



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 02:10 PM JST

PDB ID : 5YDH
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 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	:	2.18
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)	:	2.18

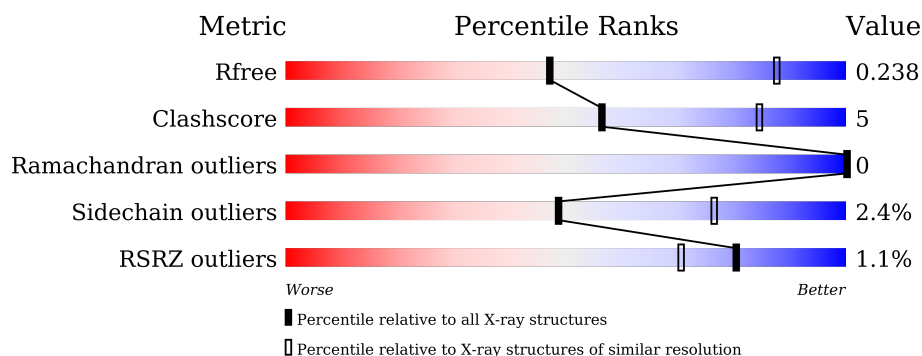
1 Overall quality at a glance

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}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (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	<div> <div></div> <div>80%14%7%</div> </div>
1	B	576	<div> <div></div> <div>79%14%7%</div> </div>
2	C	4	<div> <div>25%50%25%</div> </div>
3	D	5	<div> <div>100%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	C	3	-	-	-	X
2	MAN	C	4	-	-	-	X
3	BMA	D	3	-	-	-	X
3	MAN	D	4	-	-	-	X
3	MAN	D	5	-	-	-	X
4	SO4	A	807	-	-	-	X
4	SO4	A	810	-	-	-	X
4	SO4	B	807	-	-	-	X
4	SO4	B	810	-	-	-	X
4	SO4	B	813	-	-	-	X
6	EPE	B	818	-	-	-	X

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.

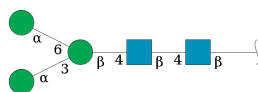
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4257	2711	743	790	13			
1	B	538	Total	C	N	O	S	0	0	0
			4257	2711	743	790	13			

- 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 (three-letter code: SO4) (formula: O₄S).



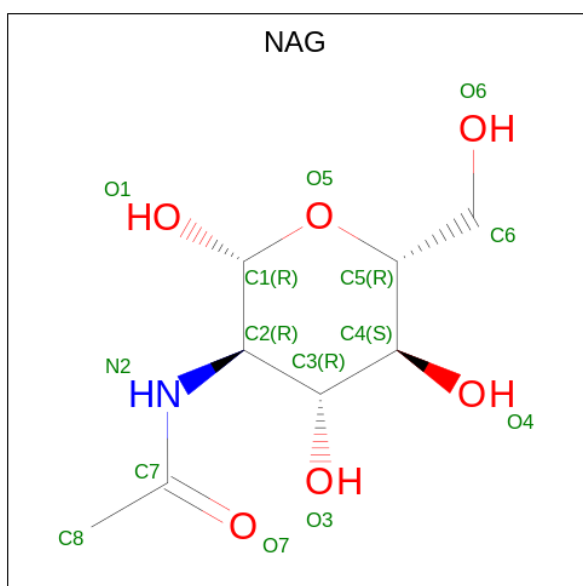
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

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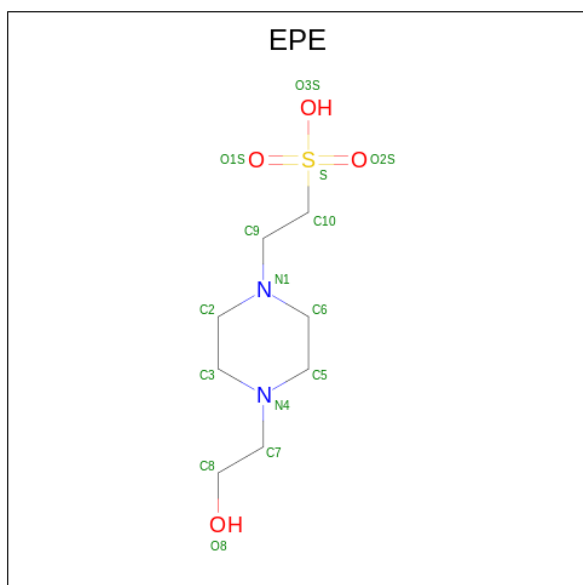
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

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



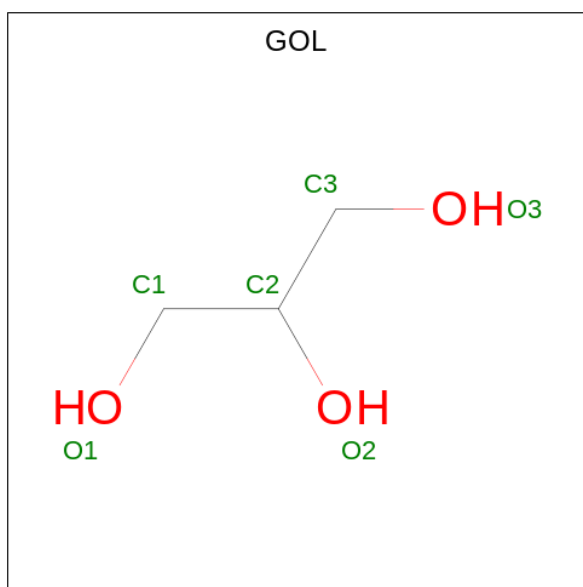
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: 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 (three-letter code: 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 (three-letter code: 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		



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

Chain 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 , 52.9	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: CO, EPE, MAN, SO4, NAG, GOL, BMA

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	0.30	0/4381	0.49	1/5979 (0.0%)
1	B	0.31	0/4381	0.48	0/5979
All	All	0.30	0/8762	0.48	1/11958 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	GLU	C-N-CD	5.61	140.18	128.40

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	41	0
1	B	4257	0	4105	48	0
2	C	50	0	43	1	0
3	D	61	0	52	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	87	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 (87) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:400:GLU:O	1:B:401:ALA:C	2.53	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: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
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:176:ARG:HH22	1:A:218:VAL:HG11	1.83	0.43
1:A:210:ARG:HH22	1:B:461:ASP:CG	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:PRO:HG3	1:B:674:VAL:HG11	1.99	0.43
1:B:264:ARG:HA	1:B:265:PRO:C	2.39	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:296:LEU:HA	1:B:630:MET:HE3	2.00	0.42
1:B:397:SER:C	1:B:399:GLU:N	2.73	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:205:ARG:C	1:B:207:ARG:H	2.24	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	444 (98%)	11 (2%)	49	76
1	B	455/489 (93%)	444 (98%)	11 (2%)	49	76
All	All	910/978 (93%)	888 (98%)	22 (2%)	49	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	A	181	ASP
1	A	199	PRO
1	A	208	HIS
1	A	285	THR
1	A	311	VAL
1	A	375	SER
1	A	520	ASN
1	A	571	TYR
1	A	653	GLU
1	A	658	THR
1	B	208	HIS
1	B	268	LYS
1	B	357	PHE
1	B	395	LEU
1	B	420	LYS
1	B	427	CYS
1	B	476	THR
1	B	505	VAL
1	B	658	THR
1	B	660	HIS
1	B	680	LEU

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

Mol	Chain	Res	Type
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	2,1	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	1.69	3 (17%)
2	BMA	C	3	2	11,11,12	0.63	0	15,15,17	0.68	0
2	MAN	C	4	2	11,11,12	0.56	0	15,15,17	1.90	4 (26%)
3	NAG	D	1	1,3	14,14,15	0.60	0	17,19,21	1.64	2 (11%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.95	2 (11%)
3	BMA	D	3	3	11,11,12	0.92	0	15,15,17	2.08	6 (40%)
3	MAN	D	4	3	11,11,12	0.59	0	15,15,17	1.15	1 (6%)
3	MAN	D	5	3	11,11,12	0.62	0	15,15,17	1.94	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	2,1	-	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	-	4/6/23/26	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 (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	6.66	121.21	112.19
2	C	4	MAN	C1-O5-C5	5.30	119.38	112.19
3	D	3	BMA	C3-C4-C5	4.81	118.81	110.24
3	D	5	MAN	C1-O5-C5	4.80	118.70	112.19
3	D	3	BMA	C1-O5-C5	-4.14	106.58	112.19
3	D	1	NAG	C4-C3-C2	4.13	117.07	111.02
2	C	2	NAG	C4-C3-C2	3.41	116.01	111.02
3	D	5	MAN	C1-C2-C3	3.31	113.74	109.67
2	C	4	MAN	C3-C4-C5	3.26	116.05	110.24
2	C	2	NAG	C2-N2-C7	3.24	127.51	122.90
2	C	2	NAG	C1-O5-C5	3.05	116.33	112.19
3	D	5	MAN	C3-C4-C5	2.87	115.36	110.24
3	D	5	MAN	C2-C3-C4	2.69	115.55	110.89
3	D	3	BMA	O5-C5-C6	2.48	111.09	107.20
2	C	4	MAN	O5-C5-C6	2.43	111.01	107.20
3	D	4	MAN	C1-O5-C5	2.32	115.34	112.19
3	D	3	BMA	C2-C3-C4	2.31	114.89	110.89
2	C	4	MAN	O5-C5-C4	2.30	116.43	110.83
3	D	1	NAG	O4-C4-C5	2.23	114.83	109.30
3	D	2	NAG	C1-C2-N2	2.22	114.28	110.49
3	D	3	BMA	O5-C1-C2	-2.11	107.51	110.77
3	D	3	BMA	O3-C3-C2	2.10	114.02	109.99
2	C	1	NAG	C3-C4-C5	2.05	113.90	110.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

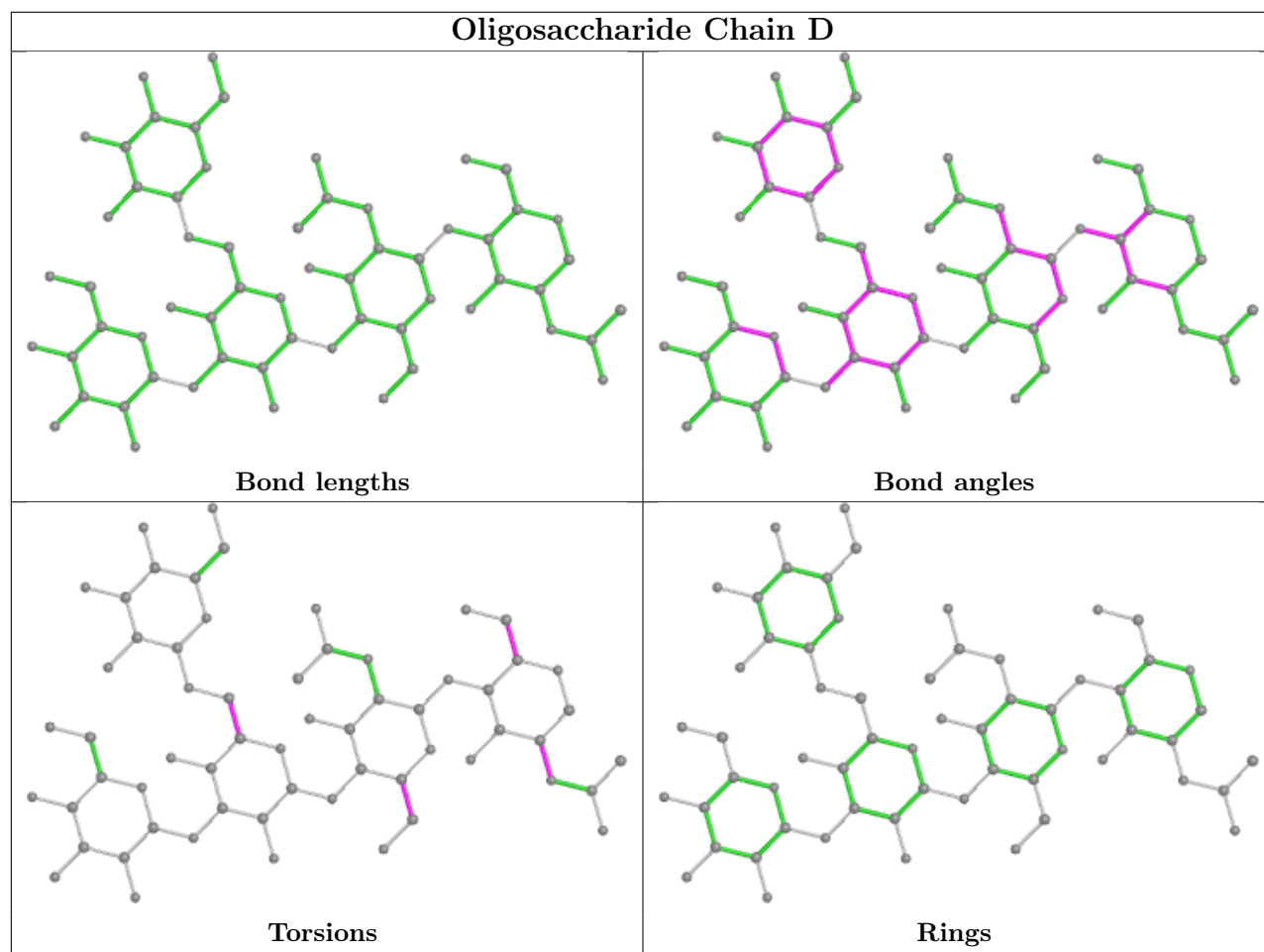
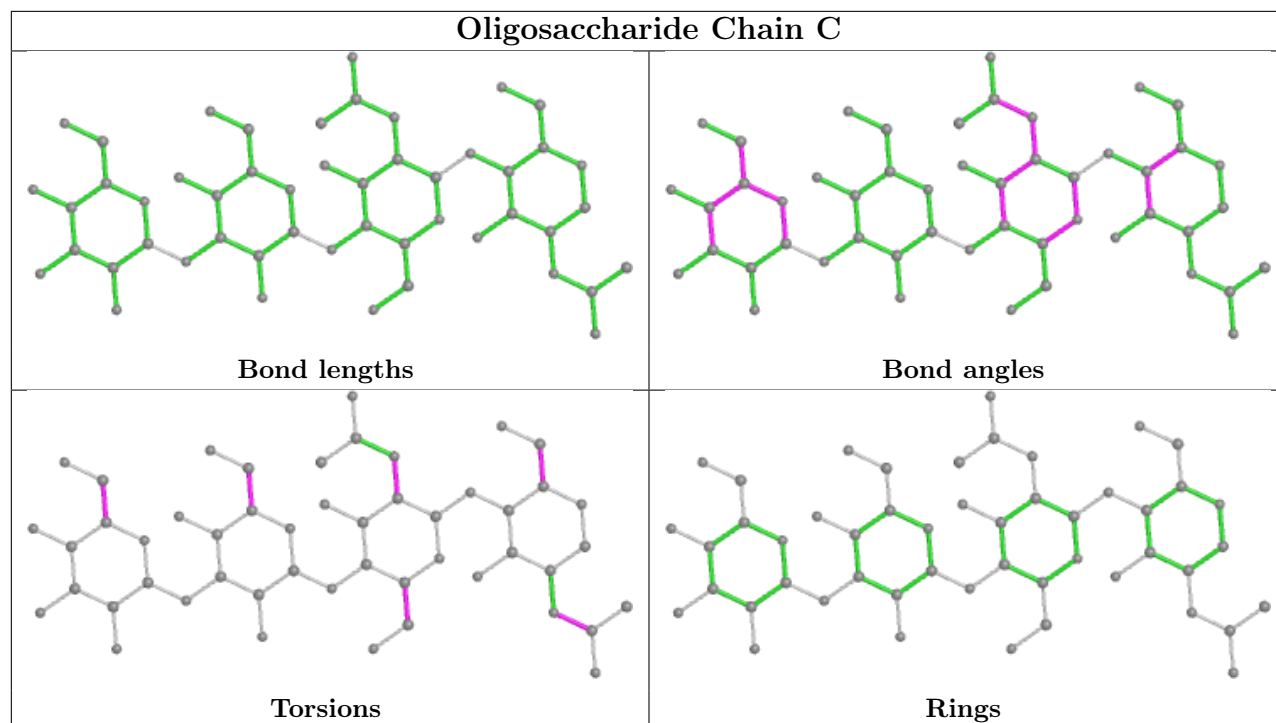
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	C	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	D	3	BMA	O5-C5-C6-O6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

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$
6	EPE	A	813	-	15,15,15	1.95	1 (6%)	18,20,20	2.76	9 (50%)
4	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	B	812	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	A	810	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	815	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	A	806	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	A	809	-	4,4,4	0.33	0	6,6,6	0.07	0
7	GOL	A	815	-	5,5,5	0.34	0	5,5,5	0.22	0
5	NAG	B	817	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	SO4	A	801	-	4,4,4	0.33	0	6,6,6	0.05	0
7	GOL	A	814	-	5,5,5	0.37	0	5,5,5	0.23	0
4	SO4	A	803	-	4,4,4	0.32	0	6,6,6	0.08	0
4	SO4	A	808	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	B	806	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	A	804	-	4,4,4	0.33	0	6,6,6	0.04	0
4	SO4	B	801	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	804	-	4,4,4	0.33	0	6,6,6	0.04	0
4	SO4	A	807	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	810	-	4,4,4	0.32	0	6,6,6	0.04	0
5	NAG	A	811	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
7	GOL	B	819	-	5,5,5	0.31	0	5,5,5	0.14	0
6	EPE	B	818	-	15,15,15	1.98	1 (6%)	18,20,20	2.78	10 (55%)
4	SO4	B	813	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	802	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	816	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	811	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	B	805	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	B	809	-	4,4,4	0.31	0	6,6,6	0.09	0
6	EPE	A	812	-	15,15,15	1.99	1 (6%)	18,20,20	2.81	11 (61%)
4	SO4	B	807	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	B	814	-	4,4,4	0.32	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	802	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	B	803	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	B	808	-	4,4,4	0.33	0	6,6,6	0.06	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
5	NAG	A	811	1	-	6/6/23/26	0/1/1/1
7	GOL	A	815	-	-	0/4/4/4	-
7	GOL	B	819	-	-	0/4/4/4	-
5	NAG	B	817	1	-	4/6/23/26	0/1/1/1
6	EPE	B	818	-	-	3/9/19/19	0/1/1/1
7	GOL	A	814	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	812	EPE	C10-S	-7.42	1.67	1.77
6	B	818	EPE	C10-S	-7.37	1.67	1.77
6	A	813	EPE	C10-S	-7.28	1.67	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	812	EPE	C6-N1-C2	5.66	121.56	108.83
6	A	813	EPE	C5-N4-C3	5.51	121.22	108.83
6	A	812	EPE	C5-N4-C3	5.48	121.17	108.83
6	A	813	EPE	C6-N1-C2	5.43	121.05	108.83
6	B	818	EPE	C5-N4-C3	5.34	120.84	108.83
6	B	818	EPE	C6-N1-C2	4.95	119.97	108.83
6	A	812	EPE	C7-N4-C3	3.70	120.69	111.23
6	B	818	EPE	C9-N1-C6	3.58	120.39	111.23
6	B	818	EPE	C7-N4-C5	3.56	120.33	111.23
6	A	813	EPE	O3S-S-C10	3.43	111.32	105.77
6	A	813	EPE	C9-N1-C2	3.37	119.84	111.23
6	B	818	EPE	C9-N1-C2	3.28	119.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	813	EPE	C7-N4-C5	3.21	119.44	111.23
6	A	813	EPE	C7-N4-C3	3.16	119.32	111.23
6	A	812	EPE	C9-N1-C2	3.13	119.25	111.23
6	A	812	EPE	O1S-S-C10	3.13	110.68	106.92
6	A	812	EPE	C9-N1-C6	3.10	119.17	111.23
6	A	813	EPE	C9-N1-C6	3.08	119.10	111.23
6	B	818	EPE	C7-N4-C3	2.96	118.81	111.23
6	B	818	EPE	O1S-S-C10	2.94	110.45	106.92
6	A	812	EPE	C7-N4-C5	2.69	118.11	111.23
6	A	812	EPE	C6-C5-N4	-2.62	105.27	110.64
6	A	812	EPE	C5-C6-N1	-2.59	105.33	110.64
6	B	818	EPE	C3-C2-N1	-2.51	105.48	110.64
6	B	818	EPE	O3S-S-C10	2.27	109.44	105.77
6	A	813	EPE	O2S-S-C10	2.10	109.44	106.92
6	A	812	EPE	O2S-S-C10	2.09	109.44	106.92
6	A	812	EPE	O3S-S-C10	2.06	109.11	105.77
6	B	818	EPE	C2-C3-N4	-2.06	106.42	110.64
5	A	811	NAG	C3-C4-C5	2.03	113.85	110.24
5	B	817	NAG	C3-C4-C5	2.01	113.83	110.24
6	A	813	EPE	C5-C6-N1	-2.00	106.53	110.64

There are no chirality outliers.

All (26) 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	A	811	NAG	C1-C2-N2-C7
5	A	811	NAG	C4-C5-C6-O6
5	B	817	NAG	C4-C5-C6-O6
6	A	813	EPE	C9-C10-S-O3S
6	A	813	EPE	N4-C7-C8-O8
5	A	811	NAG	O5-C5-C6-O6
6	A	812	EPE	N4-C7-C8-O8
6	A	812	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
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
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
7	B	819	GOL	1	0
6	B	818	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.12	7 (1%) 77 66	53, 78, 114, 136	0
1	B	538/576 (93%)	-0.12	5 (0%) 84 76	56, 79, 110, 139	0
All	All	1076/1152 (93%)	-0.12	12 (1%) 80 70	53, 79, 112, 139	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	648	SER	3.8
1	A	648	SER	3.6
1	A	646	THR	3.1
1	B	699	ASN	2.5
1	A	650	GLU	2.5
1	B	577	ASN	2.5
1	A	166	LEU	2.4
1	A	699	ASN	2.1
1	B	646	THR	2.1
1	A	163	ASN	2.1
1	B	649	SER	2.1
1	A	162	ASP	2.0

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

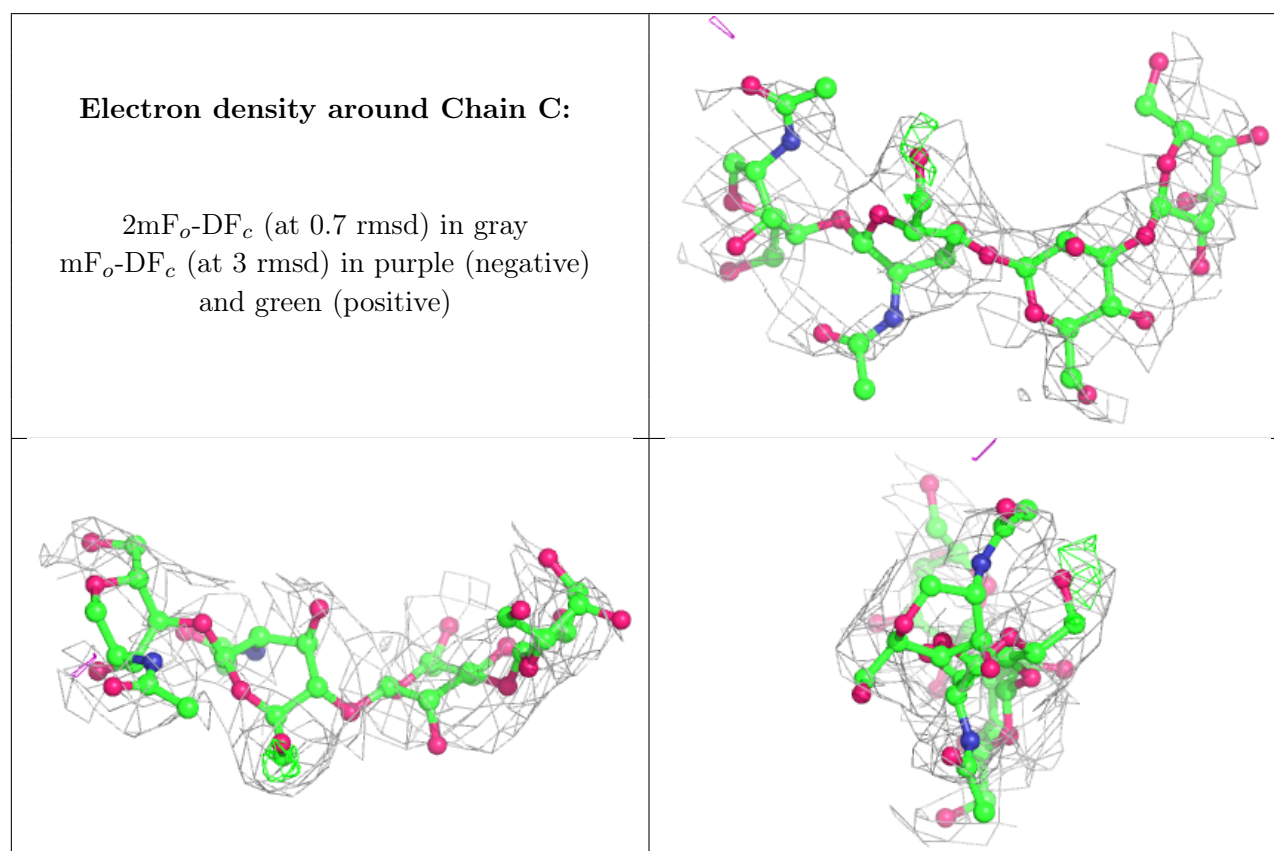
There are no non-standard protein/DNA/RNA residues in this entry.

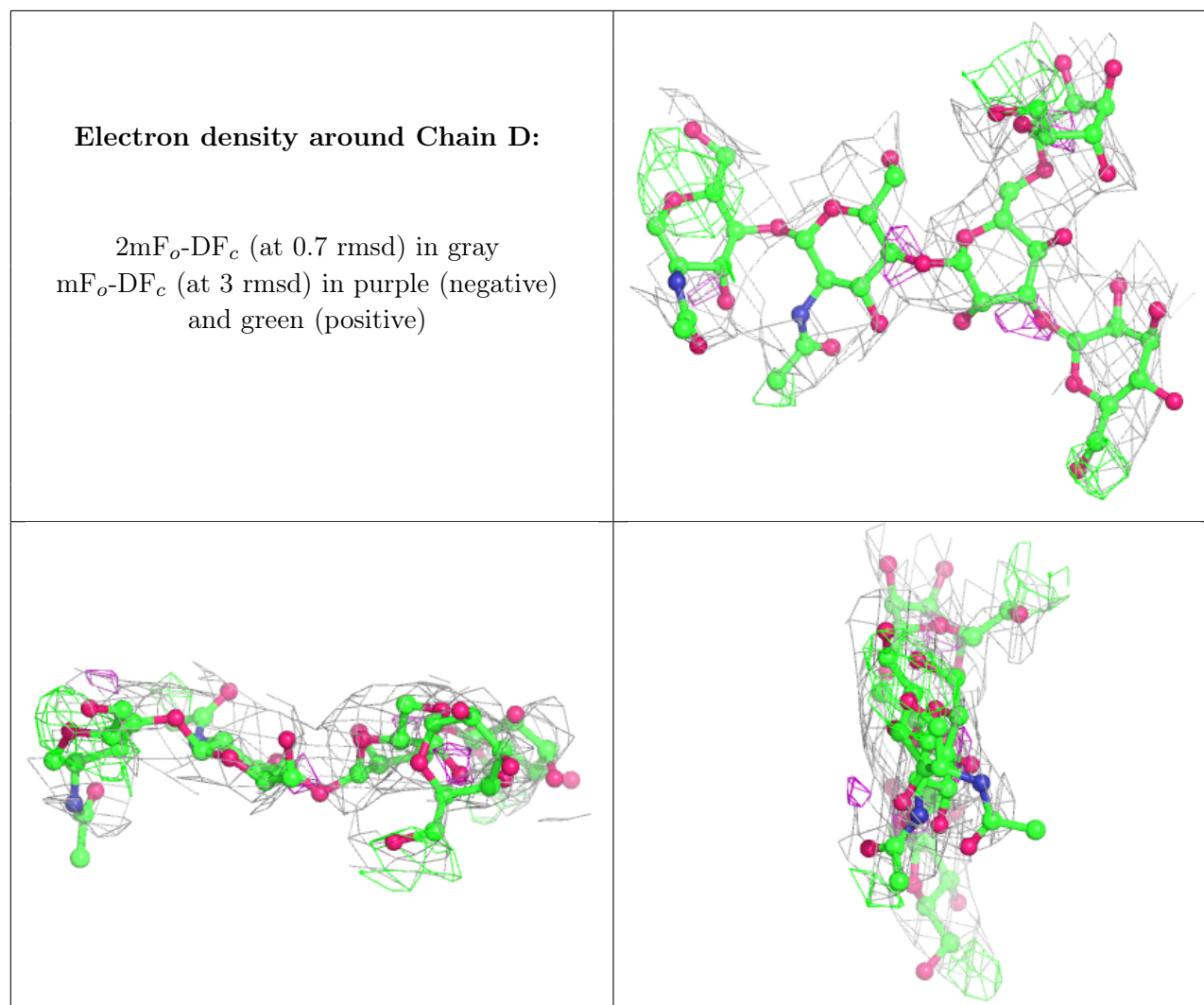
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
3	MAN	D	4	11/12	0.45	0.56	174,183,185,186	0
3	MAN	D	5	11/12	0.48	0.49	170,185,186,187	0
3	BMA	D	3	11/12	0.64	0.51	173,180,184,186	0
2	BMA	C	3	11/12	0.71	0.43	164,174,179,185	0
2	MAN	C	4	11/12	0.73	0.49	179,190,192,193	0
3	NAG	D	2	14/15	0.75	0.34	128,140,151,162	0
2	NAG	C	2	14/15	0.80	0.35	142,149,155,164	0
3	NAG	D	1	14/15	0.83	0.26	104,114,122,124	0
2	NAG	C	1	14/15	0.87	0.32	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.





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, 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
4	SO4	B	804	5/5	0.58	0.37	181,182,184,186	0
4	SO4	A	808	5/5	0.62	0.27	155,155,157,157	0
4	SO4	B	810	5/5	0.67	0.49	189,189,190,190	0
4	SO4	B	813	5/5	0.70	0.51	172,173,174,177	0
7	GOL	A	815	6/6	0.70	0.31	105,107,109,109	0
4	SO4	B	816	5/5	0.71	0.35	163,163,164,164	0
4	SO4	A	810	5/5	0.72	0.61	163,164,167,168	0
4	SO4	A	806	5/5	0.72	0.28	188,190,191,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EPE	B	818	15/15	0.73	0.50	132,152,168,170	0
4	SO4	B	814	5/5	0.73	0.30	180,181,181,183	0
4	SO4	B	808	5/5	0.74	0.25	142,143,144,145	0
4	SO4	B	807	5/5	0.75	0.52	186,186,189,189	0
4	SO4	A	803	5/5	0.75	0.22	153,153,155,156	0
4	SO4	B	803	5/5	0.76	0.24	142,142,144,146	0
4	SO4	A	807	5/5	0.79	0.45	167,168,169,172	0
4	SO4	B	802	5/5	0.80	0.23	163,164,165,166	0
7	GOL	A	814	6/6	0.80	0.32	64,68,69,69	0
4	SO4	B	809	5/5	0.80	0.29	135,137,138,139	0
6	EPE	A	813	15/15	0.81	0.34	133,145,147,148	0
4	SO4	B	812	5/5	0.81	0.28	159,160,162,163	0
6	EPE	A	812	15/15	0.82	0.37	144,145,149,150	0
4	SO4	A	805	5/5	0.83	0.24	152,152,154,154	0
4	SO4	B	815	5/5	0.83	0.33	152,154,155,157	0
5	NAG	A	811	14/15	0.84	0.54	133,140,147,148	0
4	SO4	B	811	5/5	0.84	0.35	145,146,147,147	0
4	SO4	B	805	5/5	0.84	0.21	133,134,136,137	0
5	NAG	B	817	14/15	0.85	0.41	142,148,152,153	0
4	SO4	A	809	5/5	0.86	0.42	147,147,147,148	0
7	GOL	B	819	6/6	0.86	0.28	67,73,74,74	0
4	SO4	A	802	5/5	0.87	0.21	142,142,144,145	0
4	SO4	B	806	5/5	0.89	0.22	134,135,136,137	0
4	SO4	A	801	5/5	0.90	0.13	124,125,125,126	0
4	SO4	A	804	5/5	0.91	0.25	125,125,126,128	0
4	SO4	B	801	5/5	0.96	0.09	124,125,126,127	0
8	CO	A	816	1/1	0.97	0.42	30,30,30,30	0
8	CO	B	820	1/1	0.98	0.45	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.