



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 5YDH / pdb_00005ydh
Title : Crystal structure of acetylcholinesterase catalytic subunits of the malaria vector *Anopheles gambiae*, 3.2 Å
Authors : Han, Q.; Guan, H.; Robinson, H.; Ding, H.; Liao, C.; Li, J.
Deposited on : 2017-09-13
Resolution : 3.21 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

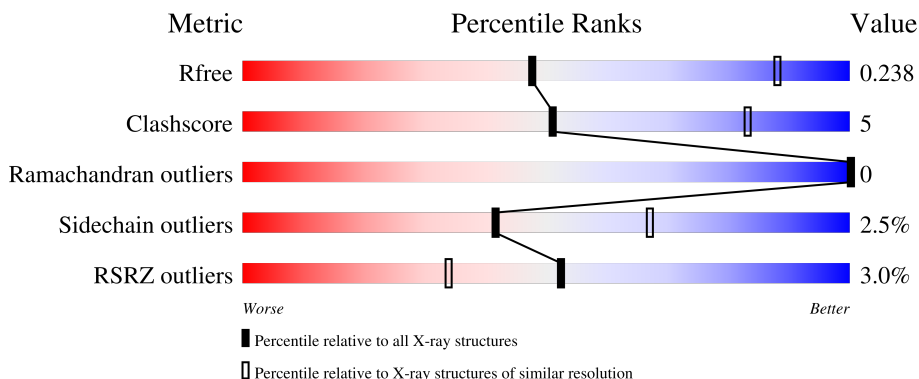
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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 $\leq 5\%$. 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	576	 2% 80% 14% 7%
1	B	576	 3% 78% 14% 7%
2	C	4	 25% 50% 25%
3	D	5	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8860 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.

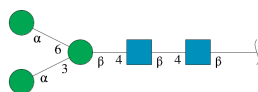
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4257	2711	743	790	13			
1	B	538	Total	C	N	O	S	0	0	0
			4257	2711	743	790	13			

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



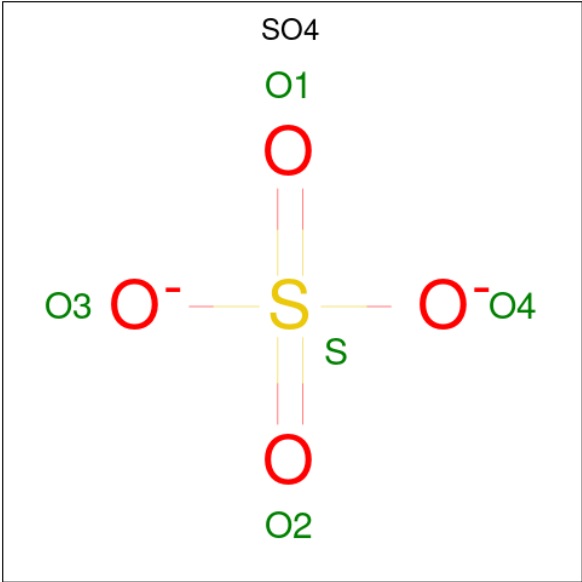
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 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	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



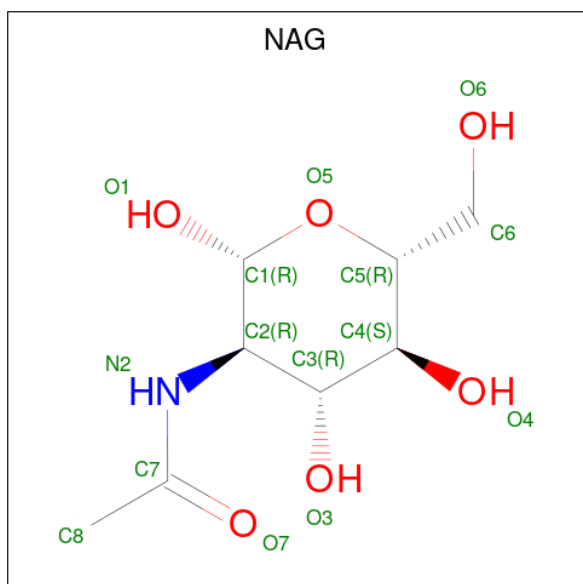
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

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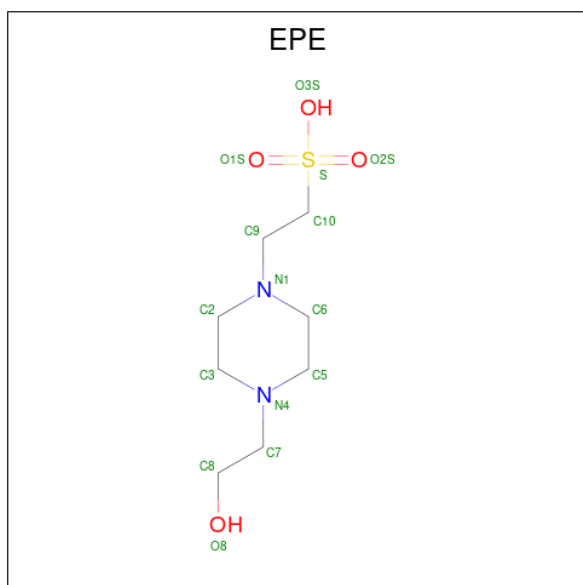
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



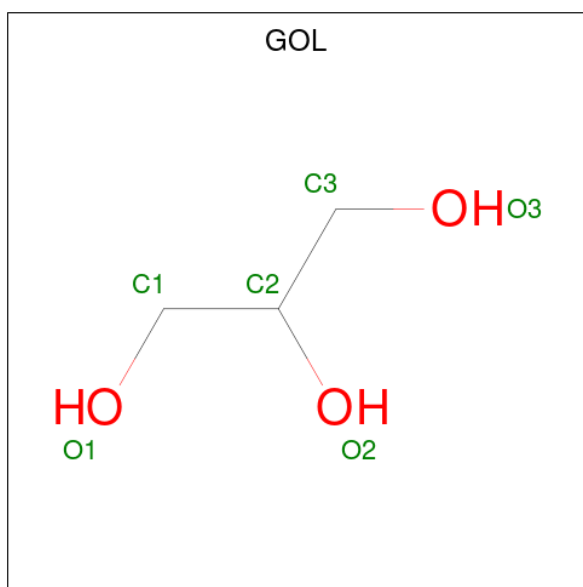
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Co	0	0
			1	1		
8	B	1	Total	Co	0	0
			1	1		

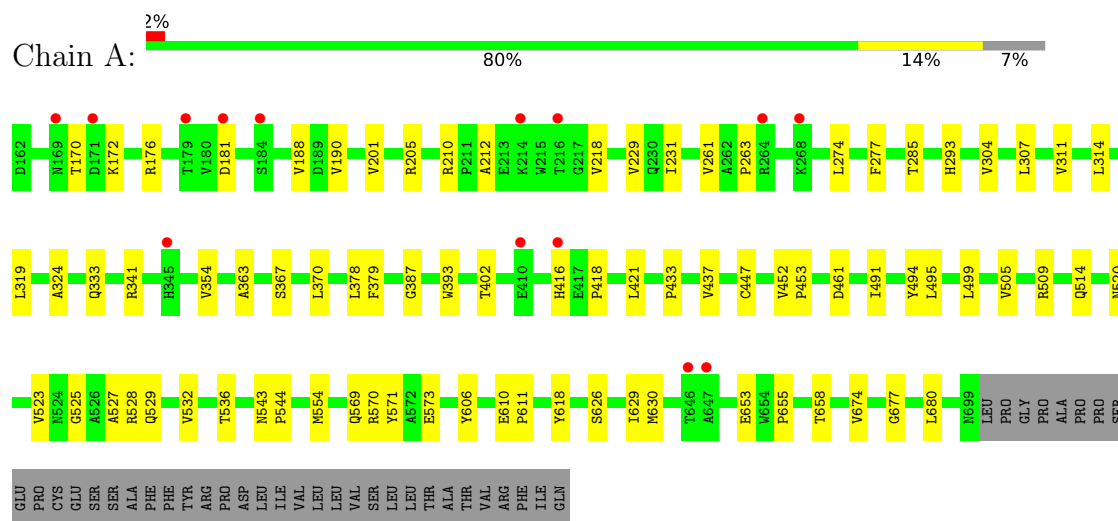
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	B	5	Total	O	0	0
			5	5		

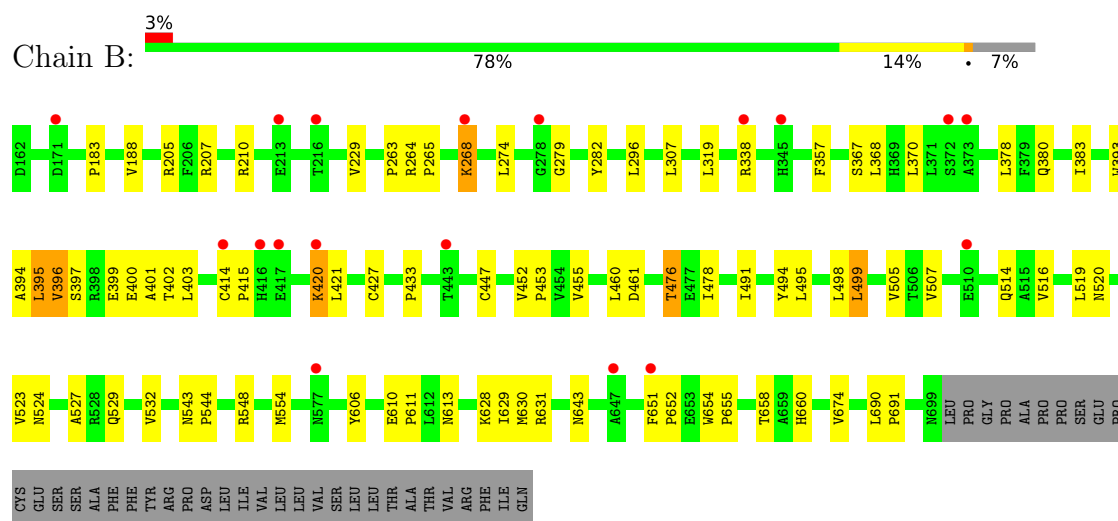
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



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





● Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	148.66Å 148.66Å 226.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.93 – 3.21 55.93 – 3.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.93-3.21) 100.0 (55.93-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.207 , 0.231 0.214 , 0.238	Depositor DCC
R_{free} test set	2339 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8860	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GOL, EPE, MAN, CO, 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	0.39	1/4381 (0.0%)	0.80	0/5979
1	B	0.41	0/4381	0.78	1/5979 (0.0%)
All	All	0.40	1/8762 (0.0%)	0.79	1/11958 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	PRO	N-CD	5.01	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	524	ASN	N-CA-C	5.64	118.36	111.82

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	4257	0	4106	43	0
1	B	4257	0	4105	49	0
2	C	50	0	43	1	0
3	D	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	0	0	0
4	B	80	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	30	0	36	0	0
6	B	15	0	18	1	0
7	A	12	0	16	0	0
7	B	6	0	8	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	7	0	0	0	0
9	B	5	0	0	0	0
All	All	8860	0	8410	90	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 5.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ALA:O	1:B:395:LEU:HD12	1.87	0.75
1:B:643:ASN:ND2	1:B:654:TRP:H	1.88	0.70
1:A:499:LEU:HA	1:A:505:VAL:HG11	1.76	0.66
1:B:274:LEU:HD21	1:B:307:LEU:HD23	1.76	0.66
1:B:643:ASN:HD21	1:B:654:TRP:H	1.43	0.63
1:B:396:VAL:CG2	1:B:401:ALA:HB2	2.30	0.62
1:B:400:GLU:O	1:B:403:LEU:N	2.35	0.59
1:A:188:VAL:HG12	1:A:263:PRO:HA	1.83	0.59
1:A:532:VAL:O	1:A:536:THR:HG22	2.03	0.58
1:A:274:LEU:HD21	1:A:307:LEU:HD23	1.86	0.58
1:B:631:ARG:HG2	1:B:651:PHE:HE2	1.71	0.56
1:B:188:VAL:HG12	1:B:263:PRO:HA	1.87	0.55
1:A:611:PRO:HA	1:A:618:TYR:CD1	2.42	0.55
1:A:176:ARG:HD2	2:C:1:NAG:O7	2.07	0.55
1:A:520:ASN:OD1	1:A:554:MET:HE1	2.07	0.54
1:B:296:LEU:HA	1:B:630:MET:HE3	1.90	0.54
1:A:172:LYS:HE2	1:A:212:ALA:O	2.08	0.54
1:B:631:ARG:HG2	1:B:651:PHE:CE2	2.43	0.53
1:A:341:ARG:HD2	1:A:378:LEU:HA	1.91	0.53
1:B:396:VAL:HG13	1:B:452:VAL:CG2	2.39	0.53
1:A:525:GLY:HA2	1:A:528:ARG:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:HB	1:B:453:PRO:HD2	1.91	0.52
1:B:319:LEU:HD22	1:B:421:LEU:HD22	1.92	0.52
1:B:420:LYS:HA	1:B:420:LYS:HE2	1.92	0.52
1:A:319:LEU:HB3	1:A:421:LEU:HD23	1.91	0.52
1:A:367:SER:HA	1:A:370:LEU:HD12	1.91	0.51
1:A:452:VAL:HB	1:A:453:PRO:HD2	1.91	0.51
1:B:319:LEU:HA	1:B:402:THR:HG22	1.92	0.51
1:A:611:PRO:HG2	1:A:626:SER:HB2	1.92	0.51
1:B:400:GLU:O	1:B:401:ALA:C	2.53	0.51
1:A:523:VAL:HB	1:A:527:ALA:HB3	1.94	0.49
1:A:205:ARG:HD2	1:A:314:LEU:HD22	1.93	0.49
1:A:416:HIS:N	1:A:416:HIS:ND1	2.61	0.49
1:B:368:LEU:HD22	1:B:460:LEU:HD11	1.94	0.49
1:A:293:HIS:HB3	1:A:304:VAL:HB	1.94	0.49
1:A:229:VAL:HG11	1:A:433:PRO:HB2	1.95	0.49
1:A:570:ARG:NH1	1:A:573:GLU:HG3	2.28	0.48
1:A:210:ARG:HH22	1:B:461:ASP:CG	2.22	0.48
1:B:264:ARG:HA	1:B:265:PRO:C	2.39	0.47
1:A:491:ILE:O	1:A:494:TYR:O	2.32	0.47
1:A:319:LEU:HA	1:A:402:THR:HG22	1.97	0.47
1:B:491:ILE:O	1:B:494:TYR:O	2.32	0.47
1:B:498:LEU:HD11	1:B:507:VAL:HG22	1.97	0.47
1:B:414:CYS:HB3	1:B:415:PRO:HD2	1.95	0.47
1:A:461:ASP:OD2	1:B:210:ARG:NH2	2.48	0.47
1:B:357:PHE:CB	1:B:383:ILE:HB	2.45	0.47
1:B:393:TRP:HB3	1:B:447:CYS:O	2.15	0.47
1:B:529:GLN:HA	1:B:532:VAL:HG22	1.97	0.46
1:A:529:GLN:HA	1:A:532:VAL:HG22	1.98	0.46
1:B:282:TYR:OH	6:B:818:EPE:H71	2.16	0.46
1:A:363:ALA:HB3	1:A:387:GLY:HA3	1.98	0.46
1:A:569:GLN:O	1:A:573:GLU:HG2	2.16	0.45
1:B:523:VAL:HB	1:B:527:ALA:HB3	1.98	0.45
1:A:190:VAL:HG12	1:A:261:VAL:HG22	1.99	0.45
1:B:205:ARG:C	1:B:207:ARG:H	2.24	0.45
1:B:380:GLN:O	1:B:476:THR:HG21	2.17	0.45
1:A:509:ARG:HH12	1:A:536:THR:HB	1.81	0.45
1:A:606:TYR:HB3	1:A:629:ILE:HD11	1.98	0.45
1:A:626:SER:O	1:A:630:MET:HB2	2.17	0.45
1:A:677:GLY:HA2	1:A:680:LEU:HG	1.98	0.45
1:A:543:ASN:HA	1:A:544:PRO:HD3	1.86	0.45
1:B:367:SER:HA	1:B:370:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:SER:C	1:B:399:GLU:N	2.73	0.44
1:A:416:HIS:N	1:A:416:HIS:HD1	2.15	0.44
1:B:690:LEU:N	1:B:691:PRO:HD2	2.33	0.44
1:A:307:LEU:HD11	1:A:333:GLN:HG2	1.98	0.44
1:B:268:LYS:H	1:B:268:LYS:HG3	1.46	0.44
1:A:319:LEU:HB2	1:A:324:ALA:HB3	2.00	0.44
1:A:277:PHE:CD1	1:A:277:PHE:C	2.96	0.44
1:A:176:ARG:HH22	1:A:218:VAL:HG11	1.83	0.43
1:B:520:ASN:OD1	1:B:554:MET:HE1	2.18	0.43
1:A:231:ILE:HD11	1:A:437:VAL:O	2.19	0.43
1:B:543:ASN:HA	1:B:544:PRO:HD3	1.90	0.43
1:B:655:PRO:HG3	1:B:674:VAL:HG11	1.99	0.43
1:A:393:TRP:HB3	1:A:447:CYS:O	2.19	0.43
1:B:279:GLY:HA2	7:B:819:GOL:H31	2.00	0.42
1:B:357:PHE:HB2	1:B:383:ILE:HB	2.02	0.41
1:A:610:GLU:N	1:A:611:PRO:CD	2.83	0.41
1:B:183:PRO:HB2	1:B:613:ASN:HA	2.02	0.41
1:B:516:VAL:HG12	1:B:554:MET:SD	2.60	0.41
1:B:338:ARG:HG3	1:B:378:LEU:HD21	2.03	0.41
1:B:229:VAL:HG11	1:B:433:PRO:HB2	2.01	0.41
1:B:628:LYS:HE3	1:B:652:PRO:HD2	2.03	0.41
1:B:495:LEU:HD22	1:B:519:LEU:HD21	2.02	0.41
1:B:610:GLU:N	1:B:611:PRO:CD	2.84	0.41
1:B:499:LEU:HD11	1:B:548:ARG:HG3	2.03	0.41
1:A:354:VAL:HB	1:A:379:PHE:HA	2.04	0.40
1:A:655:PRO:HG3	1:A:674:VAL:HG11	2.03	0.40
1:B:606:TYR:HB3	1:B:629:ILE:HD11	2.03	0.40
1:B:414:CYS:CB	1:B:415:PRO:HD2	2.51	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	536/576 (93%)	518 (97%)	18 (3%)	0	100	100
1	B	536/576 (93%)	513 (96%)	23 (4%)	0	100	100
All	All	1072/1152 (93%)	1031 (96%)	41 (4%)	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	455/489 (93%)	445 (98%)	10 (2%)	45	69
1	B	455/489 (93%)	442 (97%)	13 (3%)	37	64
All	All	910/978 (93%)	887 (98%)	23 (2%)	42	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	A	181	ASP
1	A	201	VAL
1	A	285	THR
1	A	311	VAL
1	A	495	LEU
1	A	514	GLN
1	A	571	TYR
1	A	653	GLU
1	A	658	THR
1	B	268	LYS
1	B	395	LEU
1	B	396	VAL
1	B	420	LYS
1	B	427	CYS
1	B	455	VAL
1	B	476	THR
1	B	478	ILE

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Mol	Chain	Res	Type
1	B	499	LEU
1	B	505	VAL
1	B	514	GLN
1	B	658	THR
1	B	660	HIS

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	301	ASN
1	A	434	HIS
1	A	657	HIS
1	B	334	ASN
1	B	514	GLN
1	B	529	GLN
1	B	576	ASN
1	B	643	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 ⓘ

9 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	C	1	1,2	14,14,15	0.37	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.67	0	17,19,21	1.71	3 (17%)
2	BMA	C	3	2	11,11,12	0.61	0	15,15,17	0.62	0
2	MAN	C	4	2	11,11,12	0.55	0	15,15,17	1.84	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.61	0	17,19,21	1.63	2 (11%)
3	NAG	D	2	3	14,14,15	0.54	0	17,19,21	1.98	2 (11%)
3	BMA	D	3	3	11,11,12	0.90	0	15,15,17	1.97	3 (20%)
3	MAN	D	4	3	11,11,12	0.57	0	15,15,17	1.04	1 (6%)
3	MAN	D	5	3	11,11,12	0.61	0	15,15,17	1.86	4 (26%)

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	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	6.73	121.21	112.19
2	C	4	MAN	C1-O5-C5	5.37	119.38	112.19
3	D	5	MAN	C1-O5-C5	4.86	118.70	112.19
3	D	3	BMA	C3-C4-C5	4.73	118.81	110.23
3	D	3	BMA	C1-O5-C5	-4.18	106.58	112.19
3	D	1	NAG	C4-C3-C2	4.13	117.07	111.02
2	C	2	NAG	C2-N2-C7	3.44	127.51	122.90
2	C	2	NAG	C4-C3-C2	3.41	116.01	111.02
2	C	4	MAN	C3-C4-C5	3.21	116.05	110.23
2	C	2	NAG	C1-O5-C5	3.09	116.33	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C3-C4-C5	2.83	115.36	110.23
3	D	5	MAN	C1-C2-C3	2.81	113.74	109.64
3	D	5	MAN	C2-C3-C4	2.67	115.55	110.86
3	D	2	NAG	C1-C2-N2	2.44	114.28	110.43
3	D	4	MAN	C1-O5-C5	2.35	115.34	112.19
2	C	4	MAN	O5-C5-C4	2.30	116.43	110.83
3	D	3	BMA	C2-C3-C4	2.29	114.89	110.86
3	D	1	NAG	O4-C4-C5	2.24	114.83	109.32
2	C	1	NAG	C3-C4-C5	2.02	113.90	110.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

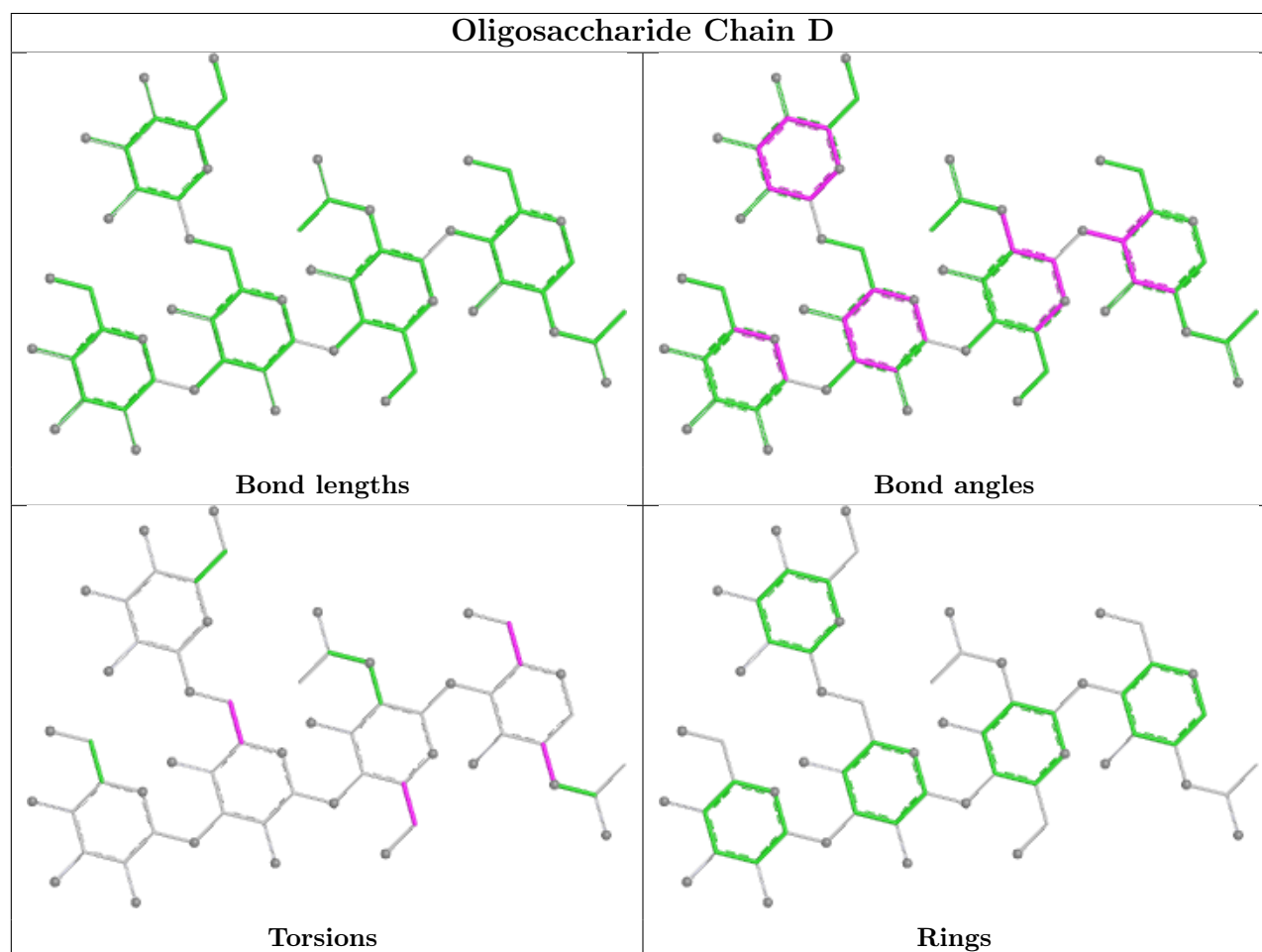
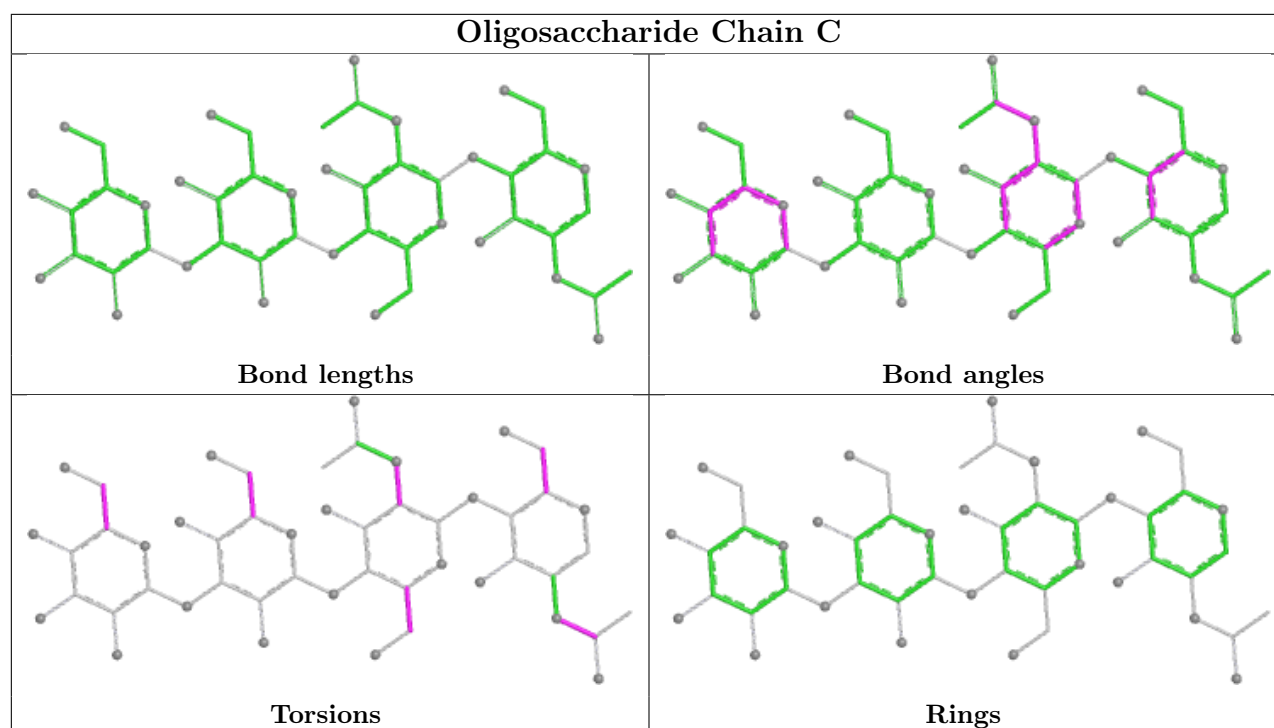
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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



5.6 Ligand geometry

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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$
4	SO4	B	804	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	A	806	-	4,4,4	0.43	0	6,6,6	0.07	0
4	SO4	B	805	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	A	807	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	B	809	-	4,4,4	0.42	0	6,6,6	0.12	0
4	SO4	A	809	-	4,4,4	0.43	0	6,6,6	0.05	0
4	SO4	B	803	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	B	807	-	4,4,4	0.44	0	6,6,6	0.08	0
4	SO4	A	803	-	4,4,4	0.42	0	6,6,6	0.11	0
4	SO4	A	802	-	4,4,4	0.43	0	6,6,6	0.07	0
4	SO4	B	802	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	B	810	-	4,4,4	0.42	0	6,6,6	0.08	0
4	SO4	A	801	-	4,4,4	0.43	0	6,6,6	0.06	0
4	SO4	A	810	-	4,4,4	0.43	0	6,6,6	0.07	0
4	SO4	B	801	-	4,4,4	0.43	0	6,6,6	0.08	0
5	NAG	A	811	1	14,14,15	0.38	0	17,19,21	0.72	0
4	SO4	B	816	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	B	806	-	4,4,4	0.43	0	6,6,6	0.07	0
7	GOL	A	815	-	5,5,5	0.35	0	5,5,5	0.23	0
6	EPE	B	818	-	15,15,15	2.02	1 (6%)	19,20,20	2.68	10 (52%)
4	SO4	B	812	-	4,4,4	0.42	0	6,6,6	0.09	0
4	SO4	A	805	-	4,4,4	0.43	0	6,6,6	0.08	0
6	EPE	A	813	-	15,15,15	2.00	1 (6%)	19,20,20	2.67	8 (42%)
4	SO4	A	808	-	4,4,4	0.43	0	6,6,6	0.07	0
4	SO4	B	811	-	4,4,4	0.44	0	6,6,6	0.07	0
6	EPE	A	812	-	15,15,15	2.03	1 (6%)	19,20,20	2.73	9 (47%)
4	SO4	B	808	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	B	814	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	B	815	-	4,4,4	0.43	0	6,6,6	0.11	0
7	GOL	A	814	-	5,5,5	0.38	0	5,5,5	0.24	0
4	SO4	A	804	-	4,4,4	0.44	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	819	-	5,5,5	0.32	0	5,5,5	0.15	0
5	NAG	B	817	1	14,14,15	0.38	0	17,19,21	0.71	0
4	SO4	B	813	-	4,4,4	0.43	0	6,6,6	0.08	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
6	EPE	A	813	-	-	5/9/19/19	0/1/1/1
6	EPE	A	812	-	-	4/9/19/19	0/1/1/1
7	GOL	B	819	-	-	0/4/4/4	-
7	GOL	A	814	-	-	4/4/4/4	-
7	GOL	A	815	-	-	0/4/4/4	-
6	EPE	B	818	-	-	3/9/19/19	0/1/1/1
5	NAG	A	811	1	-	5/6/23/26	0/1/1/1
5	NAG	B	817	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	812	EPE	C10-S	-7.57	1.67	1.77
6	B	818	EPE	C10-S	-7.53	1.67	1.77
6	A	813	EPE	C10-S	-7.44	1.67	1.77

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	812	EPE	C6-N1-C2	5.90	121.56	108.84
6	A	813	EPE	C5-N4-C3	5.75	121.22	108.84
6	A	812	EPE	C5-N4-C3	5.73	121.17	108.84
6	A	813	EPE	C6-N1-C2	5.67	121.05	108.84
6	B	818	EPE	C5-N4-C3	5.57	120.84	108.84
6	B	818	EPE	C6-N1-C2	5.17	119.97	108.84
6	A	812	EPE	C7-N4-C3	3.55	120.69	111.24
6	B	818	EPE	C9-N1-C6	3.44	120.39	111.24
6	B	818	EPE	C7-N4-C5	3.41	120.33	111.24
6	A	813	EPE	C9-N1-C2	3.23	119.84	111.24
6	B	818	EPE	C9-N1-C2	3.15	119.62	111.24
6	A	813	EPE	C7-N4-C5	3.08	119.44	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	813	EPE	C7-N4-C3	3.03	119.32	111.24
6	A	812	EPE	C9-N1-C2	3.01	119.25	111.24
6	A	812	EPE	C9-N1-C6	2.98	119.17	111.24
6	A	813	EPE	C9-N1-C6	2.95	119.10	111.24
6	B	818	EPE	C7-N4-C3	2.84	118.81	111.24
6	A	813	EPE	O3S-S-C10	2.72	111.32	106.00
6	A	812	EPE	C6-C5-N4	-2.67	105.27	110.65
6	A	812	EPE	C5-C6-N1	-2.64	105.33	110.65
6	A	812	EPE	O1S-S-C10	2.62	110.68	106.73
6	A	812	EPE	C7-N4-C5	2.58	118.11	111.24
6	B	818	EPE	C3-C2-N1	-2.56	105.48	110.65
6	B	818	EPE	O1S-S-C10	2.47	110.45	106.73
6	B	818	EPE	C2-C3-N4	-2.10	106.42	110.65
6	A	813	EPE	C5-C6-N1	-2.04	106.53	110.65
6	B	818	EPE	C5-C6-N1	-2.03	106.56	110.65

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	811	NAG	C8-C7-N2-C2
5	A	811	NAG	O7-C7-N2-C2
6	A	813	EPE	C9-C10-S-O1S
6	A	813	EPE	C9-C10-S-O2S
7	A	814	GOL	O1-C1-C2-O2
7	A	814	GOL	O1-C1-C2-C3
7	A	814	GOL	C1-C2-C3-O3
7	A	814	GOL	O2-C2-C3-O3
5	B	817	NAG	O5-C5-C6-O6
5	B	817	NAG	C4-C5-C6-O6
5	A	811	NAG	C4-C5-C6-O6
6	A	813	EPE	C9-C10-S-O3S
5	A	811	NAG	O5-C5-C6-O6
6	A	813	EPE	N4-C7-C8-O8
6	A	812	EPE	N4-C7-C8-O8
6	A	812	EPE	C10-C9-N1-C2
6	A	813	EPE	C10-C9-N1-C6
6	A	812	EPE	C8-C7-N4-C5
5	A	811	NAG	C3-C2-N2-C7
6	A	812	EPE	C10-C9-N1-C6
6	B	818	EPE	C10-C9-N1-C2
5	B	817	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	B	818	EPE	C8-C7-N4-C3
5	B	817	NAG	O7-C7-N2-C2
6	B	818	EPE	N4-C7-C8-O8

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	818	EPE	1	0
7	B	819	GOL	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

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, 95th 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	538/576 (93%)	0.18	14 (2%) 57 38	53, 78, 114, 136	0
1	B	538/576 (93%)	0.23	18 (3%) 49 31	56, 79, 110, 139	0
All	All	1076/1152 (93%)	0.20	32 (2%) 52 34	53, 79, 112, 139	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	ALA	4.0
1	B	416	HIS	3.6
1	A	268	LYS	3.5
1	B	268	LYS	3.3
1	B	213	GLU	3.1
1	A	647	ALA	3.0
1	B	651	PHE	2.9
1	B	372	SER	2.8
1	A	416	HIS	2.7
1	A	214	LYS	2.6
1	A	181	ASP	2.6
1	B	647	ALA	2.6
1	A	646	THR	2.4
1	B	577	ASN	2.4
1	B	417	GLU	2.4
1	B	510	GLU	2.3
1	B	171	ASP	2.3
1	A	179	THR	2.2
1	A	171	ASP	2.2
1	A	216	THR	2.2
1	A	169	ASN	2.2
1	B	414	CYS	2.2
1	B	216	THR	2.1
1	B	278	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	345	HIS	2.1
1	B	420	LYS	2.1
1	A	264	ARG	2.1
1	B	338	ARG	2.1
1	A	410	GLU	2.1
1	B	345	HIS	2.0
1	B	443	THR	2.0
1	A	184	SER	2.0

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

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

6.3 Carbohydrates [i](#)

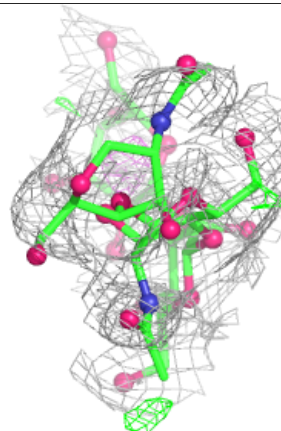
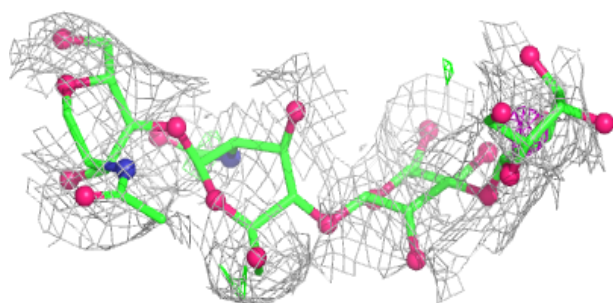
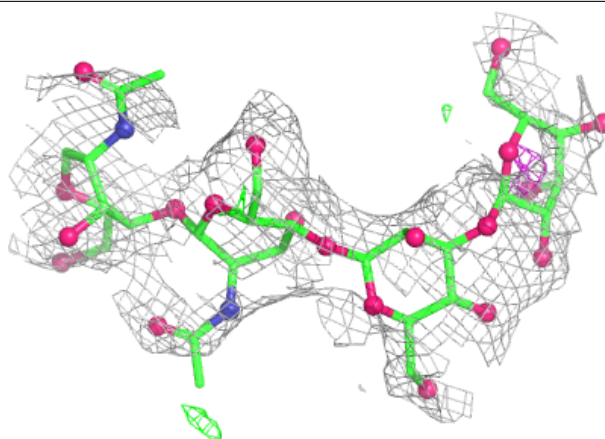
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

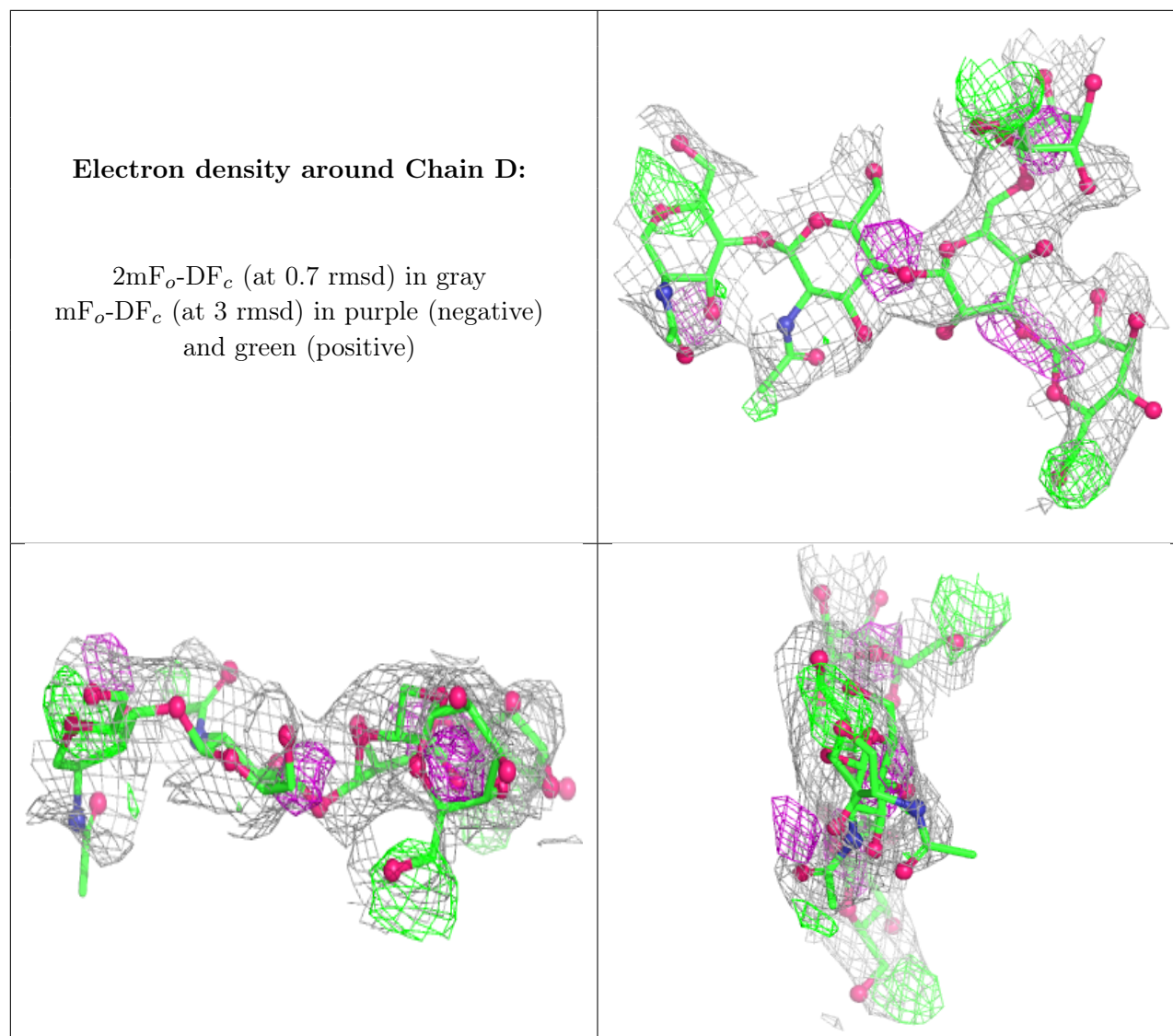
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	D	4	11/12	0.14	0.17	174,183,185,186	0
3	MAN	D	5	11/12	0.18	0.19	170,185,186,187	0
2	MAN	C	4	11/12	0.35	0.15	179,190,192,193	0
2	BMA	C	3	11/12	0.50	0.12	164,174,179,185	0
3	BMA	D	3	11/12	0.57	0.14	173,180,184,186	0
2	NAG	C	2	14/15	0.64	0.16	142,149,155,164	0
3	NAG	D	2	14/15	0.74	0.15	128,140,151,162	0
3	NAG	D	1	14/15	0.80	0.18	104,114,122,124	0
2	NAG	C	1	14/15	0.82	0.14	130,136,143,146	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 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 [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, 95th 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	NAG	B	817	14/15	0.32	0.18	142,148,152,153	0
4	SO4	B	804	5/5	0.36	0.15	181,182,184,186	0
7	GOL	A	815	6/6	0.54	0.32	105,107,109,109	0
5	NAG	A	811	14/15	0.55	0.18	133,140,147,148	0
4	SO4	B	811	5/5	0.56	0.26	145,146,147,147	0
4	SO4	B	814	5/5	0.62	0.09	180,181,181,183	0
4	SO4	A	808	5/5	0.65	0.13	155,155,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	813	5/5	0.65	0.16	172,173,174,177	0
4	SO4	B	812	5/5	0.66	0.10	159,160,162,163	0
4	SO4	A	803	5/5	0.67	0.14	153,153,155,156	0
4	SO4	B	802	5/5	0.67	0.09	163,164,165,166	0
4	SO4	B	810	5/5	0.68	0.14	189,189,190,190	0
4	SO4	A	806	5/5	0.69	0.11	188,190,191,192	0
4	SO4	B	808	5/5	0.69	0.17	142,143,144,145	0
6	EPE	A	813	15/15	0.72	0.29	133,145,147,148	0
4	SO4	A	802	5/5	0.74	0.12	142,142,144,145	0
4	SO4	A	807	5/5	0.75	0.16	167,168,169,172	0
4	SO4	A	810	5/5	0.76	0.18	163,164,167,168	0
4	SO4	A	804	5/5	0.77	0.21	125,125,126,128	0
4	SO4	B	806	5/5	0.77	0.12	134,135,136,137	0
4	SO4	B	803	5/5	0.78	0.14	142,142,144,146	0
4	SO4	B	809	5/5	0.80	0.14	135,137,138,139	0
6	EPE	B	818	15/15	0.81	0.35	132,152,168,170	0
4	SO4	B	807	5/5	0.82	0.14	186,186,189,189	0
6	EPE	A	812	15/15	0.82	0.33	144,145,149,150	0
4	SO4	B	805	5/5	0.82	0.14	133,134,136,137	0
4	SO4	B	816	5/5	0.82	0.13	163,163,164,164	0
4	SO4	A	805	5/5	0.82	0.18	152,152,154,154	0
7	GOL	A	814	6/6	0.85	0.23	64,68,69,69	0
7	GOL	B	819	6/6	0.85	0.23	67,73,74,74	0
4	SO4	A	801	5/5	0.87	0.13	124,125,125,126	0
4	SO4	B	815	5/5	0.88	0.26	152,154,155,157	0
4	SO4	B	801	5/5	0.89	0.10	124,125,126,127	0
8	CO	A	816	1/1	0.89	0.45	30,30,30,30	0
4	SO4	A	809	5/5	0.92	0.32	147,147,147,148	0
8	CO	B	820	1/1	0.95	0.47	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.