Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:57 PM EDT

PDB ID	:	1XLV
Title	:	Ethylphosphorylated Butyrylcholinesterase (Aged) Obtained By Reaction With Echothiophate
Authors	:	Nachon, F.; Asojo, O.A.; Borgstahl, G.E.O.; Masson, P.; Lockridge, O.
Deposited on	:	2004-09-30
Resolution	:	2.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

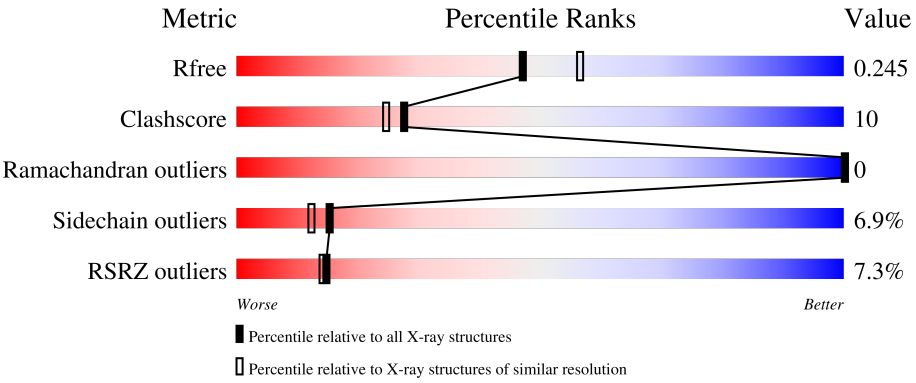
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	529	7%, 76%, 20%
2	B	3	33%, 67%
3	C	2	100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4676 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.

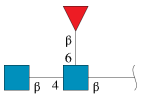
- Molecule 1 is a protein called BUTYRYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	11	0
			4286	2765	723	781	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

- 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.

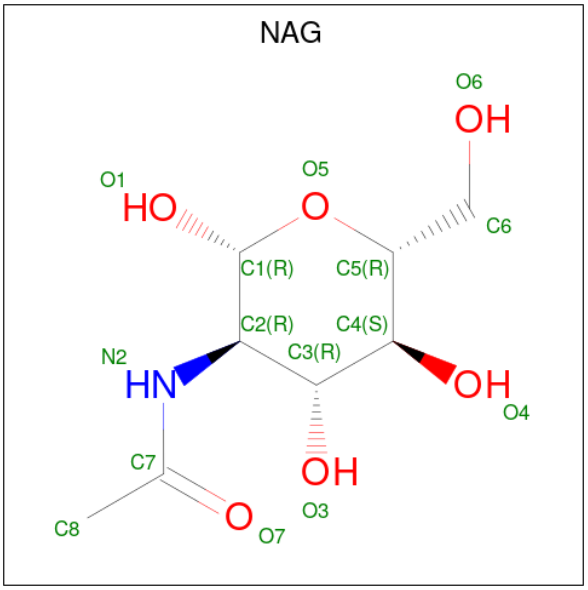


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

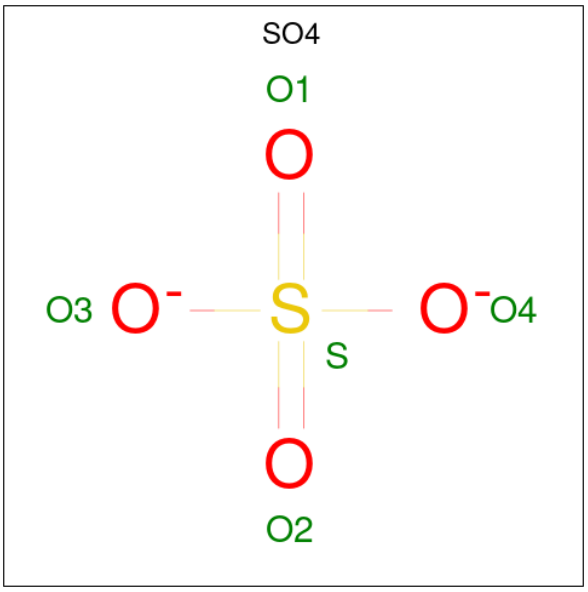
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	2	Total C N O 28 16 2 10	0	0	0

- 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 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

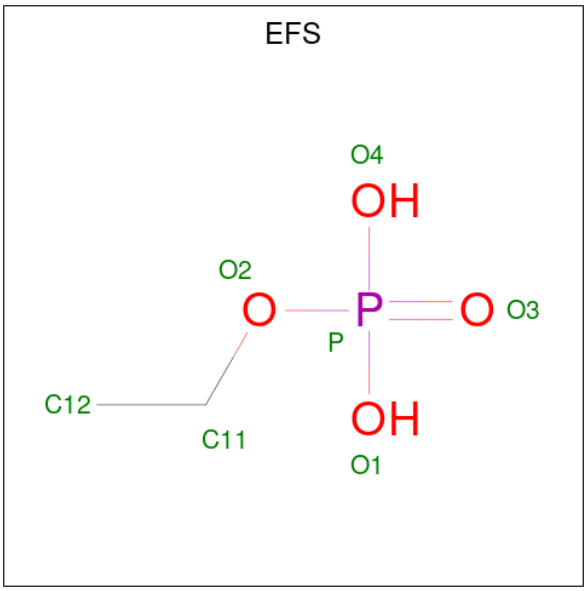


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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

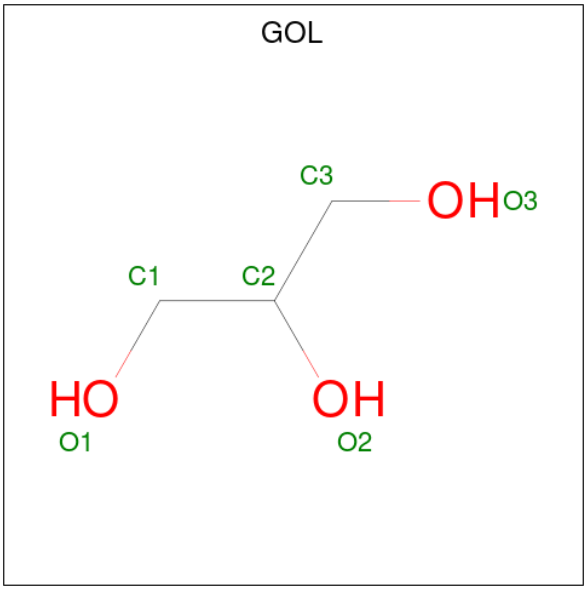
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0

- Molecule 7 is ETHYL DIHYDROGEN PHOSPHATE (three-letter code: EFS) (formula: $C_2H_7O_4P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 6 2 3 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 9 is water.

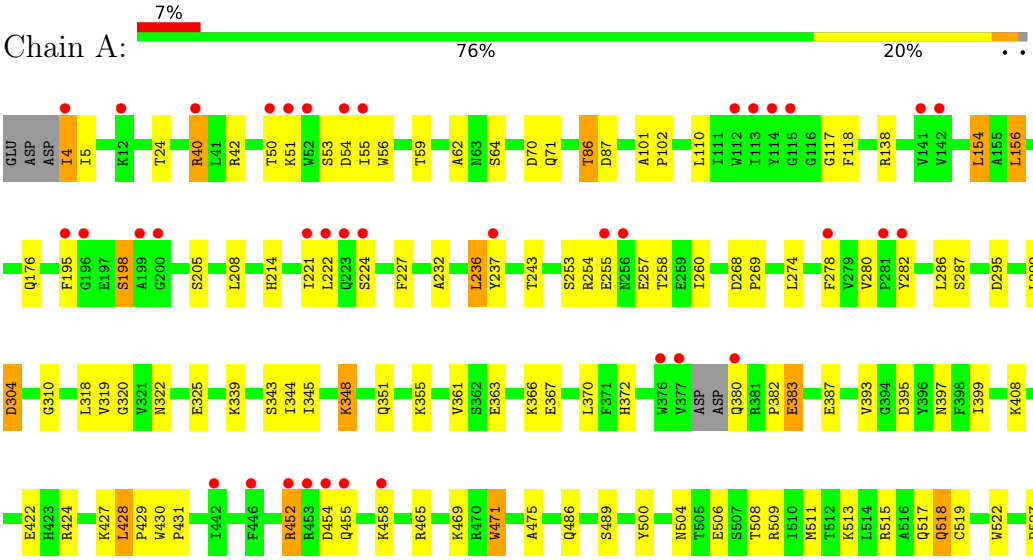
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	220	Total	O	0	0
			220	220		

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: BUTYRYLCHOLINESTERASE

Chain A:

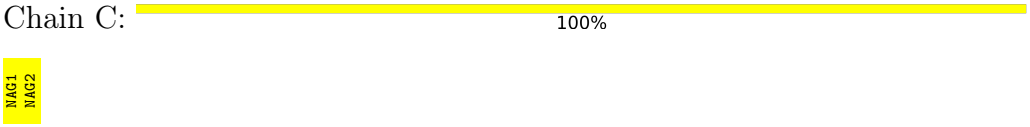


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	154.59Å 154.59Å 126.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.25 30.34 – 2.25	Depositor EDS
% Data completeness (in resolution range)	78.2 (40.00-2.25) 78.2 (30.34-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.183 , 0.247 0.181 , 0.245	Depositor DCC
R_{free} test set	1596 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4676	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: CL, EFS, NAG, FUL, GOL, CSS, SO4

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	0.87	1/4400 (0.0%)	0.88	11/5968 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TRP	CB-CG	5.10	1.59	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ASP	CB-CG-OD2	7.26	124.84	118.30
1	A	395	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	465	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	301	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	295	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	87[A]	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	87[B]	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	268	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	465	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	304	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	198	SER	CA-CB-OG	5.02	124.75	111.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4286	0	4163	87	0
2	B	38	0	34	3	0
3	C	28	0	25	0	0
4	A	56	0	52	1	0
5	A	15	0	0	0	0
6	A	3	0	0	0	0
7	A	6	0	5	1	0
8	A	24	0	32	2	0
9	A	220	0	0	14	0
All	All	4676	0	4311	88	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 10.

All (88) 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:508:THR:HG22	9:A:1171:HOH:O	1.53	1.09
1:A:408:LYS:HE3	9:A:1265:HOH:O	1.55	1.05
1:A:518:GLN:HE21	1:A:518:GLN:H	0.92	0.88
1:A:62:ALA:O	1:A:86:THR:HG21	1.74	0.88
1:A:518:GLN:H	1:A:518:GLN:NE2	1.73	0.87
1:A:71:GLN:HG2	9:A:1223:HOH:O	1.84	0.77
1:A:518:GLN:HE21	1:A:518:GLN:N	1.77	0.71
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.71	0.71
1:A:427:LYS:C	8:A:607:GOL:H32	2.13	0.69
1:A:452:ARG:HH22	1:A:458:LYS:HA	1.56	0.69
1:A:304:ASP:HB3	9:A:1242:HOH:O	1.94	0.68
1:A:257:GLU:HA	1:A:260:ILE:HD12	1.76	0.67
1:A:253:SER:O	1:A:254:ARG:HD3	1.96	0.66
1:A:159:ASN:OD1	1:A:161:GLU:HB2	1.96	0.65
1:A:236:LEU:HB2	9:A:1281:HOH:O	1.96	0.65
1:A:522:TRP:O	1:A:527:PRO:HD3	1.96	0.65
1:A:62:ALA:O	1:A:86:THR:CG2	2.46	0.64
1:A:254:ARG:HB2	1:A:260:ILE:HG13	1.79	0.62
1:A:452:ARG:NH2	1:A:458:LYS:HA	2.14	0.61
1:A:237:TYR:HE1	2:B:1:NAG:H83	1.66	0.61
1:A:64:SER:H	1:A:86:THR:HG22	1.67	0.59
1:A:383:GLU:CD	1:A:383:GLU:H	2.07	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLU:HG2	1:A:258:THR:HG23	1.86	0.58
1:A:221:ILE:HG23	1:A:318:LEU:HD22	1.86	0.57
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.39	0.57
1:A:5:ILE:HG12	1:A:55:ILE:HD13	1.85	0.57
1:A:361:VAL:O	1:A:366:LYS:HE2	2.05	0.56
1:A:339:LYS:O	1:A:431:PRO:HG3	2.06	0.55
1:A:227[B]:PHE:CE2	1:A:303:PRO:HB2	2.42	0.55
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.38	0.54
1:A:383:GLU:O	1:A:387:GLU:HG3	2.08	0.53
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.89	0.52
1:A:4:ILE:HD12	1:A:4:ILE:N	2.25	0.52
1:A:319:VAL:O	1:A:418:PHE:HA	2.09	0.52
1:A:343:SER:O	1:A:345:ILE:HG23	2.10	0.51
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.92	0.51
1:A:278:PHE:O	2:B:3:FUL:H4	2.11	0.50
1:A:408:LYS:CD	9:A:1265:HOH:O	2.57	0.50
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.28	0.49
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.96	0.49
1:A:454:ASP:O	1:A:455:GLN:HB2	2.13	0.48
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.78	0.48
1:A:348:LYS:HE3	1:A:351:GLN:OE1	2.13	0.48
1:A:227[B]:PHE:CD2	1:A:303:PRO:HB2	2.48	0.48
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.48	0.48
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.49	0.48
1:A:393:VAL:O	1:A:397:ASN:HB2	2.14	0.47
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.95	0.47
1:A:515:ARG:HH21	1:A:515:ARG:HG2	1.78	0.47
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.49	0.47
1:A:348:LYS:HB2	9:A:1247:HOH:O	2.13	0.47
1:A:117:GLY:HA2	7:A:1001:EFS:H111	1.96	0.47
1:A:322:ASN:O	1:A:325:GLU:HG2	2.14	0.47
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.68	0.47
1:A:513:LYS:HD2	9:A:1275:HOH:O	2.14	0.46
1:A:399:ILE:HG21	1:A:515:ARG:HG3	1.97	0.46
1:A:51:LYS:HG2	9:A:1320:HOH:O	2.15	0.46
1:A:222:LEU:HD12	1:A:222:LEU:N	2.32	0.45
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.32	0.45
1:A:254:ARG:HB2	1:A:260:ILE:CG1	2.46	0.45
1:A:64:SER:N	1:A:86:THR:HG22	2.31	0.44
1:A:372[A]:HIS:CD2	9:A:1289:HOH:O	2.70	0.44
1:A:40:ARG:CZ	1:A:40:ARG:HB2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.53	0.44
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.81	0.44
1:A:214[A]:HIS:HE1	9:A:1203:HOH:O	2.01	0.44
1:A:24:THR:O	1:A:101:ALA:HB3	2.18	0.43
1:A:56:TRP:CD1	1:A:56:TRP:C	2.91	0.43
1:A:227[B]:PHE:O	1:A:232:ALA:HB3	2.19	0.43
1:A:198:SER:HA	1:A:224:SER:O	2.19	0.43
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.76	0.43
1:A:227[B]:PHE:CD2	1:A:227[B]:PHE:C	2.93	0.42
1:A:504:ASN:OD1	1:A:506:GLU:HG3	2.20	0.42
4:A:536:NAG:H83	4:A:536:NAG:H2	2.01	0.42
1:A:422:GLU:HG3	1:A:504:ASN:HB3	2.01	0.41
1:A:237:TYR:CE1	2:B:1:NAG:H83	2.51	0.41
1:A:154:LEU:HD23	1:A:162:ALA:HB1	2.02	0.41
1:A:519:CYS:HB3	9:A:1116:HOH:O	2.20	0.41
1:A:344:ILE:HD12	1:A:382:PRO:HB2	2.01	0.41
1:A:370:LEU:HD23	1:A:370:LEU:C	2.41	0.41
1:A:367[A]:GLU:OE1	1:A:370:LEU:HD22	2.21	0.41
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.99	0.41
1:A:101:ALA:HA	1:A:102:PRO:C	2.41	0.41
1:A:117:GLY:O	1:A:118:PHE:HB2	2.21	0.41
1:A:517:GLN:NE2	9:A:1254:HOH:O	2.53	0.40
1:A:427:LYS:HB2	8:A:607:GOL:H32	2.03	0.40
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.90	0.40
1:A:138[A]:ARG:NH1	9:A:1139:HOH:O	2.55	0.40

There are no symmetry-related clashes.

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	530/529 (100%)	505 (95%)	25 (5%)	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	459/453 (101%)	425 (93%)	34 (7%)	13 10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	40	ARG
1	A	50	THR
1	A	53	SER
1	A	54	ASP
1	A	59	THR
1	A	86	THR
1	A	154	LEU
1	A	156	LEU
1	A	161	GLU
1	A	176[A]	GLN
1	A	176[B]	GLN
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	274	LEU
1	A	280	VAL
1	A	282[A]	TYR
1	A	282[B]	TYR
1	A	286	LEU
1	A	287	SER
1	A	299	LEU
1	A	348	LYS
1	A	355	LYS
1	A	363[A]	GLU
1	A	363[B]	GLU
1	A	380	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	383	GLU
1	A	428	LEU
1	A	452	ARG
1	A	471	TRP
1	A	486	GLN
1	A	489	SER
1	A	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	GLN
1	A	71	GLN
1	A	119	GLN
1	A	172	GLN
1	A	270	GLN
1	A	311	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	CSS	A	66	1	4,6,7	0.70	0	1,6,8	0.36	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
1	CSS	A	66	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

5 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	2,1	14,14,15	0.64	0	17,19,21	1.30	3 (17%)
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	2.05	7 (41%)
2	FUL	B	3	2	10,10,11	0.97	0	14,14,16	2.61	6 (42%)
3	NAG	C	1	3,1	14,14,15	0.58	0	17,19,21	2.26	4 (23%)
3	NAG	C	2	3	14,14,15	0.78	0	17,19,21	2.21	5 (29%)

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	2,1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	FUL	C1-C2-C3	-7.00	101.06	109.67
3	C	2	NAG	C1-O5-C5	6.30	120.72	112.19
3	C	1	NAG	C2-N2-C7	6.20	131.73	122.90
3	C	1	NAG	C1-O5-C5	4.56	118.38	112.19
3	C	2	NAG	O5-C5-C6	4.26	113.88	107.20
2	B	2	NAG	C4-C3-C2	3.62	116.33	111.02
2	B	2	NAG	C3-C4-C5	3.32	116.16	110.24
2	B	2	NAG	C2-N2-C7	3.24	127.51	122.90
3	C	1	NAG	C8-C7-N2	3.19	121.50	116.10
2	B	2	NAG	C1-O5-C5	3.17	116.49	112.19
2	B	3	FUL	O5-C1-C2	-3.11	105.98	110.77
2	B	3	FUL	O4-C4-C5	2.73	115.71	109.67
2	B	3	FUL	C1-O5-C5	-2.58	106.92	112.78
2	B	1	NAG	C4-C3-C2	2.51	114.70	111.02
2	B	1	NAG	O5-C1-C2	-2.46	107.40	111.29
3	C	2	NAG	C4-C3-C2	2.46	114.63	111.02
2	B	2	NAG	O5-C5-C4	2.42	116.72	110.83
2	B	3	FUL	O3-C3-C4	2.38	115.86	110.35
3	C	2	NAG	O7-C7-C8	-2.29	117.80	122.06
2	B	3	FUL	O2-C2-C1	2.19	113.64	109.15
2	B	2	NAG	O7-C7-N2	2.12	125.84	121.95
3	C	1	NAG	O7-C7-C8	-2.09	118.18	122.06
2	B	1	NAG	C2-N2-C7	-2.09	119.93	122.90
2	B	2	NAG	O3-C3-C4	-2.03	105.66	110.35
3	C	2	NAG	C8-C7-N2	2.02	119.52	116.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

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	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

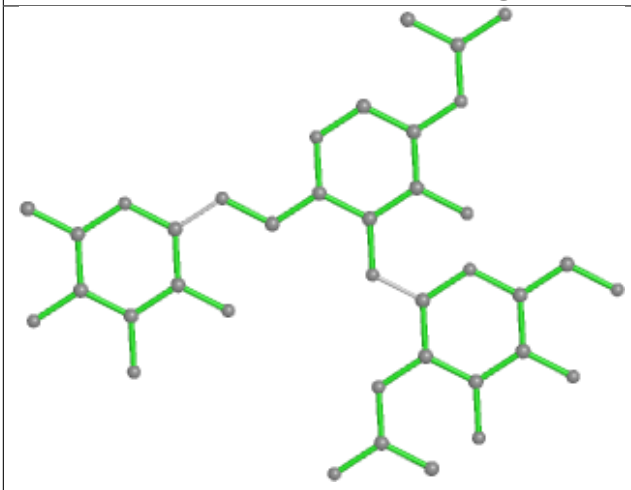
There are no ring outliers.

2 monomers are involved in 3 short contacts:

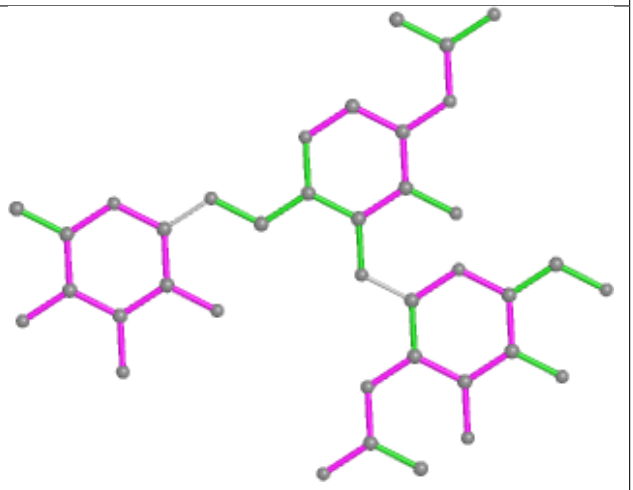
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	FUL	1	0
2	B	1	NAG	2	0

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

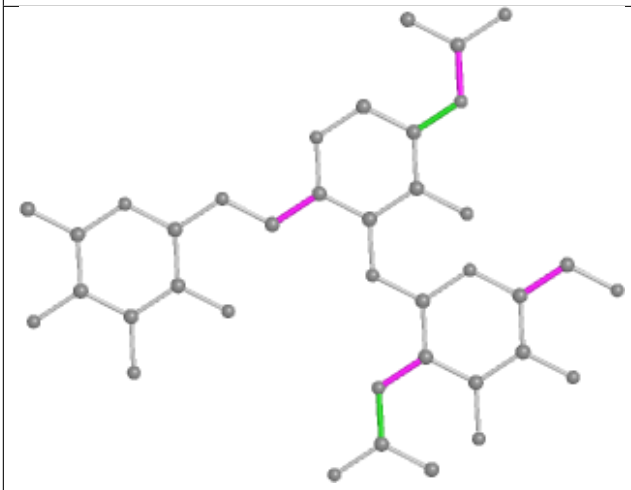
Oligosaccharide Chain B



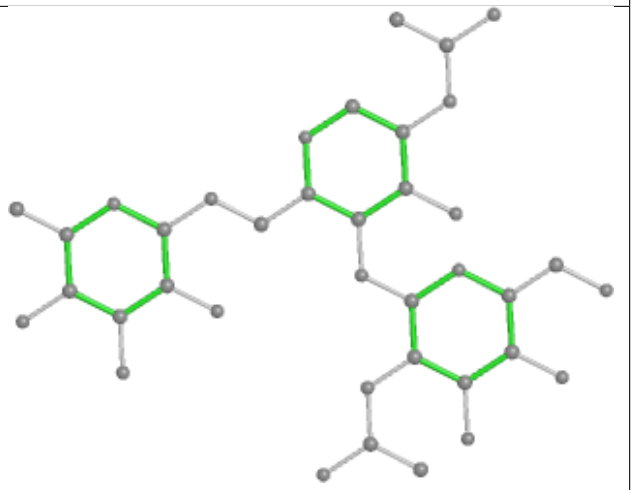
Bond lengths



Bond angles

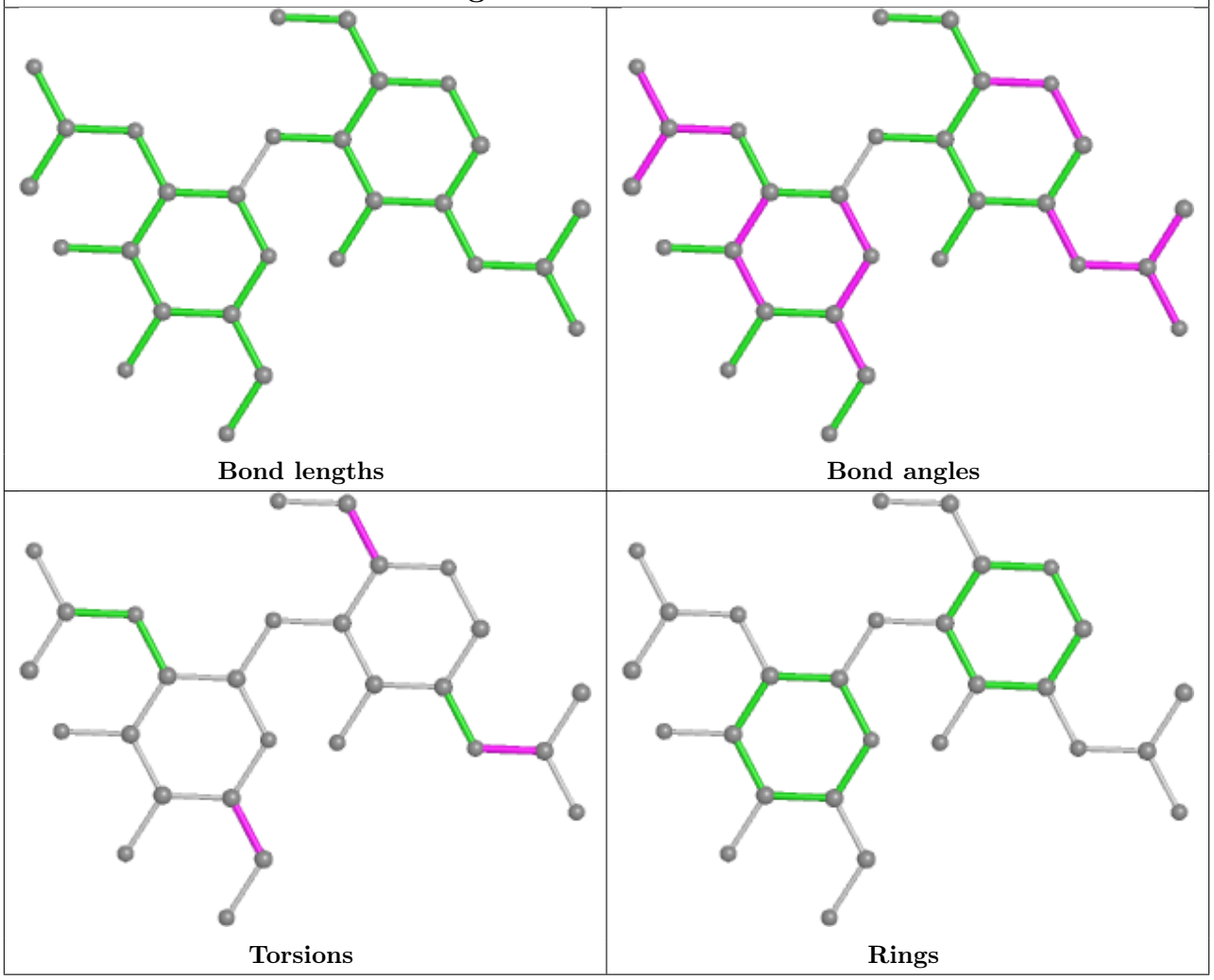


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
8	GOL	A	604	-	5,5,5	0.68	0	5,5,5	0.81	0
8	GOL	A	605	-	5,5,5	0.33	0	5,5,5	0.83	0
5	SO4	A	601	-	4,4,4	0.22	0	6,6,6	0.35	0
7	EFS	A	1001	1	2,5,6	1.04	0	0,5,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.23	0
5	SO4	A	602	-	4,4,4	0.27	0	6,6,6	0.30	0
4	NAG	A	536	1	14,14,15	0.66	0	17,19,21	2.07	6 (35%)
8	GOL	A	606	-	5,5,5	0.27	0	5,5,5	0.74	0
4	NAG	A	538	1	14,14,15	0.50	0	17,19,21	1.02	1 (5%)
4	NAG	A	537	1	14,14,15	0.78	0	17,19,21	1.91	5 (29%)
8	GOL	A	607	-	5,5,5	0.38	0	5,5,5	1.05	0
4	NAG	A	535	1	14,14,15	1.03	1 (7%)	17,19,21	1.82	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	604	-	-	2/4/4/4	-
8	GOL	A	605	-	-	0/4/4/4	-
7	EFS	A	1001	1	-	0/1/3/4	-
4	NAG	A	536	1	-	4/6/23/26	0/1/1/1
8	GOL	A	606	-	-	2/4/4/4	-
4	NAG	A	538	1	-	4/6/23/26	0/1/1/1
4	NAG	A	537	1	-	4/6/23/26	0/1/1/1
8	GOL	A	607	-	-	2/4/4/4	-
4	NAG	A	535	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	535	NAG	C1-C2	2.71	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	536	NAG	C1-O5-C5	4.90	118.83	112.19
4	A	536	NAG	O5-C1-C2	-4.23	104.60	111.29
4	A	537	NAG	C4-C3-C2	4.23	117.21	111.02
4	A	535	NAG	C2-N2-C7	4.09	128.73	122.90
4	A	537	NAG	C2-N2-C7	3.60	128.03	122.90
4	A	538	NAG	C1-O5-C5	3.28	116.63	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	535	NAG	C8-C7-N2	3.14	121.42	116.10
4	A	535	NAG	O7-C7-C8	-2.99	116.50	122.06
4	A	537	NAG	O7-C7-N2	2.95	127.37	121.95
4	A	537	NAG	C3-C4-C5	2.88	115.38	110.24
4	A	536	NAG	O7-C7-C8	-2.56	117.31	122.06
4	A	536	NAG	C8-C7-N2	2.33	120.04	116.10
4	A	535	NAG	O4-C4-C5	2.23	114.83	109.30
4	A	535	NAG	C1-O5-C5	2.20	115.17	112.19
4	A	535	NAG	C1-C2-N2	2.17	114.20	110.49
4	A	536	NAG	C3-C4-C5	2.12	114.02	110.24
4	A	537	NAG	O7-C7-C8	-2.04	118.26	122.06
4	A	536	NAG	O5-C5-C6	2.01	110.36	107.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	536	NAG	C8-C7-N2-C2
4	A	536	NAG	O7-C7-N2-C2
4	A	538	NAG	C8-C7-N2-C2
4	A	538	NAG	O7-C7-N2-C2
4	A	537	NAG	O5-C5-C6-O6
4	A	536	NAG	O5-C5-C6-O6
4	A	537	NAG	C4-C5-C6-O6
4	A	535	NAG	C8-C7-N2-C2
4	A	535	NAG	O7-C7-N2-C2
4	A	538	NAG	C4-C5-C6-O6
8	A	606	GOL	C1-C2-C3-O3
8	A	607	GOL	O1-C1-C2-C3
4	A	536	NAG	C4-C5-C6-O6
4	A	538	NAG	O5-C5-C6-O6
4	A	537	NAG	C8-C7-N2-C2
8	A	604	GOL	O2-C2-C3-O3
8	A	607	GOL	O1-C1-C2-O2
4	A	537	NAG	O7-C7-N2-C2
8	A	606	GOL	O2-C2-C3-O3
8	A	604	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	EFS	1	0
4	A	536	NAG	1	0
8	A	607	GOL	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^{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	523/529 (98%)	0.02	38 (7%)	15	14	31, 45, 66, 81	16 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282[A]	TYR	12.6
1	A	40	ARG	4.3
1	A	453	ARG	4.2
1	A	455	GLN	4.2
1	A	452	ARG	3.9
1	A	50	THR	3.6
1	A	55	ILE	3.6
1	A	237	TYR	3.6
1	A	255	GLU	3.5
1	A	380	GLN	3.4
1	A	442	ILE	3.4
1	A	52	TRP	3.2
1	A	51	LYS	3.2
1	A	195	PHE	3.1
1	A	115	GLY	3.0
1	A	196	GLY	3.0
1	A	221	ILE	3.0
1	A	256	ASN	3.0
1	A	112	TRP	3.0
1	A	4	ILE	2.9
1	A	113	ILE	2.9
1	A	377	VAL	2.8
1	A	54	ASP	2.7
1	A	278	PHE	2.6
1	A	200	GLY	2.6
1	A	224	SER	2.5
1	A	376	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	281	PRO	2.4
1	A	222	LEU	2.4
1	A	142	VAL	2.3
1	A	454	ASP	2.2
1	A	114	TYR	2.1
1	A	199	ALA	2.1
1	A	12	LYS	2.1
1	A	446	PHE	2.1
1	A	223	GLN	2.1
1	A	141	VAL	2.1
1	A	458	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSS	A	66	7/8	0.96	0.07	41,43,51,66	0

6.3 Carbohydrates (i)

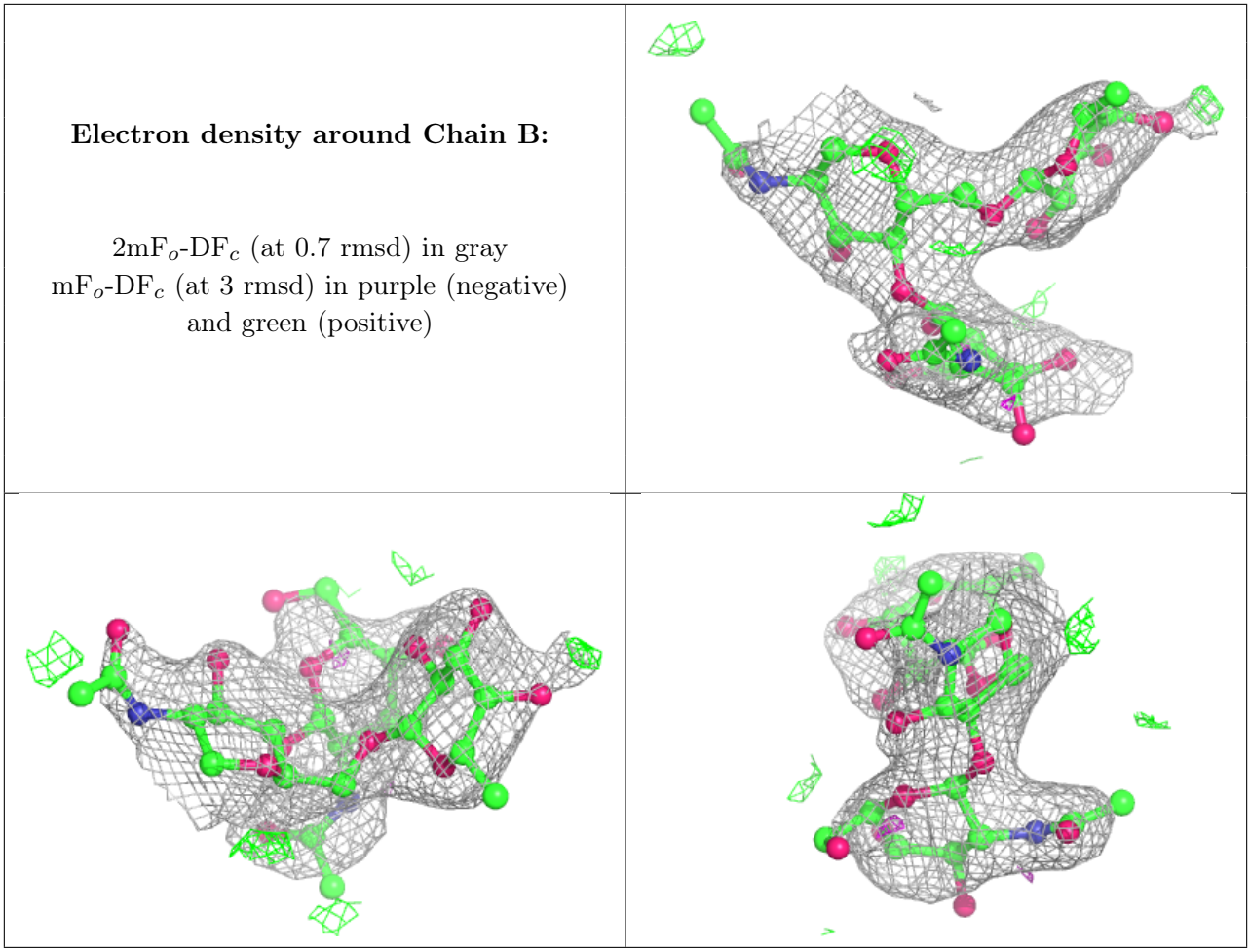
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	NAG	C	2	14/15	0.78	0.27	77,81,86,87	0
2	NAG	B	2	14/15	0.85	0.41	88,91,93,93	0
2	NAG	B	1	14/15	0.92	0.27	76,81,87,88	0
3	NAG	C	1	14/15	0.94	0.11	58,63,70,70	0
2	FUL	B	3	10/11	0.95	0.25	79,81,83,83	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.

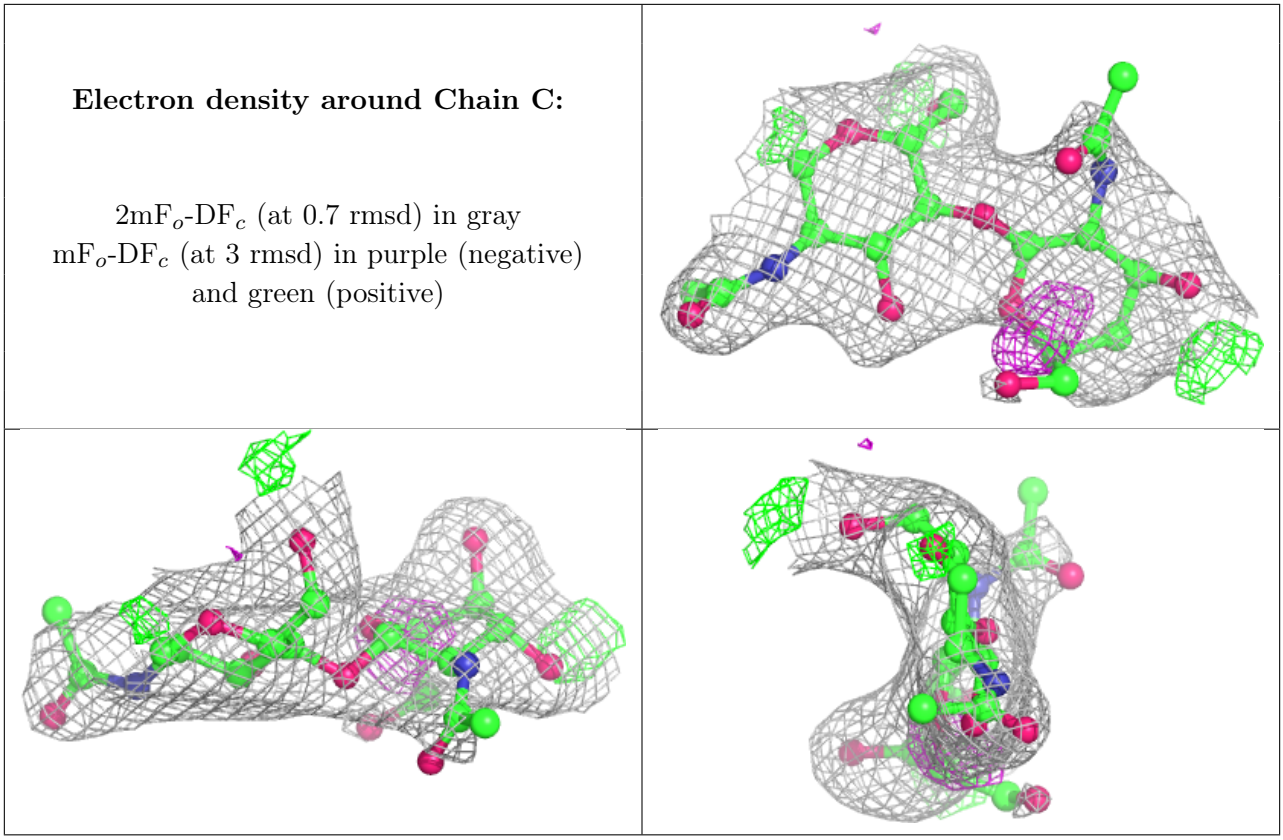
Electron density around Chain B:

$2mF_o$-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
4	NAG	A	536	14/15	0.77	0.32	82,86,87,88	0
4	NAG	A	535	14/15	0.87	0.25	68,73,74,74	0
4	NAG	A	537	14/15	0.87	0.23	64,75,78,79	5
4	NAG	A	538	14/15	0.91	0.30	78,81,83,84	10
8	GOL	A	604	6/6	0.92	0.16	56,60,63,65	0
6	CL	A	703	1/1	0.94	0.07	73,73,73,73	0
8	GOL	A	605	6/6	0.95	0.23	54,58,60,62	0
8	GOL	A	607	6/6	0.95	0.19	57,62,62,63	0
8	GOL	A	606	6/6	0.96	0.12	60,62,66,68	0
6	CL	A	701	1/1	0.96	0.14	74,74,74,74	0
6	CL	A	702	1/1	0.97	0.19	65,65,65,65	0
5	SO4	A	603	5/5	0.97	0.08	52,54,55,55	5
5	SO4	A	602	5/5	0.98	0.12	44,44,45,47	5
5	SO4	A	601	5/5	0.99	0.10	59,60,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EFS	A	1001	6/7	0.99	0.19	34,34,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.