Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:48 PM BST

PDB ID	:	4AXB
Title	:	Crystal structure of soman-aged human butyrylcholinesterase in complex with 2-PAM
Authors	:	Wandhammer, M.; de Koning, M.; Noort, D.; Goeldner, M.; Nachon, F.
Deposited on	:	2012-06-12
Resolution	:	2.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

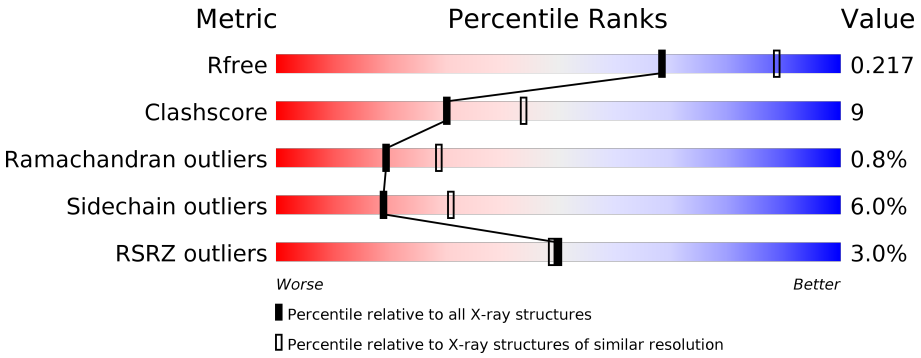
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 >=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 <=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	527	3% 79% 17%
2	B	3	100%
2	C	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
2	NAG	C	1	X	-	-	-
2	NAG	C	2	-	-	-	X
4	SO4	A	1531	-	-	X	-

2 Entry composition

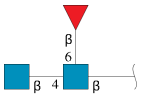
There are 9 unique types of molecules in this entry. The entry contains 4792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	527	4261	2751	713	780	1	16	0	10	0

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

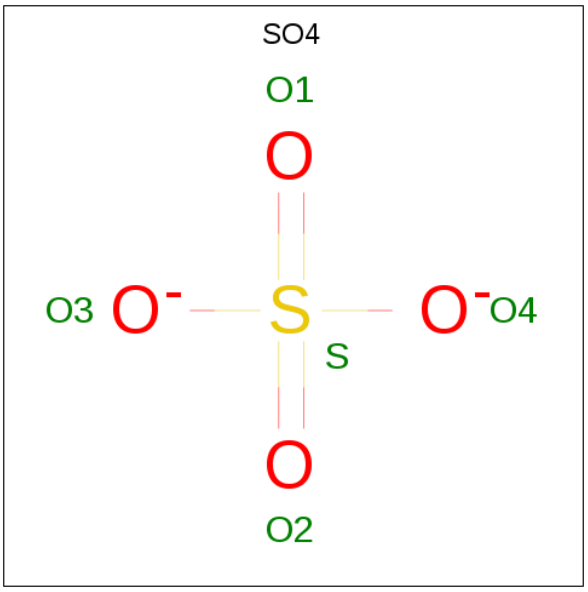


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	C	3	38	22	2	14	0	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

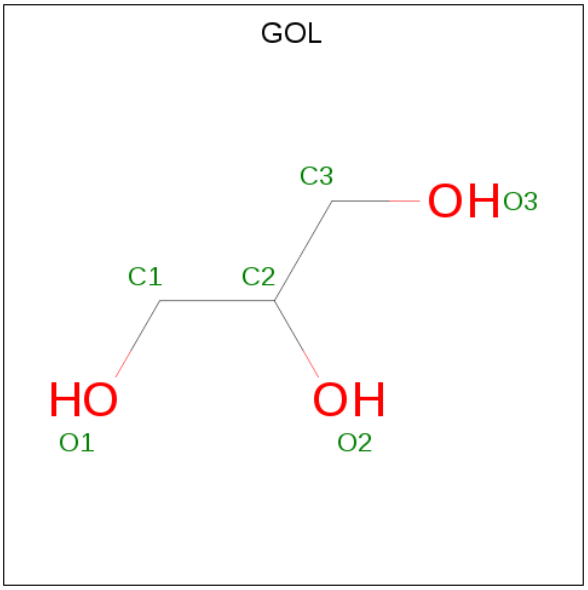
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	2	2	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- 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

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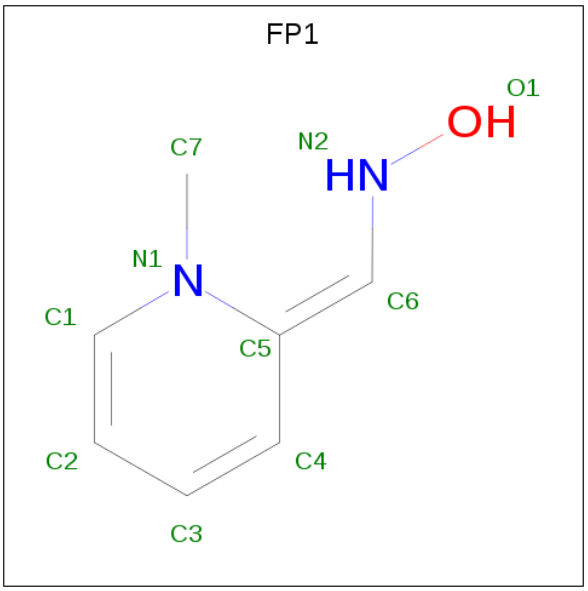
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

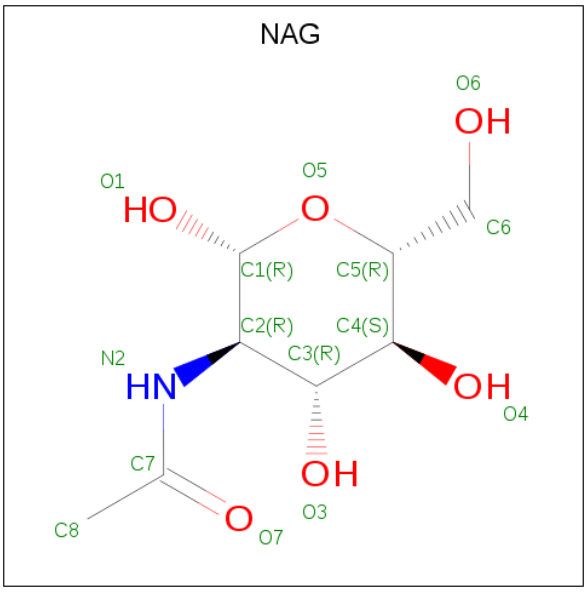
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0

- Molecule 7 is N-hydroxy-1-(1-methylpyridin-2(1H)-ylidene)methanamine (three-letter code: FP1) (formula: $C_7H_{10}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 10 7 2 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

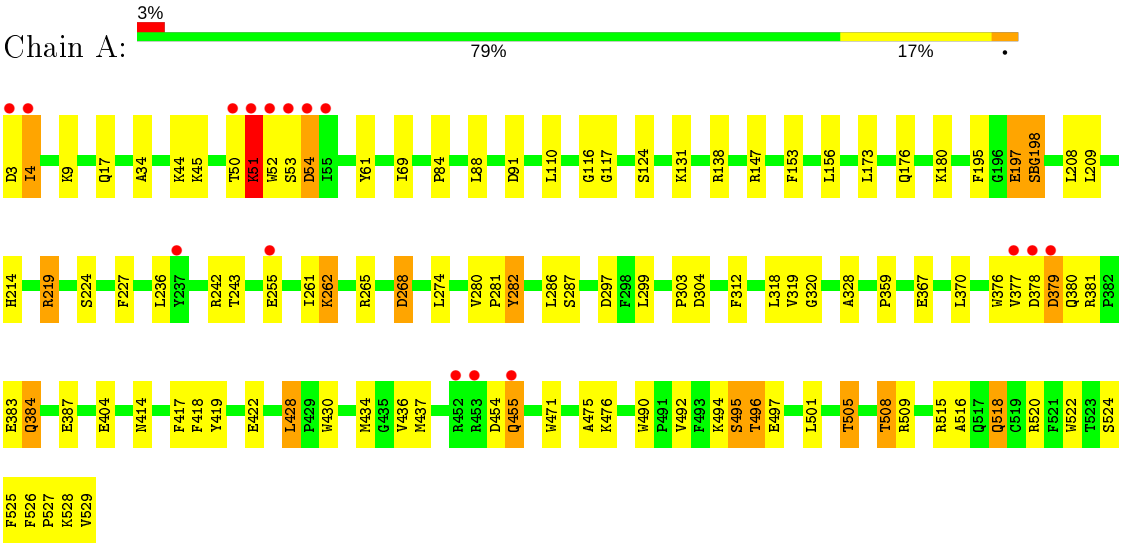
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	356	Total O 356 356	0	0

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.

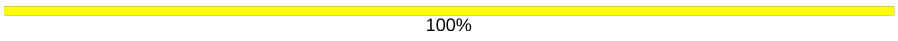
• Molecule 1: CHOLINESTERASE

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	155.95Å 155.95Å 127.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.27 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (110.27-2.40) 99.6 (49.32-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.221 0.165 , 0.217	Depositor DCC
R_{free} test set	1563 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4792	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL, K, FP1, SO4, FUL, SBG

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	3.50	7/4406 (0.2%)	1.07	10/5978 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	155.49	5.21	1.32
1	A	455[B]	GLN	CD-NE2	155.49	5.21	1.32
1	A	436	VAL	CB-CG2	6.42	1.66	1.52
1	A	153	PHE	CE1-CZ	5.99	1.48	1.37
1	A	404	GLU	CG-CD	5.88	1.60	1.51
1	A	497	GLU	CD-OE1	5.80	1.32	1.25
1	A	197	GLU	CB-CG	5.25	1.62	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455[A]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[B]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[A]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	455[B]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	219	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	236	LEU	CA-CB-CG	-6.10	101.27	115.30
1	A	91	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	147	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	138	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	265	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	4261	0	4165	77	0
2	B	38	0	34	0	0
2	C	38	0	34	3	0
3	A	2	0	0	0	1
4	A	10	0	0	2	0
5	A	18	0	24	3	0
6	A	3	0	0	1	0
7	A	10	0	10	2	0
8	A	56	0	52	1	0
9	A	356	0	0	12	0
All	All	4792	0	4319	81	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 9.

All (81) 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:4:ILE:N	1:A:4:ILE:HD12	1.79	0.96
6:A:1536:CL:CL	9:A:2230:HOH:O	2.20	0.95
1:A:381:ARG:HH11	1:A:384:GLN:HE22	1.18	0.92
4:A:1531:SO4:O2	9:A:2269:HOH:O	1.93	0.87
1:A:518:GLN:H	1:A:518:GLN:HE21	1.28	0.81
1:A:281:PRO:HG3	2:C:1:NAG:H83	1.66	0.77
1:A:496:THR:N	9:A:2317:HOH:O	2.03	0.76
1:A:376:TRP:O	9:A:2241:HOH:O	2.05	0.73
1:A:44:LYS:HE3	9:A:2030:HOH:O	1.91	0.70
1:A:50:THR:O	1:A:51:LYS:HB3	1.92	0.70
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.75	0.68
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.29	0.68
1:A:495:SER:HA	9:A:2317:HOH:O	1.93	0.67
1:A:242:ARG:HH12	5:A:1540:GOL:H31	1.62	0.65
1:A:381:ARG:HH11	1:A:384:GLN:NE2	1.93	0.64
1:A:516:ALA:O	1:A:520:ARG:HG3	1.98	0.64
1:A:4:ILE:N	1:A:4:ILE:CD1	2.54	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:O	1:A:384:GLN:HG2	1.98	0.63
2:C:2:NAG:H2	2:C:3:FUL:O2	1.98	0.63
1:A:4:ILE:H	1:A:4:ILE:HD12	1.62	0.63
1:A:281:PRO:HG3	2:C:1:NAG:C8	2.29	0.62
1:A:381:ARG:NH1	1:A:384:GLN:HE22	1.93	0.61
1:A:495:SER:CA	9:A:2317:HOH:O	2.48	0.60
1:A:262:LYS:NZ	9:A:2179:HOH:O	2.35	0.59
1:A:209:LEU:HD12	1:A:312:PHE:HB3	1.83	0.59
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.85	0.59
1:A:501:LEU:HD11	1:A:508:THR:HG23	1.84	0.59
1:A:304:ASP:HB3	9:A:2086:HOH:O	2.02	0.58
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.40	0.57
1:A:53:SER:O	1:A:54:ASP:CG	2.43	0.57
1:A:378:ASP:O	1:A:379:ASP:C	2.42	0.56
1:A:131:LYS:HD3	5:A:1533:GOL:H32	1.87	0.56
1:A:319:VAL:O	1:A:418:PHE:HA	2.06	0.55
8:A:1545:NAG:C6	9:A:2348:HOH:O	2.54	0.55
1:A:522:TRP:O	1:A:527:PRO:HD3	2.07	0.54
1:A:524:SER:O	1:A:528:LYS:HE3	2.08	0.53
1:A:384:GLN:HE21	1:A:384:GLN:HA	1.74	0.53
1:A:198:SBG:HA	1:A:224:SER:O	2.09	0.53
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.73	0.52
1:A:227:PHE:CD1	1:A:227:PHE:C	2.82	0.52
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.39	0.52
1:A:378:ASP:O	1:A:379:ASP:O	2.28	0.51
1:A:117:GLY:H	1:A:198:SBG:H1	1.57	0.51
1:A:282:TYR:CD1	1:A:359:PRO:HB2	2.46	0.50
1:A:383:GLU:O	1:A:387:GLU:HG3	2.11	0.50
1:A:378:ASP:O	1:A:380:GLN:NE2	2.45	0.49
1:A:45:LYS:NZ	5:A:1532:GOL:H12	2.27	0.49
1:A:381:ARG:NH1	1:A:384:GLN:NE2	2.56	0.49
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.44	0.47
1:A:45:LYS:NZ	1:A:297:ASP:OD2	2.43	0.47
1:A:54:ASP:C	1:A:54:ASP:OD1	2.53	0.47
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.50	0.46
1:A:116:GLY:HA2	7:A:1535:FP1:HB	1.97	0.46
1:A:268:ASP:OD1	1:A:268:ASP:N	2.40	0.46
1:A:495:SER:O	1:A:496:THR:OG1	2.27	0.46
1:A:492:VAL:CG2	1:A:494:LYS:HE3	2.47	0.45
1:A:476:LYS:NZ	9:A:2122:HOH:O	2.48	0.45
1:A:176[B]:GLN:HG3	1:A:180:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.52	0.44
1:A:378:ASP:C	1:A:379:ASP:O	2.53	0.44
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.52	0.44
1:A:505:THR:HB	9:A:2273:HOH:O	2.18	0.44
1:A:34:ALA:HB2	1:A:173:LEU:HD23	2.00	0.44
1:A:318:LEU:HD23	1:A:318:LEU:C	2.38	0.43
1:A:84:PRO:HG2	1:A:88:LEU:HD21	1.99	0.43
1:A:3:ASP:C	1:A:4:ILE:HD12	2.35	0.43
1:A:377:VAL:HA	1:A:378:ASP:HB2	2.01	0.43
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.72	0.42
1:A:328:ALA:HA	1:A:434:MET:HE3	2.01	0.42
1:A:197:GLU:OE1	7:A:1535:FP1:H3	2.19	0.42
1:A:526:PHE:N	1:A:527:PRO:CD	2.83	0.42
1:A:515:ARG:N	4:A:1531:SO4:O1	2.53	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.55	0.42
1:A:414[B]:ASN:H	1:A:414[B]:ASN:ND2	2.18	0.41
1:A:51:LYS:HG2	1:A:52:TRP:N	2.35	0.41
1:A:526:PHE:O	1:A:529:VAL:HB	2.21	0.41
1:A:417:PHE:CE2	1:A:492:VAL:HG12	2.55	0.41
1:A:525:PHE:CZ	1:A:529:VAL:HG23	2.56	0.41
1:A:370:LEU:HD13	1:A:370:LEU:C	2.41	0.41
1:A:434:MET:HE2	1:A:437:MET:CE	2.52	0.41
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	2.04	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)
3:A:1538:K:K	3:A:1538:K:K[5_555]	1.93	0.27

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	534/527 (101%)	508 (95%)	22 (4%)	4 (1%)	22 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	379	ASP
1	A	496	THR
1	A	54	ASP

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	461/451 (102%)	432 (94%)	29 (6%)	18 28

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	17	GLN
1	A	51	LYS
1	A	69	ILE
1	A	195	PHE
1	A	219	ARG
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	280	VAL
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	299	LEU
1	A	367[A]	GLU

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Mol	Chain	Res	Type
1	A	367[B]	GLU
1	A	384	GLN
1	A	422	GLU
1	A	428	LEU
1	A	454	ASP
1	A	455[A]	GLN
1	A	455[B]	GLN
1	A	471	TRP
1	A	495	SER
1	A	505	THR
1	A	508	THR
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	275	ASN
1	A	380	GLN
1	A	384	GLN
1	A	518	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	SBG	A	198	1	8,9,10	2.74	3 (37%)	5,12,14	3.42	3 (60%)

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
1	SBG	A	198	1	-	2/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SBG	P1-OG	6.68	1.67	1.57
1	A	198	SBG	P1-O2	2.38	1.54	1.50
1	A	198	SBG	P1-C1	-2.03	1.72	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SBG	OG-P1-O2	-5.64	93.99	111.76
1	A	198	SBG	OG-CB-CA	4.45	112.48	108.14
1	A	198	SBG	OG-P1-C1	2.08	110.96	105.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SBG	N-CA-CB-OG
1	A	198	SBG	CB-OG-P1-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SBG	2	0

5.5 Carbohydrates (i)

6 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	B	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	2.30	7 (41%)
2	NAG	B	2	2	14,14,15	0.72	0	17,19,21	2.09	5 (29%)
2	FUL	B	3	2	10,10,11	1.22	0	14,14,16	2.67	5 (35%)
2	NAG	C	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	2.01	6 (35%)
2	NAG	C	2	2	14,14,15	0.99	1 (7%)	17,19,21	1.95	3 (17%)
2	FUL	C	3	2	10,10,11	0.94	0	14,14,16	2.01	4 (28%)

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	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
2	NAG	C	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	FUL	C	3	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.43	1.39	1.43
2	C	2	NAG	C1-C2	2.05	1.55	1.52
2	C	1	NAG	C1-C2	2.03	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	FUL	O5-C1-C2	-5.22	102.71	110.77
2	C	2	NAG	C1-O5-C5	4.84	118.75	112.19
2	C	2	NAG	C2-N2-C7	4.81	129.75	122.90
2	B	1	NAG	C2-N2-C7	4.58	129.43	122.90
2	B	1	NAG	C8-C7-N2	4.42	123.59	116.10
2	B	2	NAG	C4-C3-C2	4.28	117.30	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	FUL	C1-O5-C5	-4.26	103.12	112.78
2	B	3	FUL	C3-C4-C5	4.07	116.12	109.77
2	B	3	FUL	C1-O5-C5	-4.00	103.72	112.78
2	C	1	NAG	C1-O5-C5	3.94	117.53	112.19
2	B	3	FUL	C6-C5-C4	3.86	120.21	113.07
2	B	3	FUL	C1-C2-C3	-3.74	105.06	109.67
2	C	3	FUL	C3-C4-C5	3.70	115.53	109.77
2	B	1	NAG	C1-C2-N2	-3.68	104.20	110.49
2	C	1	NAG	C8-C7-N2	3.66	122.30	116.10
2	B	2	NAG	C3-C4-C5	3.33	116.18	110.24
2	C	1	NAG	O7-C7-C8	-3.33	115.88	122.06
2	B	2	NAG	O7-C7-C8	-3.24	116.05	122.06
2	B	1	NAG	O5-C5-C6	2.99	111.88	107.20
2	C	3	FUL	C1-C2-C3	-2.91	106.08	109.67
2	B	2	NAG	O5-C5-C6	2.84	111.65	107.20
2	C	1	NAG	C2-N2-C7	2.81	126.90	122.90
2	B	1	NAG	O7-C7-C8	-2.75	116.94	122.06
2	B	2	NAG	C1-C2-N2	2.74	115.18	110.49
2	C	3	FUL	O5-C5-C6	2.42	112.54	107.33
2	C	1	NAG	C3-C4-C5	-2.42	105.92	110.24
2	C	2	NAG	C3-C4-C5	2.28	114.30	110.24
2	B	1	NAG	O6-C6-C5	2.22	118.91	111.29
2	B	1	NAG	O4-C4-C5	-2.16	103.93	109.30
2	C	1	NAG	O4-C4-C5	2.04	114.36	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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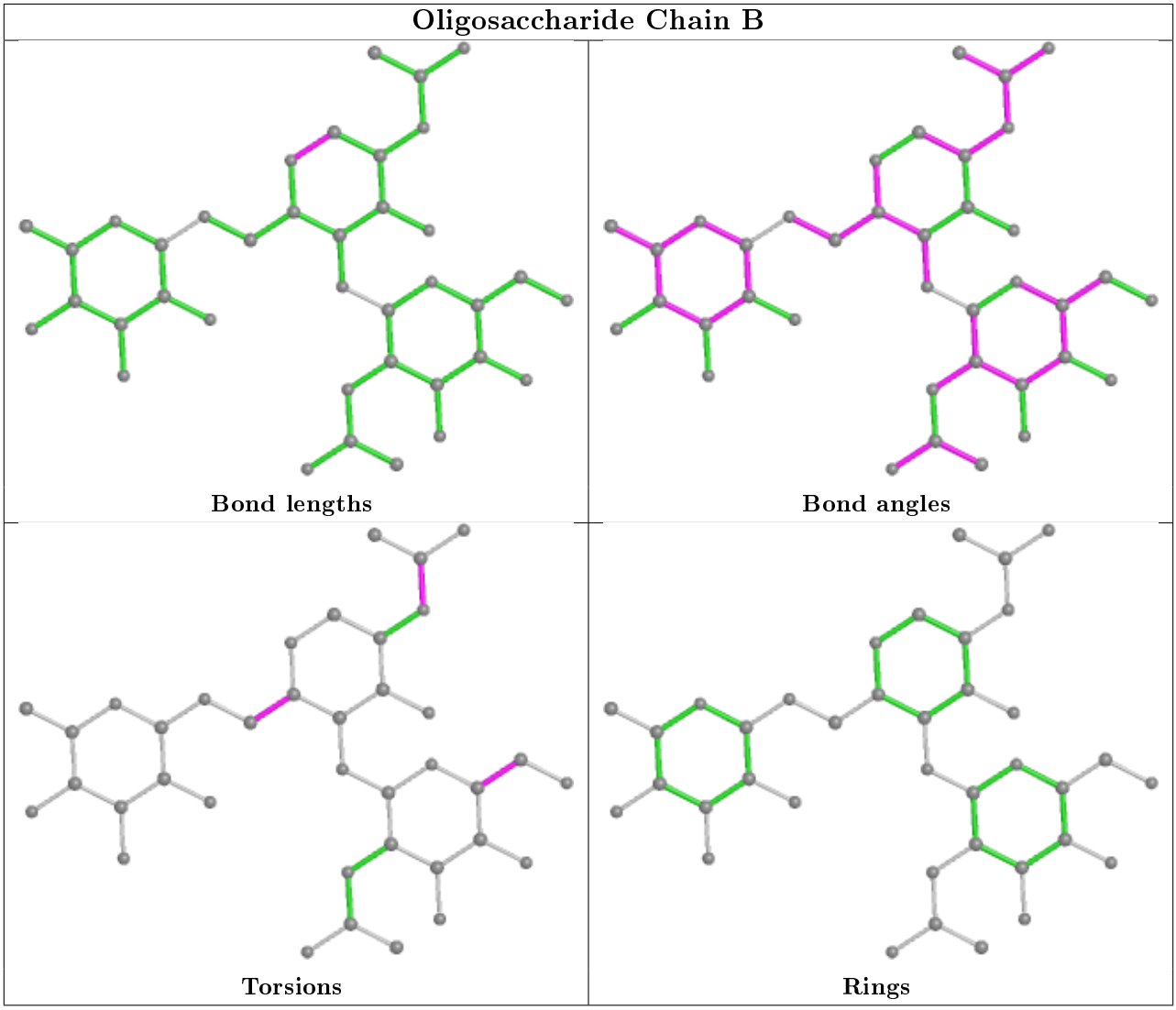
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

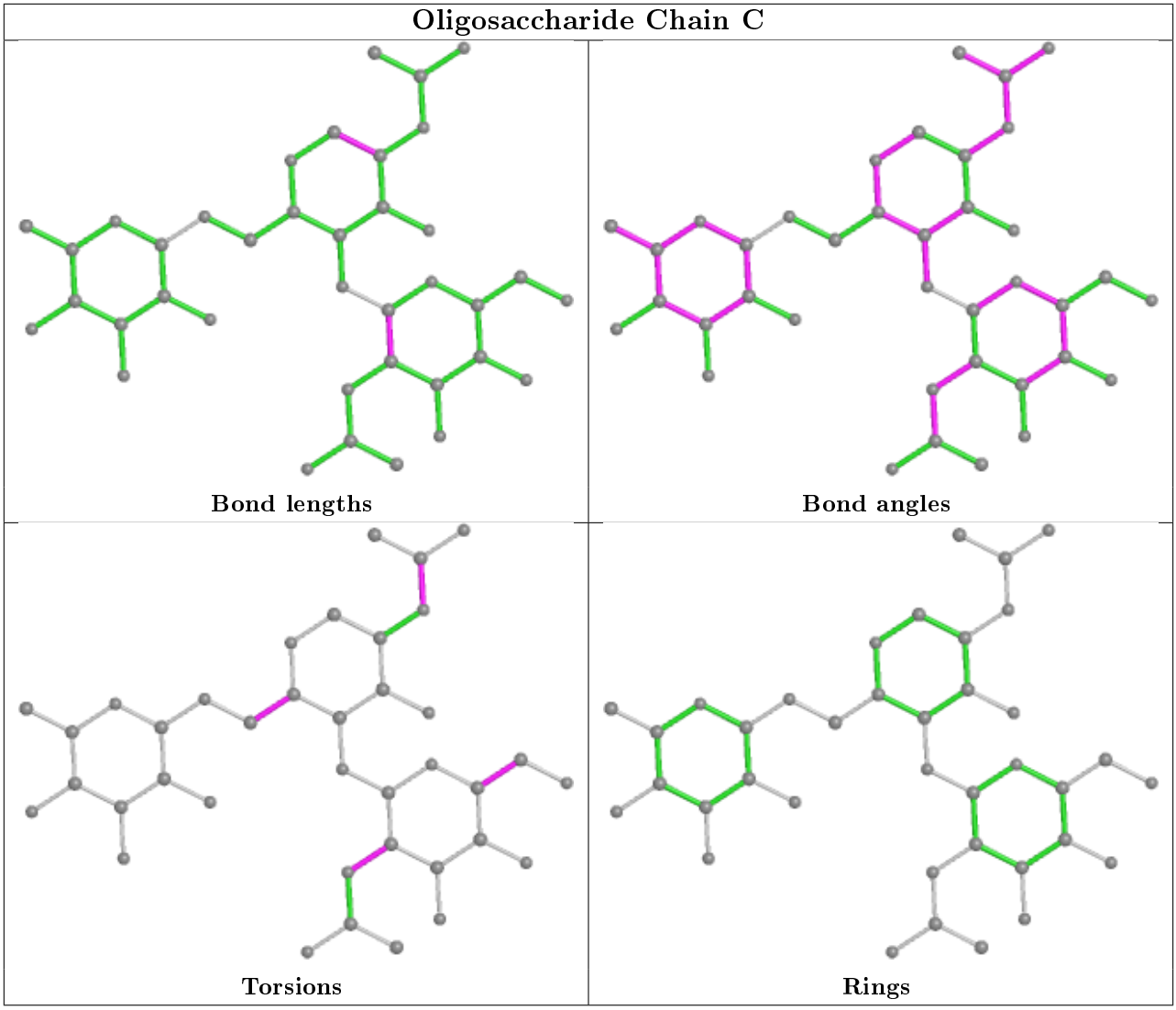
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUL	1	0
2	C	2	NAG	1	0
2	C	1	NAG	2	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

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	A	1533	-	5,5,5	0.32	0	5,5,5	1.52	1 (20%)
4	SO4	A	1531	-	4,4,4	0.39	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	1547	1	14,14,15	0.79	0	17,19,21	1.59	1 (5%)
7	FP1	A	1535	-	8,10,10	2.17	4 (50%)	9,12,12	3.30	3 (33%)
8	NAG	A	1545	1	14,14,15	0.77	0	17,19,21	2.66	6 (35%)
4	SO4	A	1539	-	4,4,4	0.16	0	6,6,6	0.42	0
5	GOL	A	1532	-	5,5,5	0.41	0	5,5,5	0.78	0
8	NAG	A	1546	1	14,14,15	0.73	0	17,19,21	2.79	6 (35%)
8	NAG	A	1544	1	14,14,15	1.10	1 (7%)	17,19,21	2.02	4 (23%)
5	GOL	A	1540	-	5,5,5	0.57	0	5,5,5	0.34	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
5	GOL	A	1533	-	-	2/4/4/4	-
8	NAG	A	1547	1	-	0/6/23/26	0/1/1/1
7	FP1	A	1535	-	-	0/0/3/3	0/1/1/1
8	NAG	A	1545	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1532	-	-	4/4/4/4	-
8	NAG	A	1546	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1544	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1540	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1535	FP1	C5-N1	-4.23	1.35	1.40
7	A	1535	FP1	C6-N2	3.04	1.34	1.30
8	A	1544	NAG	C1-C2	2.98	1.56	1.52
7	A	1535	FP1	C1-N1	2.33	1.40	1.33
7	A	1535	FP1	C7-N1	2.08	1.57	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1546	NAG	C1-O5-C5	8.94	124.31	112.19
7	A	1535	FP1	C5-C6-N2	-7.39	112.48	126.88
8	A	1545	NAG	C1-O5-C5	6.10	120.45	112.19
8	A	1547	NAG	O5-C5-C6	5.06	115.14	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1545	NAG	O5-C5-C6	4.88	114.86	107.20
7	A	1535	FP1	C4-C5-N1	4.52	121.47	117.46
7	A	1535	FP1	C1-N1-C5	-4.36	117.17	121.63
8	A	1544	NAG	C2-N2-C7	4.24	128.94	122.90
8	A	1545	NAG	C6-C5-C4	-3.85	103.98	113.00
8	A	1544	NAG	C8-C7-N2	3.74	122.43	116.10
8	A	1545	NAG	O5-C1-C2	-3.58	105.64	111.29
8	A	1546	NAG	O5-C5-C6	3.47	112.64	107.20
8	A	1546	NAG	O5-C1-C2	3.40	116.66	111.29
8	A	1544	NAG	O4-C4-C5	3.15	117.12	109.30
8	A	1546	NAG	C3-C4-C5	3.02	115.63	110.24
8	A	1544	NAG	C1-O5-C5	2.87	116.08	112.19
8	A	1545	NAG	C1-C2-N2	2.76	115.20	110.49
8	A	1545	NAG	C8-C7-N2	2.63	120.56	116.10
5	A	1533	GOL	C3-C2-C1	-2.46	102.15	111.70
8	A	1546	NAG	O7-C7-N2	2.13	125.87	121.95
8	A	1546	NAG	O7-C7-C8	-2.05	118.26	122.06

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1540	GOL	C1-C2-C3-O3
5	A	1540	GOL	O2-C2-C3-O3
8	A	1545	NAG	C8-C7-N2-C2
8	A	1545	NAG	O7-C7-N2-C2
8	A	1544	NAG	C8-C7-N2-C2
8	A	1544	NAG	O7-C7-N2-C2
5	A	1533	GOL	C1-C2-C3-O3
5	A	1540	GOL	O1-C1-C2-C3
5	A	1532	GOL	O2-C2-C3-O3
5	A	1532	GOL	O1-C1-C2-O2
5	A	1532	GOL	O1-C1-C2-C3
5	A	1532	GOL	C1-C2-C3-O3
5	A	1533	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1533	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1531	SO4	2	0
7	A	1535	FP1	2	0
8	A	1545	NAG	1	0
5	A	1532	GOL	1	0
5	A	1540	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	526/527 (99%)	-0.37	16 (3%) 50 49	18, 33, 62, 80	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.2
1	A	378	ASP	3.5
1	A	55	ILE	3.4
1	A	54	ASP	3.3
1	A	453	ARG	3.2
1	A	255	GLU	3.0
1	A	379	ASP	2.9
1	A	53	SER	2.9
1	A	50	THR	2.8
1	A	52	TRP	2.8
1	A	377	VAL	2.8
1	A	237	TYR	2.7
1	A	51	LYS	2.6
1	A	4	ILE	2.5
1	A	455[A]	GLN	2.4
1	A	452	ARG	2.2

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

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SBG	A	198	10/11	0.99	0.13	11,18,22,22	0

6.3 Carbohydrates (i)

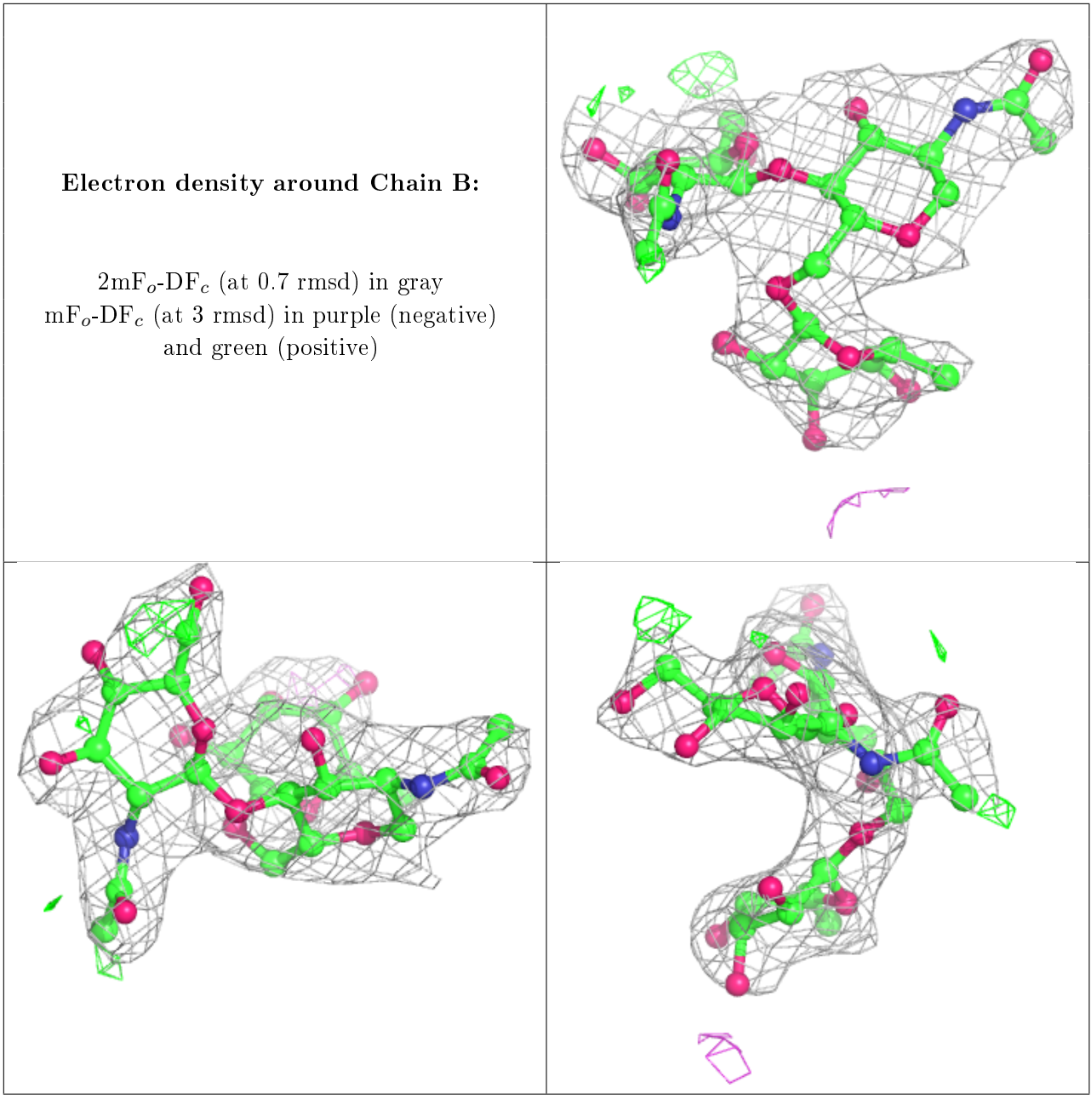
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.44	0.50	98,104,107,108	0
2	NAG	C	1	14/15	0.86	0.24	70,80,85,90	0
2	NAG	B	2	14/15	0.87	0.16	69,73,77,79	0
2	FUL	B	3	10/11	0.89	0.26	71,76,77,77	0
2	FUL	C	3	10/11	0.94	0.30	77,79,80,80	0
2	NAG	B	1	14/15	0.96	0.14	42,53,63,68	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.

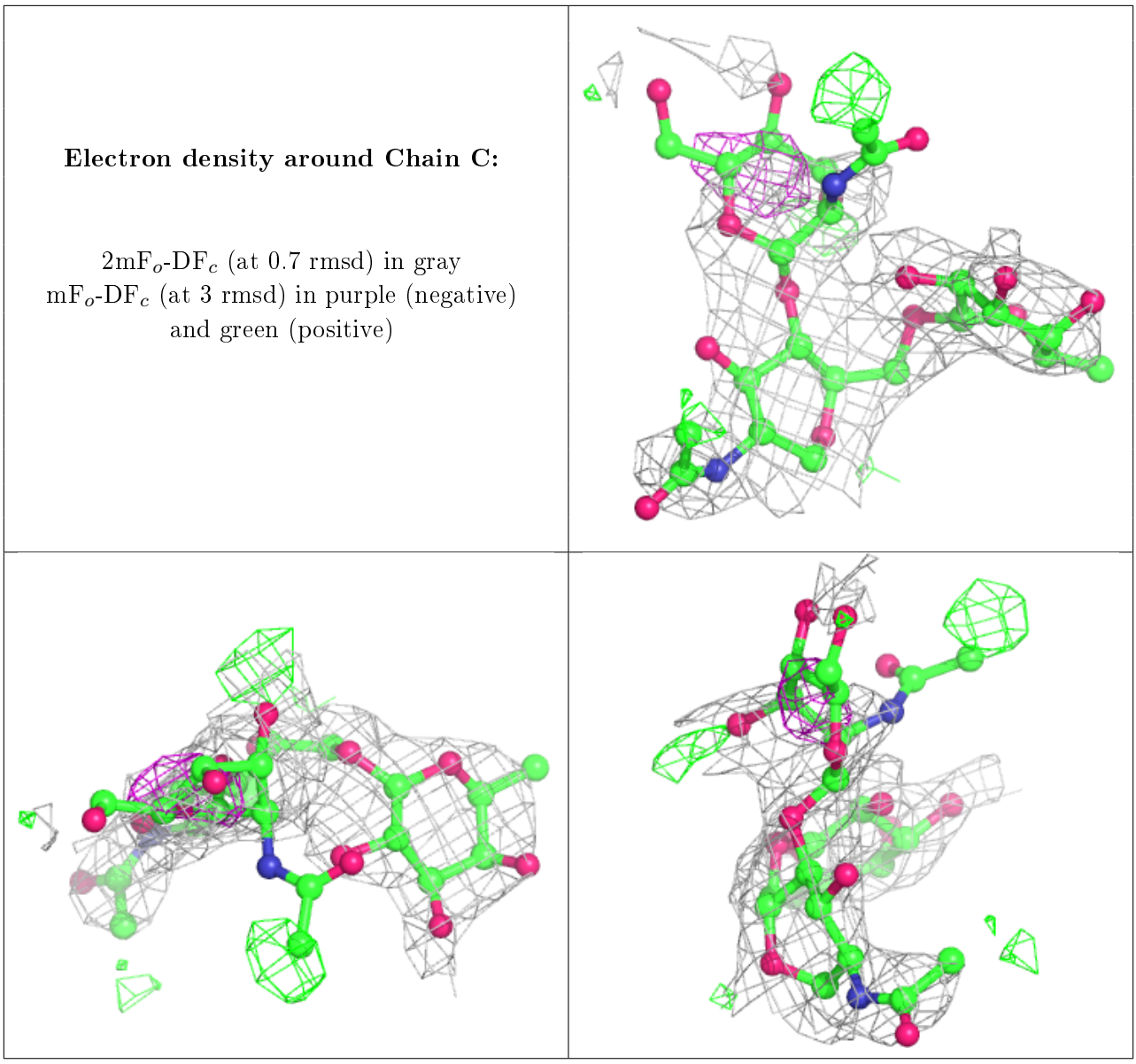
Electron density around Chain B:

$2mF_o$-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 C:

$2mF_o$-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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	1532	6/6	0.75	0.17	74,75,76,76	0
8	NAG	A	1546	14/15	0.76	0.23	60,73,80,81	0
8	NAG	A	1544	14/15	0.79	0.21	59,65,68,69	0
8	NAG	A	1545	14/15	0.81	0.29	66,72,77,79	0
8	NAG	A	1547	14/15	0.83	0.37	77,84,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	FP1	A	1535	10/10	0.84	0.27	50,56,57,59	0
4	SO4	A	1531	5/5	0.86	0.22	76,77,79,80	0
5	GOL	A	1533	6/6	0.89	0.21	47,54,55,56	0
6	CL	A	1537	1/1	0.89	0.15	73,73,73,73	0
5	GOL	A	1540	6/6	0.92	0.24	44,52,56,58	0
3	K	A	1538	1/1	0.94	0.25	112,112,112,112	0
6	CL	A	1534	1/1	0.95	0.22	52,52,52,52	0
4	SO4	A	1539	5/5	0.95	0.15	94,94,94,95	0
6	CL	A	1536	1/1	0.97	0.05	80,80,80,80	0
3	K	A	1530	1/1	0.98	0.14	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.