2	1.84	0.43
1:A:484:THR:CG2	1:A:584:THR:HG22	2.48	0.43
1:B:535:TYR:HE1	1:B:553:LYS:HB3	1.83	0.43
1:B:679:ARG:HH21	1:B:682:GLN:HG2	1.84	0.43
1:A:398:ARG:CZ	1:C:322:PRO:HD3	2.49	0.43
1:B:190:VAL:HG12	1:B:261:VAL:HG22	2.01	0.43
1:A:319:LEU:HA	1:A:402:THR:HG22	2.00	0.43
1:B:579:TYR:OH	1:B:641:ASN:ND2	2.52	0.43
1:C:404:ARG:NH1	1:C:450:PRO:O	2.51	0.43
1:A:235:VAL:CG1	1:A:493:TYR:CE2	3.03	0.42
1:A:235:VAL:HG11	1:A:493:TYR:CE2	2.55	0.42
1:A:679:ARG:HH21	1:A:682:GLN:HG2	1.84	0.42
1:A:476:THR:HG22	1:A:477:GLU:N	2.34	0.42
1:B:380:GLN:O	1:B:476:THR:HG21	2.19	0.42
1:B:333:GLN:OE1	1:B:365:SER:HB3	2.19	0.42
1:C:384:LEU:O	1:C:480:THR:HA	2.19	0.42
1:A:313:SER:O	1:A:317:LEU:HB2	2.20	0.42
1:A:352:SER:O	1:A:380:GLN:HB2	2.19	0.42
1:B:565:ASN:O	1:B:569:GLN:HB2	2.19	0.42
1:B:641:ASN:HA	1:B:642:PRO:HD3	1.87	0.42
1:B:679:ARG:NH2	1:B:682:GLN:HG2	2.35	0.42
1:C:312:ALA:HB1	1:C:440:GLU:OE1	2.20	0.42
1:B:307:LEU:HD11	1:B:333:GLN:HG2	2.02	0.42
1:B:357:PHE:HA	1:B:383:ILE:O	2.20	0.41
1:C:359:GLU:OE1	1:C:360:SER:HB2	2.20	0.41
1:A:461:ASP:OD2	1:C:210:ARG:NH2	2.53	0.41
1:B:476:THR:CG2	1:B:477:GLU:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ALA:HB2	1:C:335:LEU:HD23	2.03	0.41
1:B:357:PHE:CB	1:B:383:ILE:HB	2.50	0.41
1:B:569:GLN:CG	1:B:662:ARG:HE	2.33	0.41
1:C:357:PHE:HA	1:C:383:ILE:O	2.20	0.41
1:A:432:ASP:HB3	1:A:435:VAL:HG12	2.01	0.41
1:A:529:GLN:CA	1:A:532:VAL:HG22	2.37	0.41
1:B:682:GLN:O	1:B:685:PHE:HB3	2.20	0.41
1:B:197:ALA:HB3	1:B:256:LEU:HD23	2.03	0.41
1:A:434:HIS:O	1:A:438:ASN:ND2	2.47	0.40
1:A:510:GLU:O	1:A:514:GLN:HG2	2.21	0.40
1:A:682:GLN:O	1:A:685:PHE:HB3	2.21	0.40
1:B:527:ALA:HB1	1:B:690:LEU:HD11	2.03	0.40
1:A:487:GLY:O	1:A:491:ILE:HG13	2.22	0.40
1:B:202:GLY:HA3	1:B:203:PRO:HD3	1.97	0.40
1:B:239:PHE:HA	1:B:240:PRO:HD3	1.90	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	535/553 (97%)	517 (97%)	18 (3%)	0	100	100
1	B	535/553 (97%)	518 (97%)	17 (3%)	0	100	100
1	C	535/553 (97%)	519 (97%)	16 (3%)	0	100	100
All	All	1605/1659 (97%)	1554 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	454/467 (97%)	442 (97%)	12 (3%)	46	74
1	B	454/467 (97%)	439 (97%)	15 (3%)	38	68
1	C	454/467 (97%)	439 (97%)	15 (3%)	38	68
All	All	1362/1401 (97%)	1320 (97%)	42 (3%)	40	70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	A	293	HIS
1	A	311	VAL
1	A	330	LEU
1	A	345	HIS
1	A	357	PHE
1	A	359	GLU
1	A	417	GLU
1	A	498	LEU
1	A	571	TYR
1	A	658	THR
1	A	670	ASN
1	B	188	VAL
1	B	216	THR
1	B	301	ASN
1	B	311	VAL
1	B	330	LEU
1	B	478	ILE
1	B	482	SER
1	B	495	LEU
1	B	549	ASP
1	B	571	TYR
1	B	586	ARG
1	B	603	GLU
1	B	651	PHE
1	B	658	THR

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Mol	Chain	Res	Type
1	B	697	THR
1	C	162	ASP
1	C	291	TYR
1	C	293	HIS
1	C	311	VAL
1	C	330	LEU
1	C	357	PHE
1	C	360	SER
1	C	465	GLN
1	C	482	SER
1	C	496	THR
1	C	524	ASN
1	C	576	ASN
1	C	621	ASP
1	C	658	THR
1	C	669	LEU

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

Mol	Chain	Res	Type
1	B	520	ASN
1	C	524	ASN

### 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 ⓘ

12 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	0.59	0	17,19,21	1.56	4 (23%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	1.53	2 (11%)
2	BMA	D	3	2	11,11,12	0.64	0	15,15,17	1.69	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.45	0	17,19,21	2.71	6 (35%)
3	NAG	E	2	3	14,14,15	0.70	0	17,19,21	2.21	4 (23%)
3	BMA	E	3	3	11,11,12	0.89	1 (9%)	15,15,17	2.11	5 (33%)
3	MAN	E	4	3	11,11,12	0.52	0	15,15,17	3.20	4 (26%)
3	MAN	E	5	3	11,11,12	0.60	0	15,15,17	1.67	5 (33%)
3	MAN	E	6	3	11,11,12	0.57	0	15,15,17	1.88	4 (26%)
2	NAG	F	1	1,2	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	1.97	4 (23%)
2	BMA	F	3	2	11,11,12	0.27	0	15,15,17	1.15	2 (13%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C2-C3	2.05	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	9.34	124.85	112.19
3	E	1	NAG	C1-O5-C5	8.42	123.60	112.19
3	E	2	NAG	C1-O5-C5	5.88	120.16	112.19
3	E	3	BMA	C1-C2-C3	5.81	116.81	109.67
3	E	4	MAN	C1-C2-C3	5.75	116.73	109.67
2	F	2	NAG	C4-C3-C2	5.62	119.26	111.02
3	E	2	NAG	C4-C3-C2	4.91	118.22	111.02
3	E	4	MAN	O5-C1-C2	4.84	118.24	110.77
3	E	1	NAG	O5-C1-C2	4.78	118.83	111.29
2	D	2	NAG	C4-C3-C2	4.69	117.89	111.02
3	E	6	MAN	C1-O5-C5	4.68	118.53	112.19
2	D	3	BMA	C1-O5-C5	4.46	118.24	112.19
3	E	6	MAN	C1-C2-C3	3.78	114.32	109.67
2	F	2	NAG	C1-O5-C5	3.64	117.12	112.19
3	E	5	MAN	C3-C4-C5	3.51	116.50	110.24
2	D	1	NAG	C4-C3-C2	3.51	116.16	111.02
2	D	3	BMA	C1-C2-C3	3.50	113.97	109.67
3	E	3	BMA	C2-C3-C4	3.32	116.65	110.89
3	E	2	NAG	O5-C5-C6	3.09	112.05	107.20
3	E	5	MAN	C1-O5-C5	2.99	116.24	112.19
3	E	3	BMA	O5-C5-C6	2.96	111.85	107.20
2	D	2	NAG	C1-O5-C5	2.86	116.06	112.19
2	D	1	NAG	C1-O5-C5	-2.74	108.47	112.19
3	E	2	NAG	O5-C1-C2	2.65	115.47	111.29
2	D	1	NAG	C3-C4-C5	2.62	114.90	110.24
3	E	1	NAG	C4-C3-C2	2.56	114.77	111.02
2	F	2	NAG	O5-C5-C6	2.51	111.14	107.20
2	F	3	BMA	C2-C3-C4	-2.51	106.55	110.89
3	E	6	MAN	O5-C1-C2	2.41	114.49	110.77
3	E	1	NAG	C8-C7-N2	2.34	120.07	116.10
3	E	5	MAN	C1-C2-C3	-2.32	106.81	109.67
3	E	5	MAN	O5-C5-C6	2.31	110.82	107.20
3	E	1	NAG	O5-C5-C4	2.26	116.34	110.83
3	E	3	BMA	C1-O5-C5	-2.16	109.26	112.19
2	F	3	BMA	O5-C5-C6	2.15	110.57	107.20
3	E	1	NAG	C2-N2-C7	2.14	125.95	122.90
3	E	3	BMA	C3-C4-C5	2.14	114.06	110.24
3	E	5	MAN	O5-C5-C4	2.14	116.02	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O5-C5-C6	2.12	110.53	107.20
2	F	2	NAG	C1-C2-N2	-2.12	106.86	110.49
3	E	4	MAN	C3-C4-C5	2.06	113.91	110.24
3	E	6	MAN	C3-C4-C5	2.05	113.89	110.24
2	F	1	NAG	C3-C4-C5	2.04	113.87	110.24

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	6	MAN	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

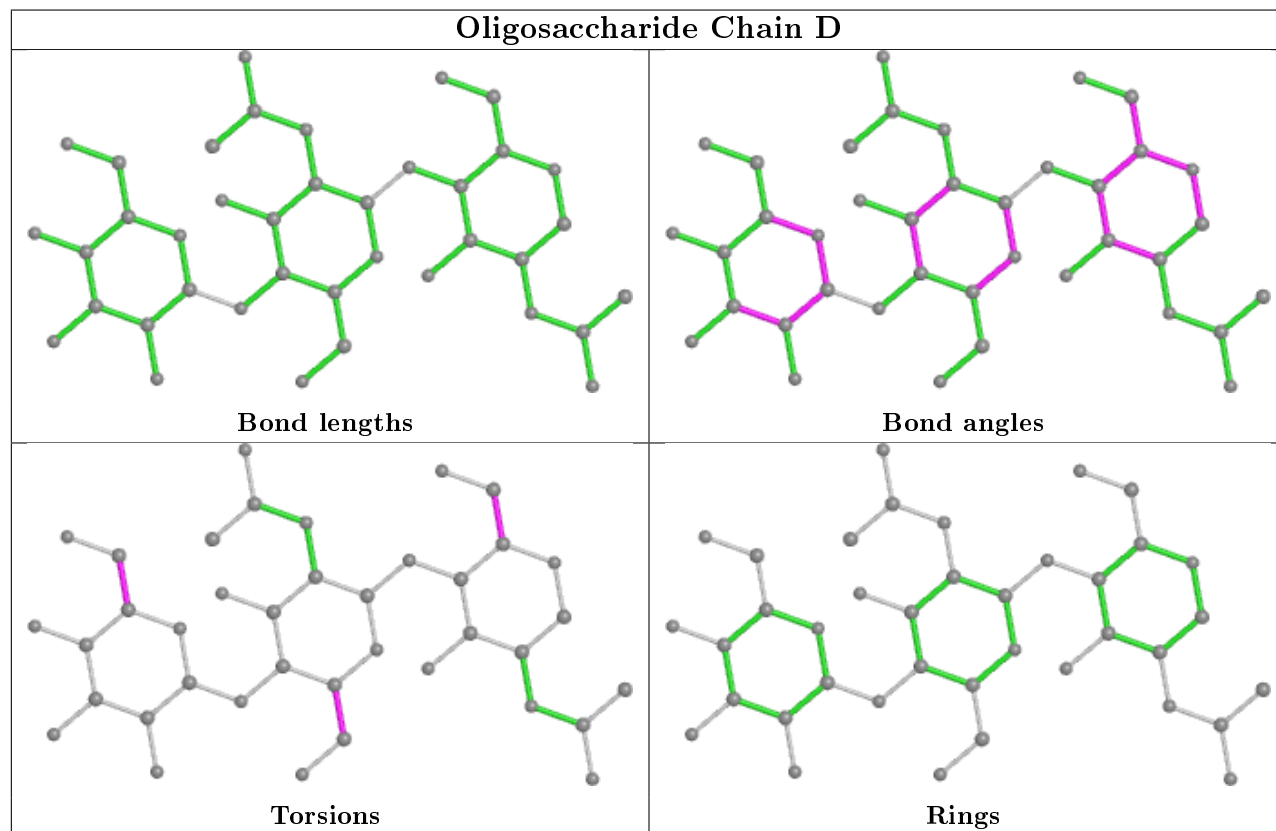
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	13	0

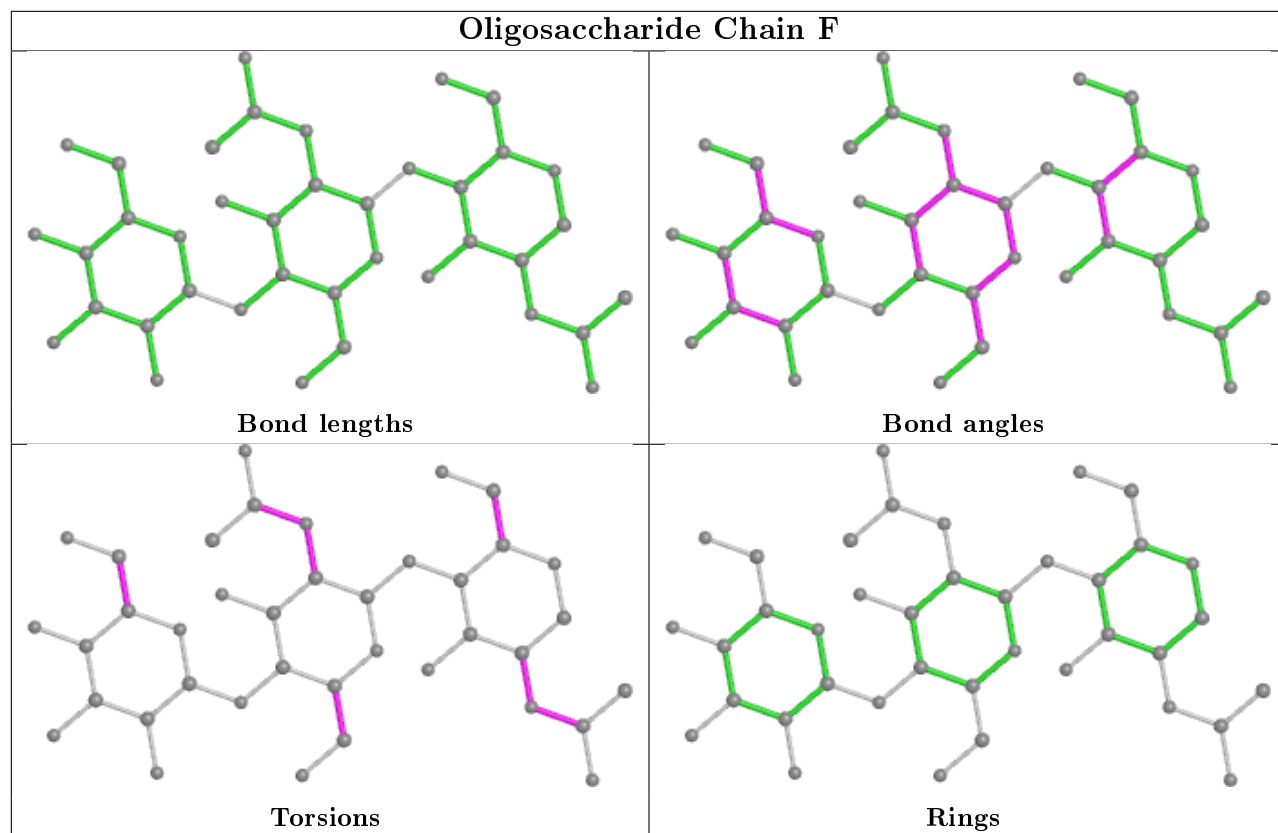
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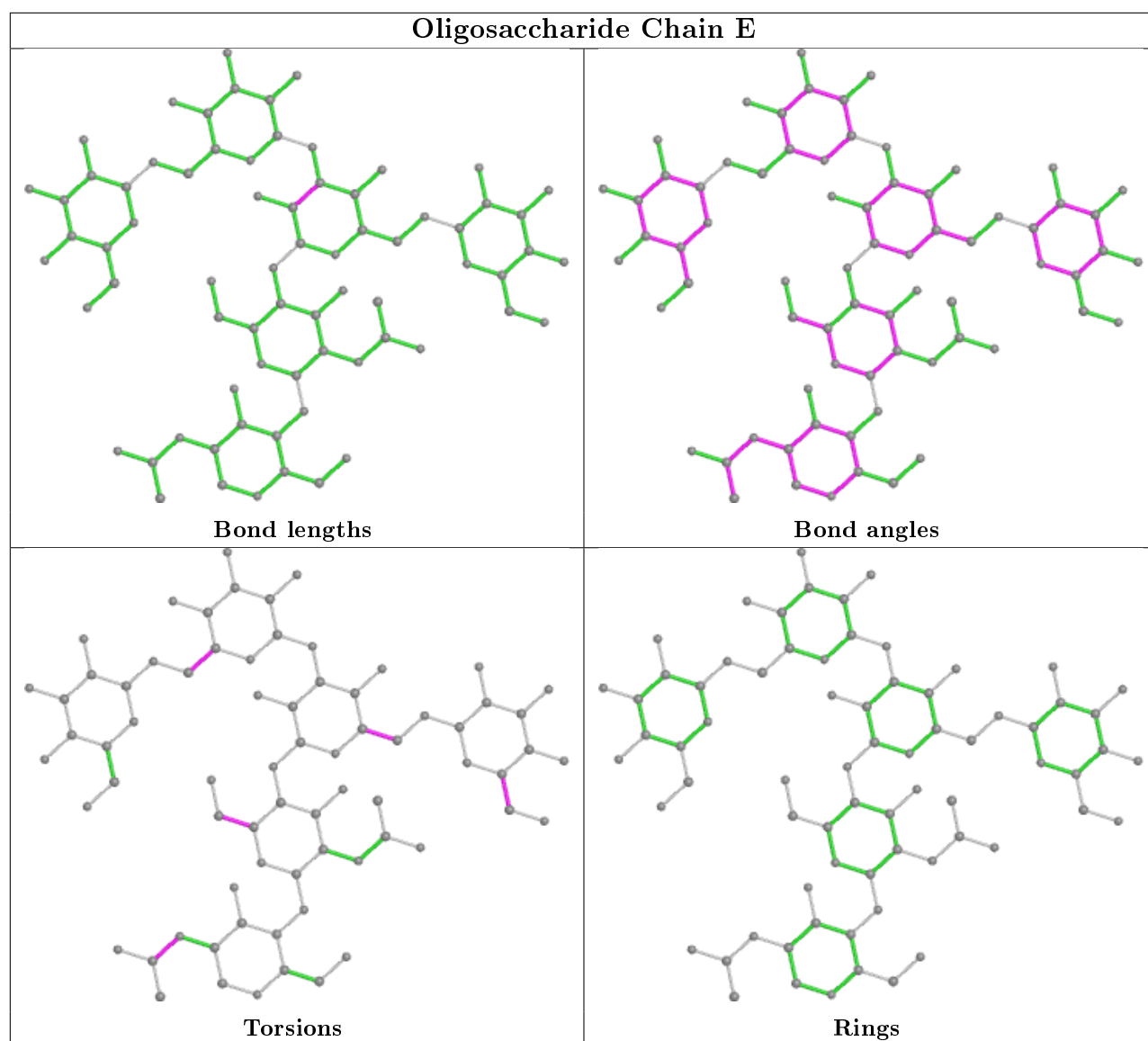
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	BMA	2	0
2	F	1	NAG	7	0

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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GOL	B	810	6	5,5,5	1.02	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.61	0
5	GOL	C	805	-	5,5,5	0.31	0	5,5,5	0.17	0
5	GOL	A	804	6	5,5,5	0.40	0	5,5,5	0.24	0
5	GOL	A	803	-	5,5,5	0.30	0	5,5,5	0.33	0
4	NAG	C	804	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	NAG	A	802	1	14,14,15	0.56	0	17,19,21	3.08	7 (41%)

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
5	GOL	B	810	6	-	0/4/4/4	-
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	GOL	C	805	-	-	0/4/4/4	-
5	GOL	A	804	6	-	2/4/4/4	-
5	GOL	A	803	-	-	2/4/4/4	-
4	NAG	C	804	1	-	3/6/23/26	0/1/1/1
4	NAG	A	802	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	NAG	C2-N2-C7	8.58	135.12	122.90
4	A	802	NAG	C1-O5-C5	5.94	120.24	112.19
4	A	802	NAG	C1-C2-N2	3.82	117.01	110.49
4	A	802	NAG	C8-C7-N2	3.69	122.35	116.10
4	A	802	NAG	O5-C5-C6	2.60	111.28	107.20
4	A	802	NAG	O7-C7-C8	-2.45	117.50	122.06
4	A	802	NAG	C3-C4-C5	2.24	114.23	110.24
4	C	804	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	801	NAG	O7-C7-N2-C2
5	A	804	GOL	O2-C2-C3-O3
5	A	803	GOL	O1-C1-C2-C3
4	C	804	NAG	C8-C7-N2-C2
4	C	804	NAG	O7-C7-N2-C2
4	A	802	NAG	C1-C2-N2-C7
4	A	802	NAG	O5-C5-C6-O6
4	A	802	NAG	C8-C7-N2-C2
4	A	802	NAG	O7-C7-N2-C2
4	C	804	NAG	C1-C2-N2-C7
5	A	804	GOL	C1-C2-C3-O3
5	A	803	GOL	O1-C1-C2-O2
4	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	805	GOL	1	0
5	A	803	GOL	2	0
4	C	804	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	537/553 (97%)	-0.21	0 100 100	34, 54, 83, 139	0
1	B	537/553 (97%)	-0.02	2 (0%) 92 90	33, 61, 90, 125	0
1	C	537/553 (97%)	-0.15	0 100 100	39, 63, 99, 136	0
All	All	1611/1659 (97%)	-0.13	2 (0%) 95 95	33, 58, 91, 139	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	648	SER	3.4
1	B	524	ASN	2.6

### 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.

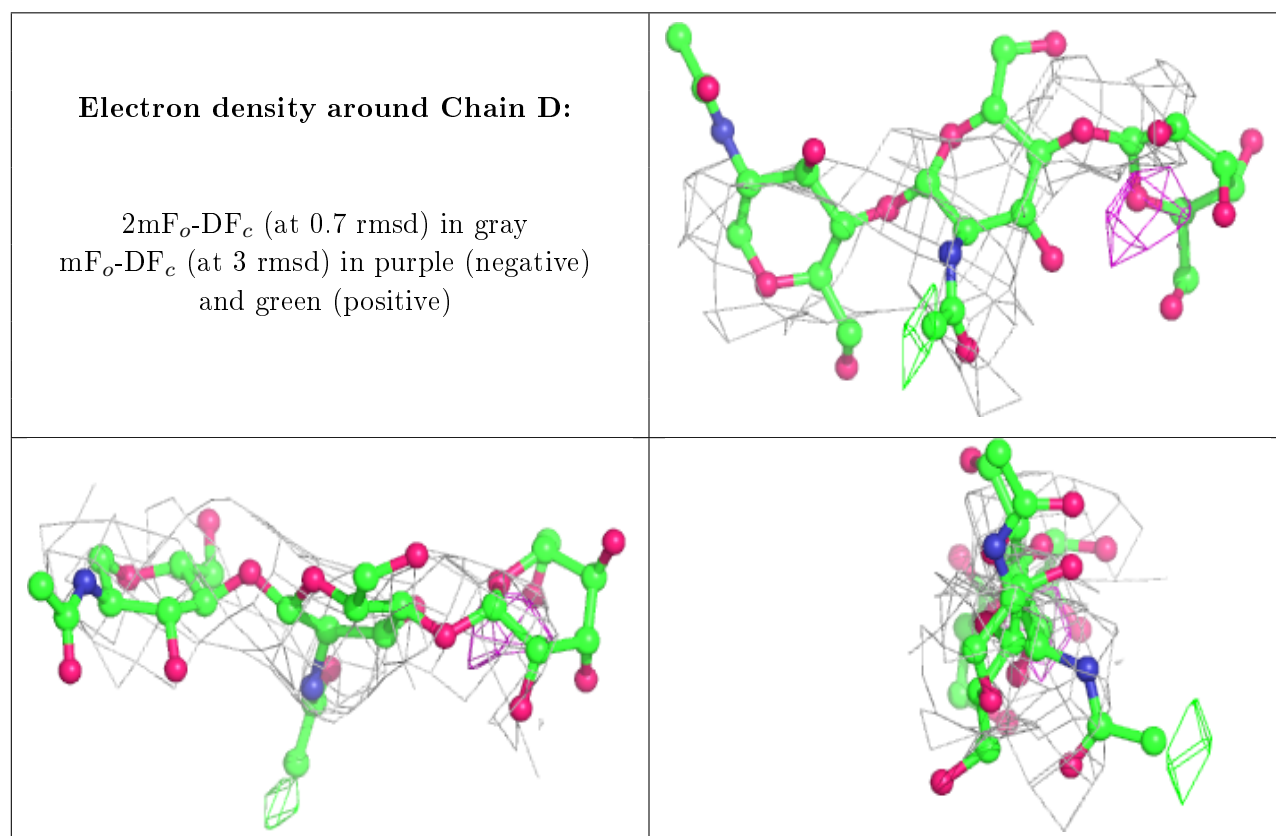
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	E	6	11/12	0.29	0.45	148,165,167,168	0
3	MAN	E	5	11/12	0.54	0.57	198,200,204,206	0
2	BMA	D	3	11/12	0.55	0.51	171,174,177,180	0
3	BMA	E	3	11/12	0.60	0.42	166,169,175,182	0
3	MAN	E	4	11/12	0.66	0.57	188,191,195,201	0
3	NAG	E	2	14/15	0.67	0.55	138,152,161,166	0

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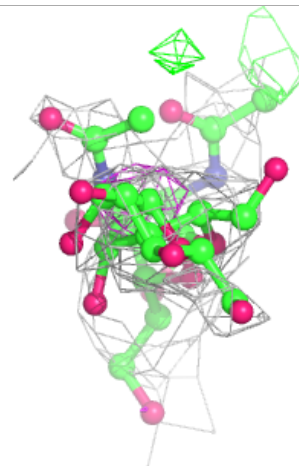
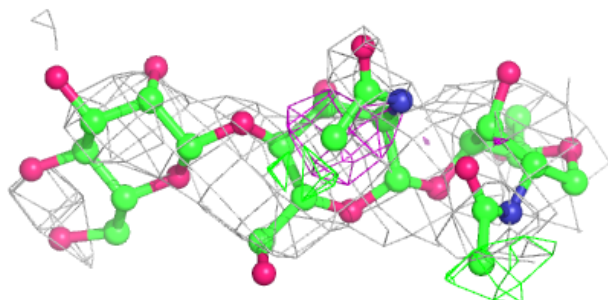
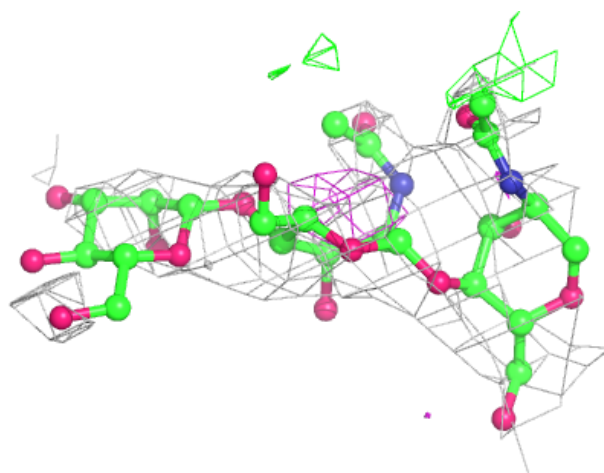
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	1	14/15	0.68	0.51	135,143,147,147	0
2	NAG	F	1	14/15	0.72	0.35	114,127,135,139	0
2	NAG	D	2	14/15	0.72	0.49	135,152,160,167	0
2	NAG	F	2	14/15	0.73	0.48	145,154,157,158	0
2	BMA	F	3	11/12	0.74	0.53	143,156,159,160	0
3	NAG	E	1	14/15	0.76	0.34	119,127,134,143	0

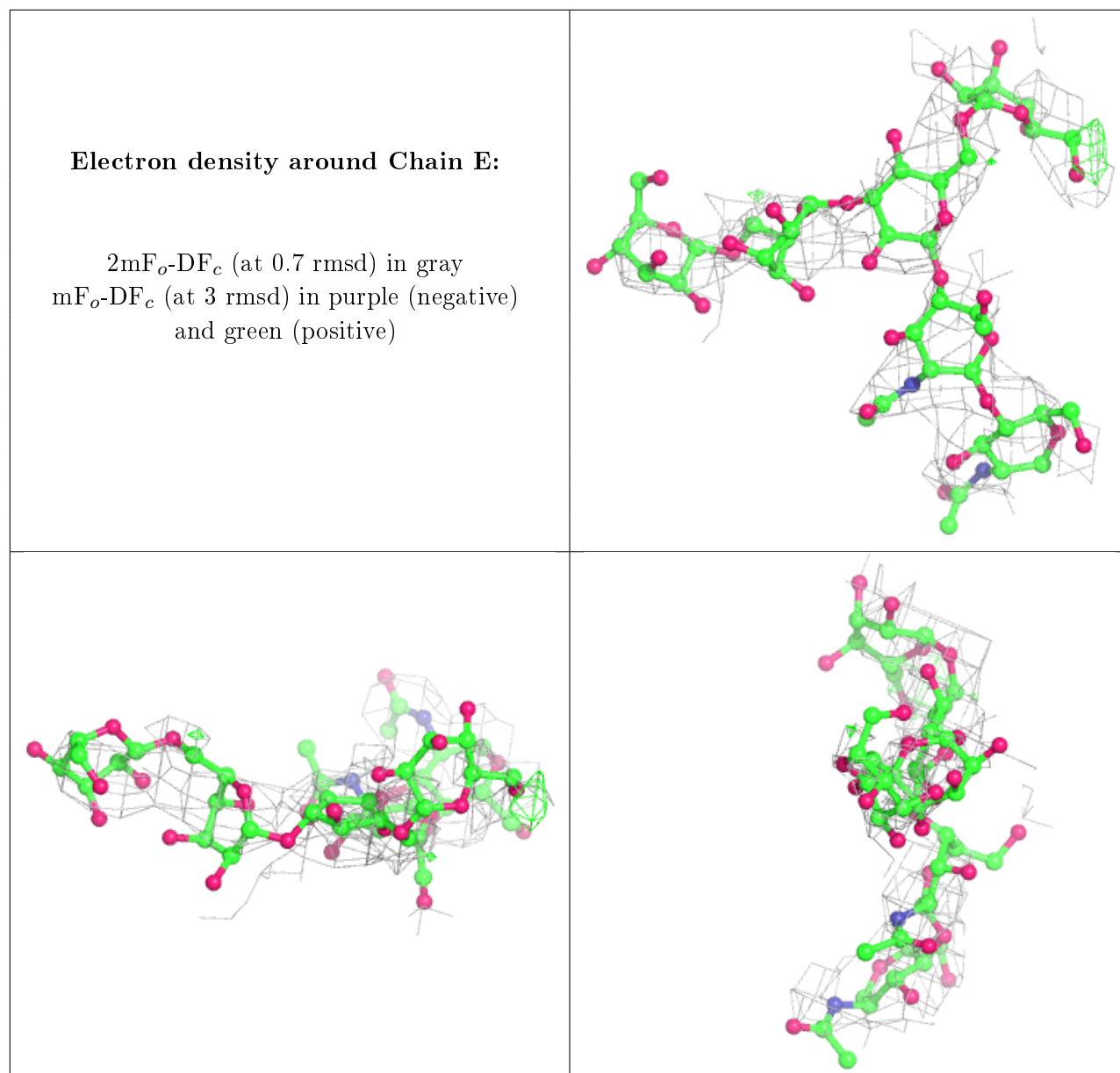
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain F:**

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





## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	804	14/15	0.75	0.32	118,127,130,130	0
4	NAG	A	801	14/15	0.76	0.46	109,115,117,120	0
4	NAG	A	802	14/15	0.80	0.38	112,119,121,122	0
5	GOL	A	803	6/6	0.82	0.30	49,51,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	810	6/6	0.83	0.32	31,31,32,32	0
5	GOL	A	804	6/6	0.86	0.24	48,53,53,53	0
5	GOL	C	805	6/6	0.88	0.21	43,46,46,46	0
6	NA	B	812	1/1	0.88	0.27	50,50,50,50	0
6	NA	A	805	1/1	0.92	0.34	22,22,22,22	0
6	NA	B	811	1/1	0.93	0.23	30,30,30,30	0
6	NA	C	806	1/1	0.94	0.27	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.