



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:48 AM UTC

PDB ID : 2WIG / pdb_00002wig
Title : NONAGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA4
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Deposited on : 2009-05-11
Resolution : 2.15 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

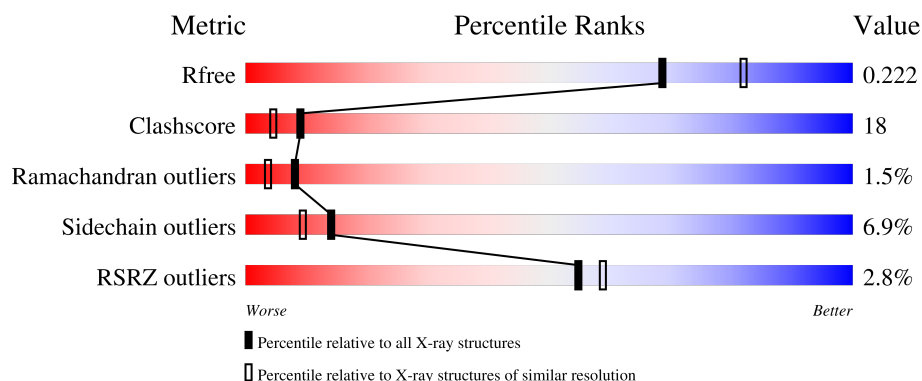
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	529	3% 75% 19% 5%
2	B	3	67% 33%
2	D	3	100%
3	C	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	A	605	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4733 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

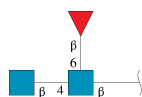
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4226	2729	710	772	15	5	3	0

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	53	THR	SER	conflict	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	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.



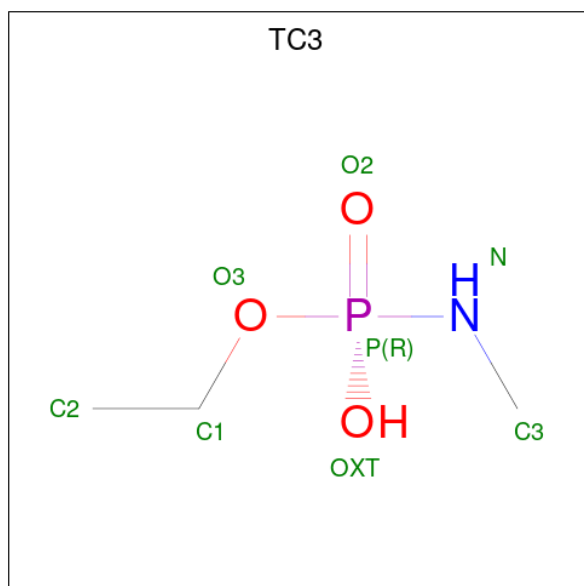
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is ETHYL HYDROGEN METHYLAMIDOPHOSPHATE (CCD ID: TC3) (formula: $C_3H_{10}NO_3P$).

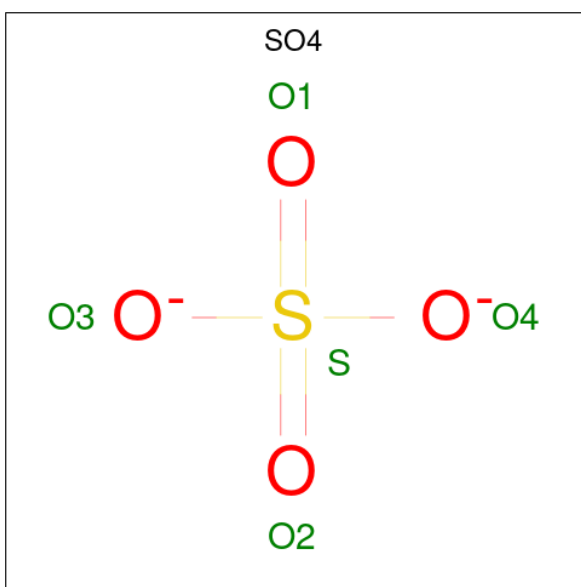


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			7	3	1	2	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

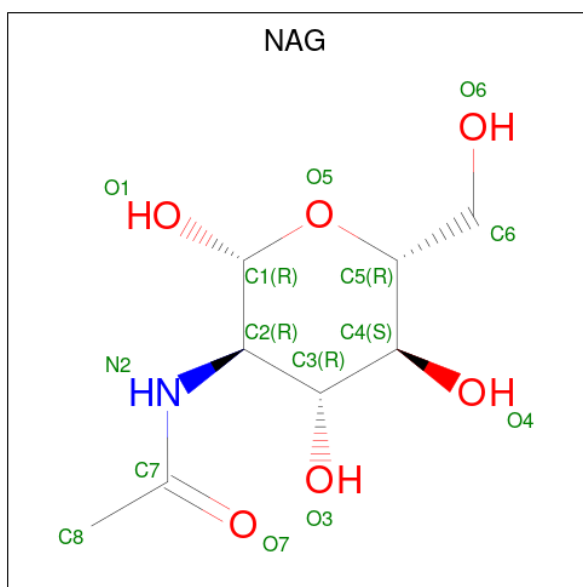


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Cl	0	0
			4	4		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

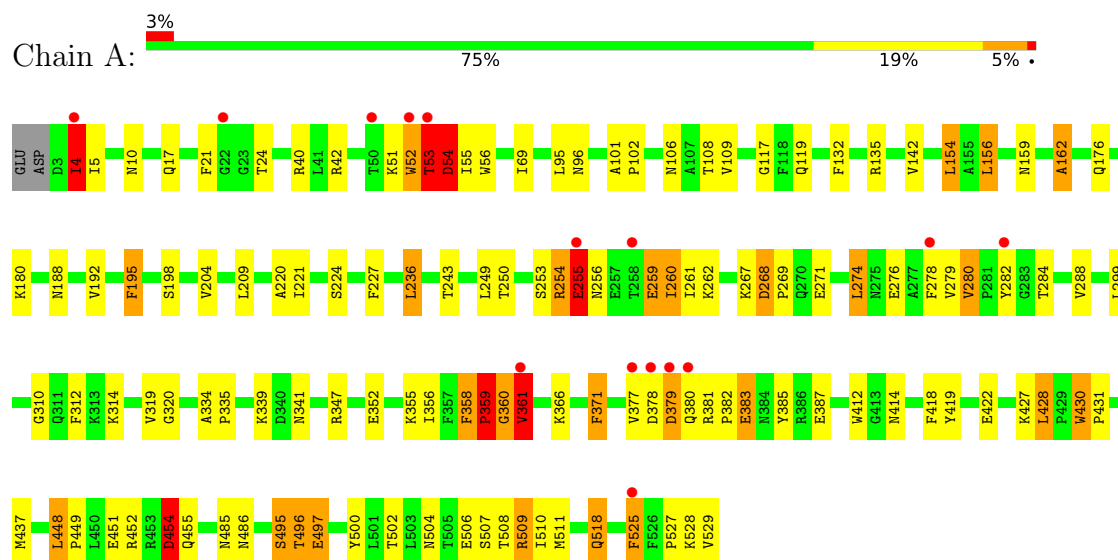
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	343	Total	O	0	0
			343	343		

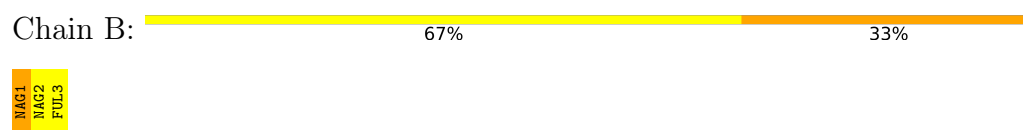
3 Residue-property plots

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

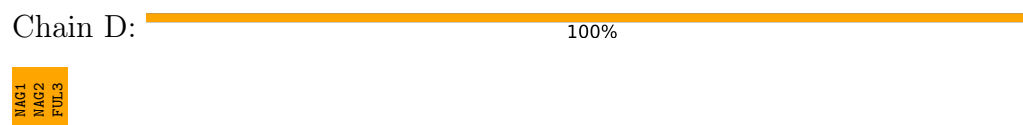
- Molecule 1: CHOLINESTERASE



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



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



- Molecule 3: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.01Å 155.01Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.15 49.09 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.15) 99.6 (49.09-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.189 , 0.253 (Not available) , 0.222	Depositor DCC
R_{free} test set	1258 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4733	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG, FUL, TC3, CL, 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	1.06	0/4351	1.12	15/5904 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	PHE	CA-C-N	10.09	132.45	119.84
1	A	358	PHE	C-N-CA	10.09	132.45	119.84
1	A	525	PHE	N-CA-C	6.90	118.69	111.03
1	A	495	SER	N-CA-C	-6.83	101.48	110.43
1	A	162	ALA	CA-C-N	-6.56	111.64	119.84
1	A	162	ALA	C-N-CA	-6.56	111.64	119.84
1	A	255	GLU	N-CA-C	-5.72	106.43	113.41
1	A	361	VAL	N-CA-C	5.36	126.00	111.00
1	A	4	ILE	N-CA-C	5.33	115.27	107.37
1	A	53	THR	N-CA-C	5.31	122.12	110.80
1	A	52	TRP	N-CA-C	-5.27	102.39	110.14
1	A	454	ASP	N-CA-C	5.25	119.79	113.17
1	A	119	GLN	N-CA-C	-5.08	107.76	114.31
1	A	430	TRP	CA-C-N	-5.02	115.39	120.21
1	A	430	TRP	C-N-CA	-5.02	115.39	120.21

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide

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	4226	0	4119	150	0
2	B	38	0	34	1	0
2	D	38	0	34	9	0
3	C	24	0	22	2	0
4	A	7	0	9	0	0
5	A	1	0	0	0	0
6	A	10	0	0	1	0
7	A	4	0	0	5	0
8	A	42	0	39	0	0
9	A	343	0	0	9	0
All	All	4733	0	4257	159	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 18.

All (159) 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:53:THR:N	1:A:54:ASP:HB2	1.14	1.42
1:A:528:LYS:CB	1:A:528:LYS:C	1.96	1.36
2:D:2:NAG:O3	2:D:2:NAG:H83	1.29	1.25
1:A:528:LYS:CB	1:A:528:LYS:N	2.04	1.21
1:A:4:ILE:HD12	1:A:4:ILE:N	1.53	1.18
1:A:53:THR:N	1:A:54:ASP:CB	2.06	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:O	1:A:53:THR:CG2	1.91	1.18
1:A:53:THR:CA	1:A:54:ASP:HB2	1.74	1.17
1:A:528:LYS:C	1:A:528:LYS:N	2.04	1.16
1:A:52:TRP:O	1:A:53:THR:HG22	1.44	1.15
1:A:256:ASN:HB3	1:A:259:GLU:HG3	1.22	1.11
1:A:53:THR:H	1:A:54:ASP:CB	1.66	1.08
1:A:52:TRP:HD1	1:A:54:ASP:HB3	1.17	1.07
1:A:4:ILE:HD12	1:A:4:ILE:H	0.91	1.07
1:A:52:TRP:C	1:A:53:THR:HG23	1.83	1.03
1:A:52:TRP:C	1:A:53:THR:CG2	2.36	0.98
1:A:255:GLU:H	1:A:255:GLU:CD	1.72	0.98
1:A:4:ILE:H	1:A:4:ILE:CD1	1.74	0.97
2:D:2:NAG:O3	2:D:2:NAG:C8	2.12	0.97
1:A:377:VAL:O	1:A:377:VAL:HG23	1.67	0.95
1:A:518:GLN:HE21	1:A:518:GLN:H	1.06	0.95
1:A:380:GLN:HB2	7:A:605:CL:CL	2.06	0.92
1:A:52:TRP:CD1	1:A:54:ASP:HB3	2.07	0.87
1:A:256:ASN:HB3	1:A:259:GLU:CG	2.05	0.86
1:A:4:ILE:N	1:A:4:ILE:CD1	2.29	0.84
1:A:156:LEU:CD2	1:A:261:ILE:HD11	2.09	0.81
1:A:495:SER:HA	9:A:703:HOH:O	1.84	0.77
1:A:253:SER:O	1:A:254:ARG:HD3	1.86	0.74
1:A:509:ARG:NH2	9:A:704:HOH:O	2.13	0.73
1:A:53:THR:H	1:A:54:ASP:HB2	0.92	0.73
1:A:496:THR:N	9:A:703:HOH:O	2.12	0.72
1:A:518:GLN:H	1:A:518:GLN:NE2	1.85	0.72
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.72	0.70
1:A:156:LEU:HD23	1:A:261:ILE:HD11	1.74	0.69
1:A:255:GLU:CD	1:A:255:GLU:N	2.47	0.69
1:A:383:GLU:O	1:A:387:GLU:HG3	1.92	0.69
1:A:495:SER:O	1:A:496:THR:OG1	2.09	0.69
6:A:603:SO4:O4	9:A:702:HOH:O	2.10	0.68
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.23	0.68
1:A:378:ASP:C	1:A:380:GLN:H	2.03	0.67
1:A:378:ASP:O	1:A:380:GLN:N	2.27	0.67
1:A:377:VAL:O	1:A:377:VAL:CG2	2.41	0.66
1:A:495:SER:CA	9:A:703:HOH:O	2.42	0.66
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.31	0.66
1:A:106:ASN:N	9:A:701:HOH:O	2.09	0.66
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.96	0.65
2:D:1:NAG:C6	2:D:3:FUL:O2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:CD2	1:A:359:PRO:HB3	2.33	0.63
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.34	0.63
1:A:380:GLN:CB	7:A:605:CL:CL	2.84	0.62
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.80	0.62
1:A:188:ASN:ND2	3:C:2:FUL:H63	2.14	0.61
1:A:176[B]:GLN:NE2	1:A:180:LYS:NZ	2.48	0.61
1:A:528:LYS:CB	1:A:528:LYS:O	2.48	0.61
1:A:361:VAL:O	1:A:366:LYS:NZ	2.34	0.61
1:A:176[B]:GLN:HG3	1:A:180:LYS:HZ2	1.64	0.60
1:A:17:GLN:NE2	1:A:24:THR:HG21	2.16	0.60
1:A:227:PHE:CD2	1:A:227:PHE:C	2.79	0.59
2:D:1:NAG:H62	2:D:2:NAG:C1	2.32	0.59
1:A:52:TRP:O	1:A:53:THR:HG23	1.79	0.59
1:A:53:THR:H	1:A:54:ASP:CG	2.11	0.58
1:A:268:ASP:O	1:A:269:PRO:C	2.47	0.57
1:A:209:LEU:HD22	1:A:312:PHE:HB3	1.86	0.57
1:A:378:ASP:CG	1:A:379:ASP:H	2.12	0.57
1:A:358:PHE:N	1:A:359:PRO:CD	2.68	0.56
1:A:276:GLU:O	1:A:279:VAL:HG22	2.05	0.56
1:A:452:ARG:C	1:A:454:ASP:H	2.14	0.56
1:A:53:THR:CA	1:A:54:ASP:CB	2.58	0.55
1:A:378:ASP:O	7:A:605:CL:CL	2.62	0.55
1:A:383:GLU:CD	1:A:383:GLU:H	2.15	0.55
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.41	0.54
1:A:278:PHE:C	1:A:280:VAL:H	2.15	0.53
1:A:176[B]:GLN:HE21	1:A:180:LYS:NZ	2.05	0.53
1:A:198:SER:HA	1:A:224:SER:O	2.09	0.53
2:D:1:NAG:H62	2:D:3:FUL:O2	2.08	0.53
1:A:414:ASN:HB2	9:A:708:HOH:O	2.09	0.53
1:A:448:LEU:N	1:A:449:PRO:CD	2.72	0.53
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.44	0.53
1:A:518:GLN:HE21	1:A:518:GLN:N	1.90	0.53
1:A:428:LEU:HD12	1:A:430:TRP:HB2	1.90	0.53
1:A:17:GLN:HE21	1:A:24:THR:HG21	1.74	0.52
1:A:377:VAL:N	1:A:378:ASP:HA	2.25	0.51
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.46	0.51
1:A:319:VAL:O	1:A:418:PHE:HA	2.11	0.50
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.93	0.50
1:A:4:ILE:HG12	1:A:17:GLN:OE1	2.12	0.50
1:A:502:THR:O	1:A:508:THR:HB	2.10	0.50
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:PHE:CZ	1:A:529:VAL:CG1	2.96	0.49
1:A:176[B]:GLN:HE21	1:A:180:LYS:HZ2	1.60	0.49
1:A:101:ALA:HA	1:A:102:PRO:C	2.37	0.49
1:A:380:GLN:HG3	7:A:605:CL:CL	2.49	0.48
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.43	0.48
1:A:55:ILE:O	1:A:55:ILE:HG22	2.10	0.48
1:A:495:SER:O	1:A:496:THR:CB	2.60	0.48
1:A:24:THR:O	1:A:101:ALA:HB3	2.14	0.48
2:D:1:NAG:C5	2:D:2:NAG:HN2	2.26	0.47
1:A:422:GLU:HG3	1:A:504:ASN:HB3	1.96	0.47
1:A:176[B]:GLN:HE21	1:A:180:LYS:HG3	1.79	0.47
1:A:109:VAL:HB	1:A:192:VAL:HG22	1.95	0.47
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.62	0.47
1:A:176[B]:GLN:CG	1:A:180:LYS:HZ2	2.28	0.47
1:A:278:PHE:C	1:A:280:VAL:N	2.74	0.46
1:A:452:ARG:C	1:A:454:ASP:N	2.72	0.46
1:A:53:THR:HG21	9:A:947:HOH:O	2.15	0.46
1:A:56:TRP:C	1:A:56:TRP:CD1	2.93	0.46
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.51	0.46
1:A:380:GLN:CG	7:A:605:CL:CL	3.00	0.46
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.80	0.46
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.96	0.46
1:A:10:ASN:O	1:A:51:LYS:HA	2.16	0.46
1:A:527:PRO:C	1:A:528:LYS:C	2.78	0.45
1:A:428:LEU:HD11	1:A:437:MET:SD	2.56	0.45
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.58	0.45
1:A:254:ARG:CG	1:A:259:GLU:HB2	2.47	0.45
1:A:253:SER:C	1:A:254:ARG:HD3	2.42	0.45
1:A:341:ASN:ND2	2:B:1:NAG:H83	2.32	0.45
1:A:267:LYS:HA	1:A:267:LYS:HD2	1.84	0.44
1:A:176[B]:GLN:NE2	1:A:180:LYS:HZ2	2.16	0.44
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.83	0.44
1:A:312:PHE:CE1	1:A:314:LYS:HE3	2.53	0.44
1:A:176[B]:GLN:NE2	1:A:180:LYS:HZ1	2.16	0.44
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.53	0.44
1:A:509:ARG:HE	1:A:509:ARG:HB3	1.29	0.43
1:A:21:PHE:O	1:A:135:ARG:NH2	2.42	0.43
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.34	0.43
1:A:195:PHE:CB	1:A:221:ILE:HB	2.48	0.43
1:A:352:GLU:HA	1:A:355:LYS:HE3	2.01	0.43
1:A:378:ASP:C	1:A:380:GLN:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:O	1:A:428:LEU:C	2.62	0.43
1:A:282:TYR:CE2	1:A:359:PRO:HB3	2.53	0.43
1:A:451:GLU:O	1:A:454:ASP:HB2	2.18	0.43
1:A:95:LEU:HD12	1:A:95:LEU:C	2.44	0.43
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.70	0.43
1:A:525:PHE:CZ	1:A:529:VAL:HG12	2.54	0.42
1:A:117:GLY:O	1:A:288:VAL:HG22	2.19	0.42
1:A:454:ASP:O	1:A:455:GLN:HB2	2.17	0.42
1:A:358:PHE:N	1:A:359:PRO:HD3	2.34	0.42
2:D:1:NAG:C6	2:D:2:NAG:HN2	2.31	0.42
1:A:339:LYS:O	1:A:431:PRO:HG3	2.19	0.42
1:A:528:LYS:N	1:A:528:LYS:CG	2.78	0.42
1:A:380:GLN:HE21	1:A:380:GLN:HB3	1.72	0.42
1:A:497:GLU:H	1:A:497:GLU:HG3	1.67	0.41
1:A:188:ASN:HD22	3:C:2:FUL:H63	1.85	0.41
1:A:284:THR:HG22	1:A:356:ILE:O	2.21	0.41
1:A:382:PRO:HD2	1:A:383:GLU:OE1	2.20	0.41
1:A:378:ASP:OD1	1:A:379:ASP:OD1	2.38	0.40
1:A:250:THR:HB	1:A:267:LYS:HE2	2.03	0.40
1:A:366:LYS:HZ3	1:A:366:LYS:HG3	1.76	0.40
1:A:381:ARG:NH2	1:A:383:GLU:HG2	2.36	0.40
1:A:452:ARG:O	1:A:454:ASP:N	2.55	0.40
1:A:485:ASN:O	1:A:486:ASN:C	2.62	0.40
2:D:1:NAG:H5	2:D:2:NAG:HN2	1.86	0.40
1:A:96:ASN:O	1:A:142:VAL:HA	2.21	0.40
1:A:159:ASN:HB2	9:A:820:HOH:O	2.20	0.40
1:A:314:LYS:HA	1:A:314:LYS:HD3	1.93	0.40
1:A:132:PHE:CE2	1:A:448:LEU:HD22	2.57	0.40
1:A:249:LEU:HG	2:D:3:FUL:H62	2.03	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	527/529 (100%)	497 (94%)	22 (4%)	8 (2%)	8 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	THR
1	A	53	THR
1	A	54	ASP
1	A	379	ASP
1	A	506	GLU
1	A	359	PRO
1	A	361	VAL
1	A	360	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	454/454 (100%)	422 (93%)	32 (7%)	14 9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	ILE
1	A	40	ARG
1	A	54	ASP
1	A	69	ILE
1	A	108	THR
1	A	154	LEU
1	A	156	LEU
1	A	195	PHE
1	A	236	LEU
1	A	254	ARG
1	A	255	GLU
1	A	259	GLU

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Mol	Chain	Res	Type
1	A	260	ILE
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	280	VAL
1	A	299	LEU
1	A	359	PRO
1	A	361	VAL
1	A	371[A]	PHE
1	A	371[B]	PHE
1	A	383	GLU
1	A	428	LEU
1	A	448	LEU
1	A	454	ASP
1	A	497	GLU
1	A	507	SER
1	A	509	ARG
1	A	510	ILE
1	A	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	126	HIS
1	A	179	GLN
1	A	289	ASN
1	A	380	GLN
1	A	517	GLN
1	A	518	GLN

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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	1.05	0	17,19,21	1.48	3 (17%)
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	1.82	3 (17%)
2	FUL	B	3	2	10,10,11	0.90	0	14,14,16	2.70	6 (42%)
3	NAG	C	1	3,1	14,14,15	0.67	0	17,19,21	1.26	3 (17%)
3	FUL	C	2	3	10,10,11	0.77	0	14,14,16	2.56	6 (42%)
2	NAG	D	1	1,2	14,14,15	0.51	0	17,19,21	1.97	4 (23%)
2	NAG	D	2	2	14,14,15	0.59	0	17,19,21	2.30	4 (23%)
2	FUL	D	3	2	10,10,11	0.86	0	14,14,16	2.29	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	6/6/23/26	0/1/1/1
2	FUL	D	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	-7.52	99.99	111.02
2	B	3	FUL	C1-C2-C3	-7.25	99.09	109.64
2	D	3	FUL	C1-C2-C3	-6.27	100.51	109.64
2	B	2	NAG	C1-O5-C5	-6.02	104.12	112.19
3	C	2	FUL	C1-C2-C3	5.72	117.97	109.64
2	D	1	NAG	C1-O5-C5	4.64	118.41	112.19
3	C	2	FUL	C2-C3-C4	4.46	118.70	110.86
2	D	3	FUL	C1-O5-C5	-4.17	103.12	112.97
2	D	1	NAG	C6-C5-C4	-3.78	103.73	113.02
2	B	3	FUL	C1-O5-C5	-3.77	104.07	112.97
2	B	3	FUL	O5-C1-C2	-3.50	102.44	110.79
2	D	1	NAG	C2-N2-C7	-3.43	118.30	122.90
3	C	2	FUL	C3-C4-C5	3.09	114.51	109.81
3	C	2	FUL	C1-O5-C5	3.02	120.10	112.97
2	B	1	NAG	O5-C1-C2	-2.94	106.75	111.29
2	D	3	FUL	C3-C4-C5	2.85	114.14	109.81
2	D	2	NAG	O3-C3-C4	2.72	116.79	110.38
2	B	3	FUL	O2-C2-C3	2.56	115.45	110.15
2	B	3	FUL	C3-C4-C5	2.55	113.68	109.81
3	C	2	FUL	O5-C5-C4	2.51	114.07	109.55
2	D	2	NAG	C1-C2-N2	2.38	114.18	110.43
2	B	1	NAG	C2-N2-C7	2.35	126.05	122.90
2	D	2	NAG	C1-O5-C5	2.32	115.30	112.19
3	C	1	NAG	C3-C4-C5	-2.28	106.09	110.23
2	B	1	NAG	O4-C4-C3	-2.23	105.11	110.38
3	C	2	FUL	O5-C1-C2	2.22	116.10	110.79
2	D	1	NAG	O4-C4-C3	-2.16	105.29	110.38
2	B	2	NAG	O6-C6-C5	-2.09	104.21	111.33
2	B	3	FUL	C6-C5-C4	2.08	116.89	113.08
3	C	1	NAG	C8-C7-N2	2.07	119.56	116.12
2	B	2	NAG	C1-C2-N2	-2.03	107.23	110.43
3	C	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (19) 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
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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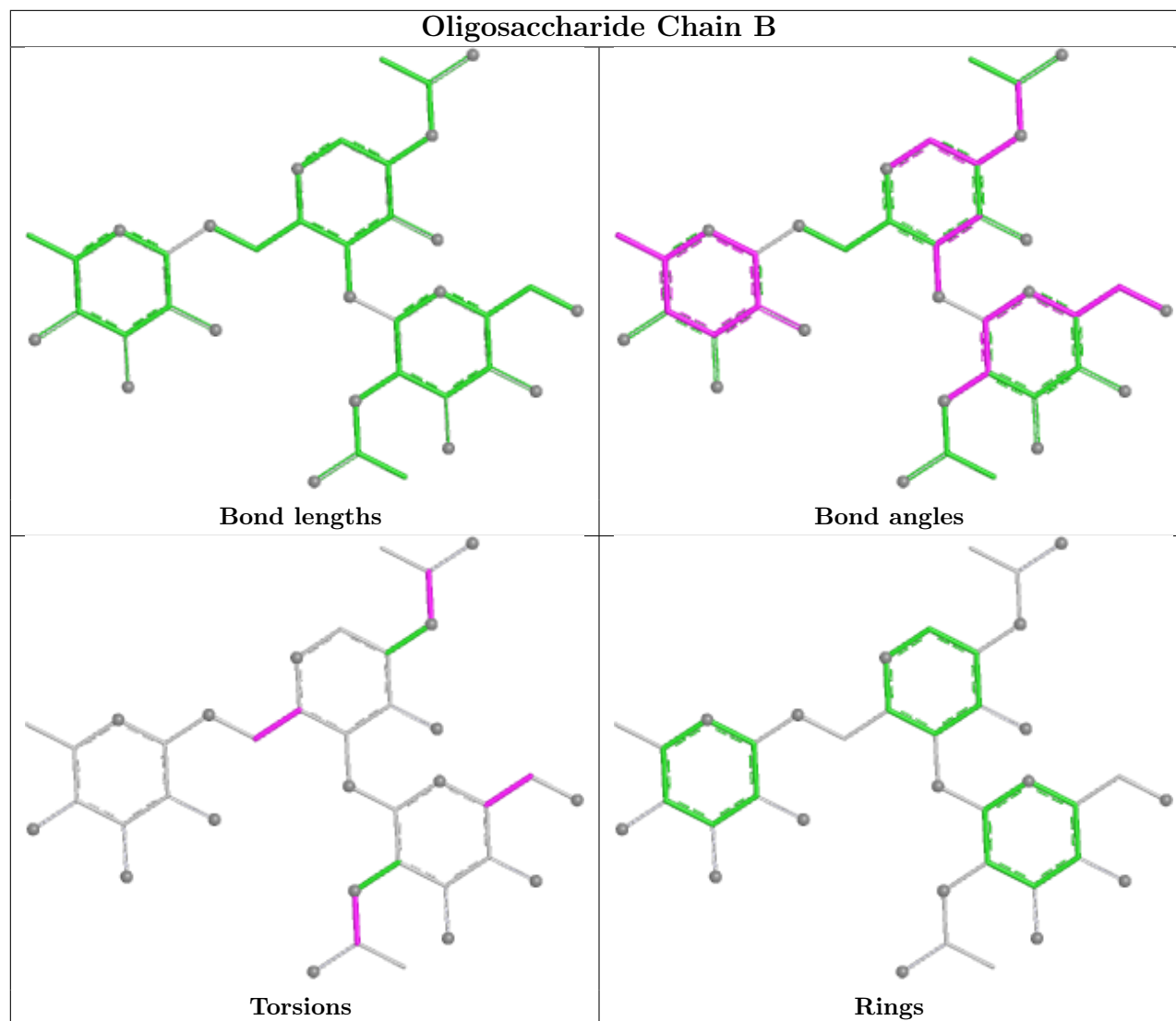
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7

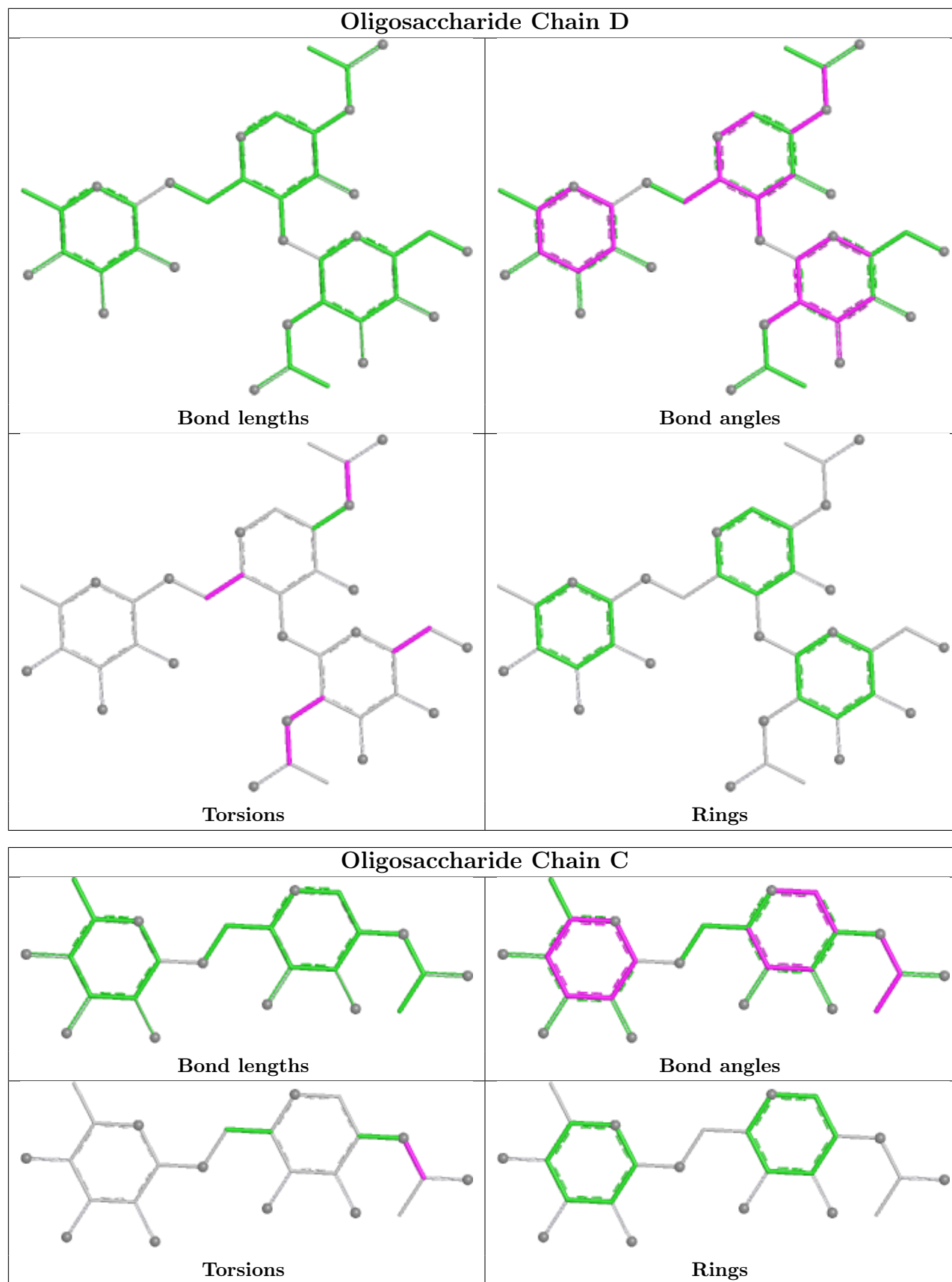
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	FUL	3	0
2	B	1	NAG	1	0
3	C	2	FUL	2	0
2	D	1	NAG	6	0
2	D	2	NAG	6	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	NAG	A	614	1	14,14,15	0.68	0	17,19,21	1.53	4 (23%)
4	TC3	A	601	1	3,6,7	1.84	1 (33%)	1,6,9	1.02	0
8	NAG	A	615	1	14,14,15	0.65	0	17,19,21	1.41	2 (11%)
6	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.44	0
6	SO4	A	607	-	4,4,4	0.44	0	6,6,6	0.27	0
8	NAG	A	616	1	14,14,15	0.52	0	17,19,21	1.60	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
8	NAG	A	614	1	-	2/6/23/26	0/1/1/1
4	TC3	A	601	1	-	0/1/5/7	-
8	NAG	A	615	1	-	1/6/23/26	0/1/1/1
8	NAG	A	616	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	TC3	C3-N	2.36	1.49	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	615	NAG	C2-N2-C7	-3.38	118.37	122.90
8	A	616	NAG	C2-N2-C7	3.28	127.30	122.90
8	A	616	NAG	O5-C1-C2	-3.18	106.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	614	NAG	O5-C1-C2	-3.11	106.48	111.29
8	A	615	NAG	O5-C5-C6	2.91	113.33	107.66
8	A	614	NAG	O5-C5-C6	2.74	112.99	107.66
8	A	614	NAG	C2-N2-C7	-2.69	119.30	122.90
8	A	614	NAG	C3-C4-C5	-2.54	105.62	110.23
8	A	616	NAG	O7-C7-C8	-2.41	117.77	122.05
8	A	616	NAG	C1-C2-N2	2.28	114.02	110.43
8	A	616	NAG	C8-C7-N2	2.10	119.59	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	NAG	C8-C7-N2-C2
8	A	614	NAG	O7-C7-N2-C2
8	A	616	NAG	C8-C7-N2-C2
8	A	616	NAG	O7-C7-N2-C2
8	A	616	NAG	O5-C5-C6-O6
8	A	615	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
6	A	603	SO4	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	527/529 (99%)	-0.01	15 (2%) 55 59	15, 30, 55, 69	11 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	5.9
1	A	22	GLY	4.0
1	A	377	VAL	3.7
1	A	379	ASP	2.9
1	A	52	TRP	2.7
1	A	361	VAL	2.5
1	A	278	PHE	2.4
1	A	282	TYR	2.3
1	A	525	PHE	2.3
1	A	53	THR	2.3
1	A	378	ASP	2.3
1	A	4	ILE	2.2
1	A	380	GLN	2.2
1	A	50	THR	2.1
1	A	255	GLU	2.0

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

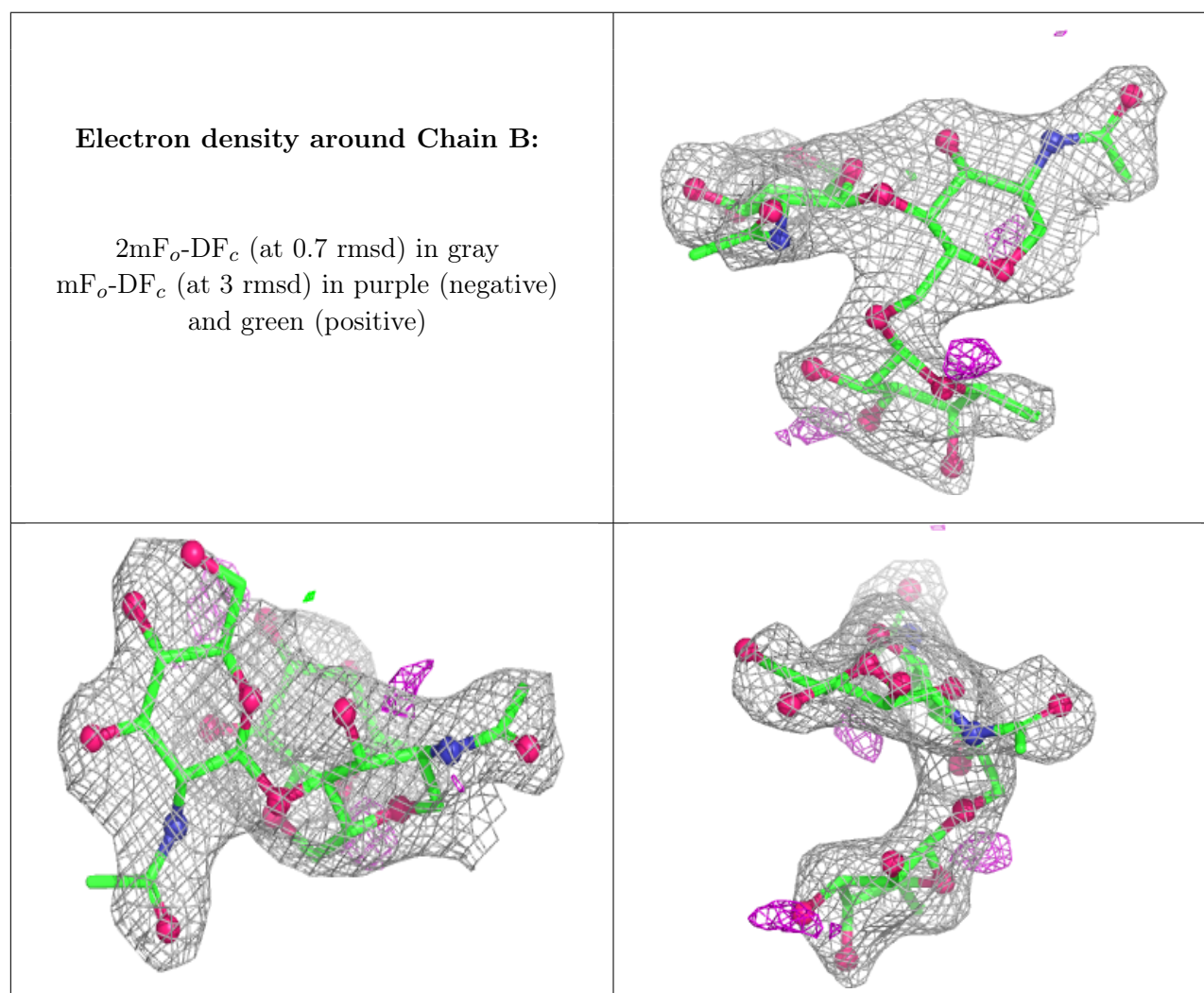
There are no non-standard protein/DNA/RNA residues in this entry.

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.

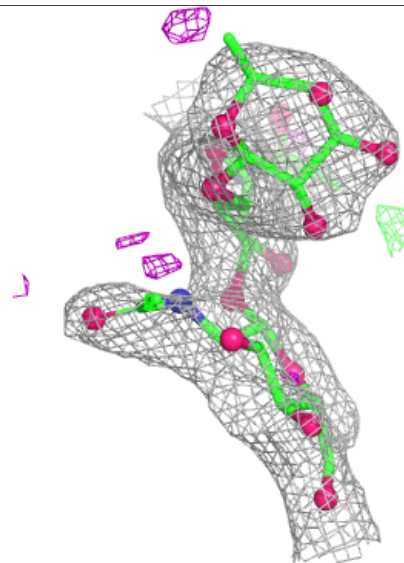
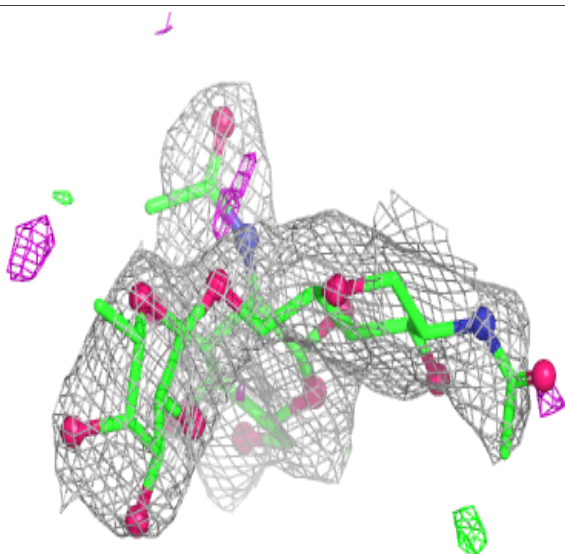
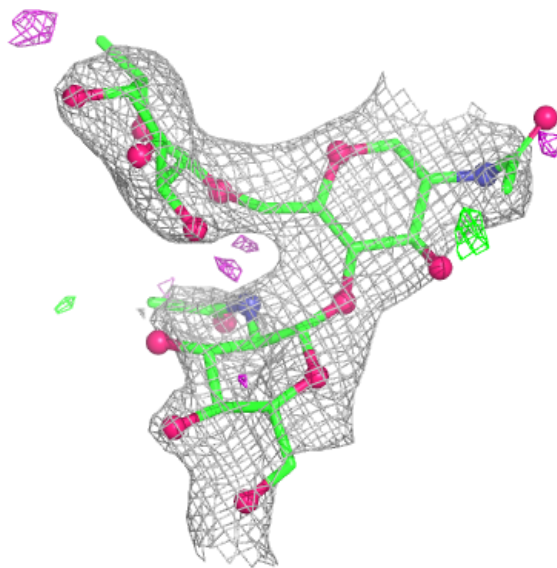
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.70	0.17	73,79,81,82	0
2	FUL	B	3	10/11	0.76	0.16	64,68,69,72	0
2	NAG	B	2	14/15	0.78	0.14	64,68,71,73	0
3	NAG	C	1	14/15	0.78	0.14	58,63,68,72	0
3	FUL	C	2	10/11	0.79	0.18	76,78,79,79	0
2	NAG	D	1	14/15	0.81	0.17	67,74,78,81	0
2	NAG	B	1	14/15	0.92	0.11	44,50,59,61	0
2	FUL	D	3	10/11	0.92	0.12	67,68,69,69	0

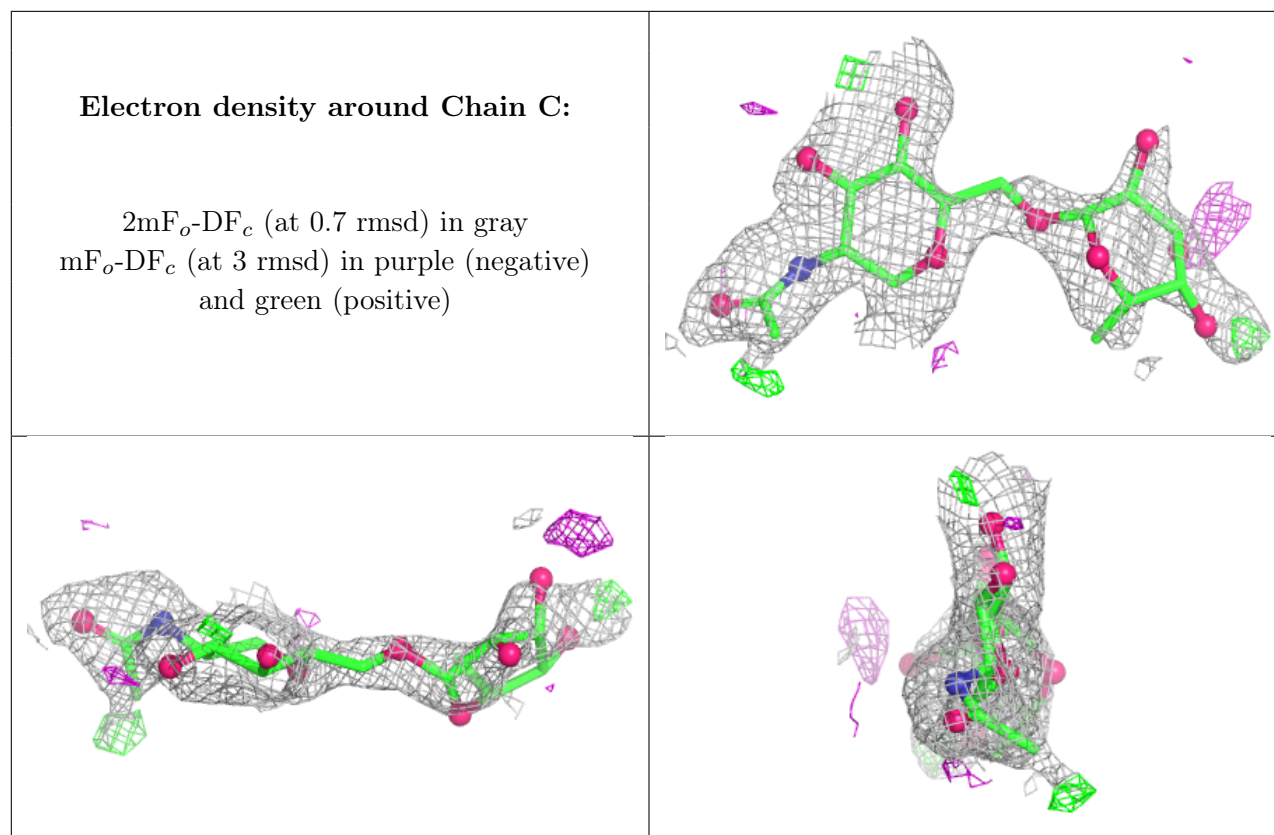
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (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, 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
8	NAG	A	614	14/15	0.62	0.18	75,80,83,83	0
8	NAG	A	616	14/15	0.63	0.17	83,87,88,89	0
8	NAG	A	615	14/15	0.79	0.14	52,67,71,71	0
7	CL	A	604	1/1	0.83	0.16	75,75,75,75	0
7	CL	A	605	1/1	0.89	0.15	73,73,73,73	0
6	SO4	A	603	5/5	0.92	0.10	47,48,49,51	5
7	CL	A	606	1/1	0.93	0.17	71,71,71,71	0
7	CL	A	608	1/1	0.94	0.17	63,63,63,63	0
5	NA	A	602	1/1	0.94	0.34	64,64,64,64	1
6	SO4	A	607	5/5	0.97	0.10	33,33,37,38	5
4	TC3	A	601	7/8	0.99	0.06	26,27,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.