



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:17 AM UTC

PDB ID : 3DKK / pdb_00003dkk
Title : Aged Form of Human Butyrylcholinesterase Inhibited by Tabun
Authors : Nachon, F.; Carletti, E.
Deposited on : 2008-06-25
Resolution : 2.31 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

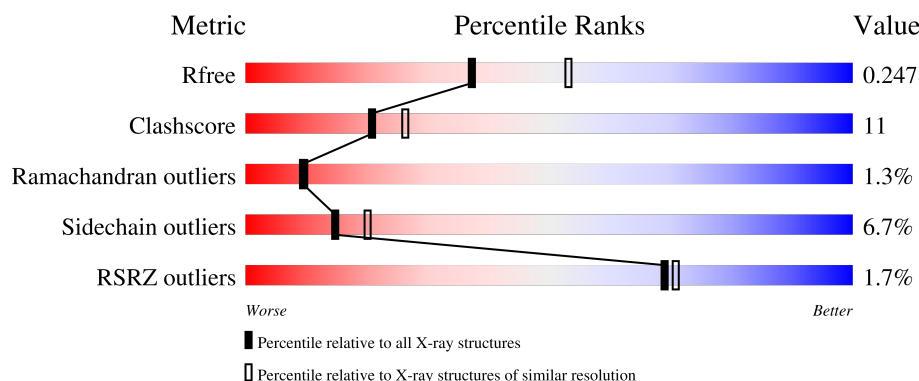
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	2% 75% 19% ..
2	B	3	33% 33% 33%
2	D	3	67% 33%
3	C	2	50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

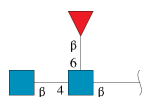
- Molecule 1 is a protein called Cholinesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	527	4215	2717	710	772	1	15	0	2	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	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl	0	0
			2 2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

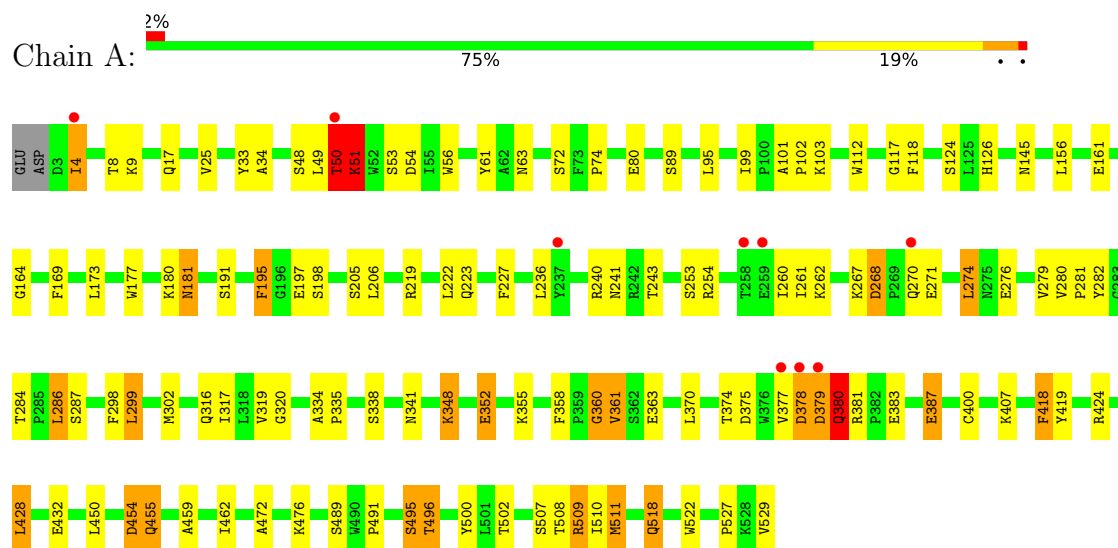
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	254	Total	O	0	0
			254	254		

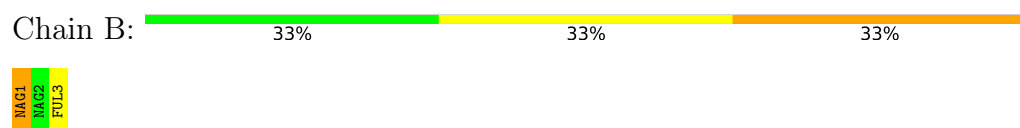
3 Residue-property plots [i](#)

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

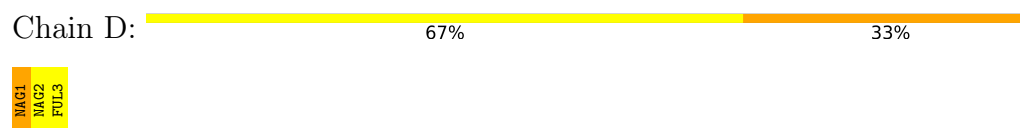
- Molecule 1: Cholinesterase



- 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	155.24Å 155.24Å 127.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.18 – 2.31 28.18 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.18-2.31) 99.0 (28.18-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.251 0.196 , 0.247	Depositor DCC
R_{free} test set	1709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: CL, SEN, NA, FUL, SO4, NAG

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	1.04	4/4327 (0.1%)	1.17	18/5873 (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	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	ILE	CA-CB	7.37	1.63	1.54
1	A	50	THR	CA-CB	5.70	1.62	1.53
1	A	418	PHE	C-O	5.16	1.30	1.24
1	A	400	CYS	CA-C	5.08	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLY	N-CA-C	-8.15	103.73	112.04
1	A	459	ALA	N-CA-C	-7.19	103.17	112.23
1	A	358	PHE	CA-C-N	7.07	128.68	119.84
1	A	358	PHE	C-N-CA	7.07	128.68	119.84
1	A	400	CYS	CA-C-N	-6.71	111.90	119.28
1	A	400	CYS	C-N-CA	-6.71	111.90	119.28
1	A	268	ASP	CB-CA-C	6.65	118.78	108.61
1	A	509	ARG	N-CA-C	6.44	119.50	109.52
1	A	352	GLU	N-CA-C	-6.43	104.35	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	SER	CA-C-N	-5.98	115.92	123.15
1	A	72	SER	C-N-CA	-5.98	115.92	123.15
1	A	302	MET	CA-C-N	-5.84	113.67	119.56
1	A	302	MET	C-N-CA	-5.84	113.67	119.56
1	A	180	LYS	N-CA-C	5.38	117.15	111.28
1	A	454	ASP	N-CA-C	5.23	119.53	113.20
1	A	450	LEU	N-CA-C	-5.19	106.46	112.89
1	A	181	ASN	N-CA-C	5.16	120.58	113.97
1	A	164	GLY	CA-C-O	-5.00	118.85	122.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	380	GLN	Peptide

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	4215	0	4113	95	2
2	B	38	0	34	1	0
2	D	38	0	34	1	0
3	C	24	0	22	1	0
4	A	42	0	39	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
8	A	254	0	0	13	2
All	All	4619	0	4242	95	2

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 11.

All (95) 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:380:GLN:HE21	1:A:380:GLN:N	1.67	0.93
1:A:4:ILE:H	1:A:4:ILE:HD12	1.33	0.92
1:A:518:GLN:HE21	1:A:518:GLN:H	1.12	0.92
1:A:518:GLN:H	1:A:518:GLN:NE2	1.71	0.88
1:A:379:ASP:O	1:A:380:GLN:HB2	1.75	0.86
1:A:4:ILE:HD12	1:A:4:ILE:N	1.94	0.82
1:A:379:ASP:HB3	1:A:381:ARG:HG3	1.63	0.80
1:A:355:LYS:HD3	8:A:743:HOH:O	1.81	0.79
1:A:495:SER:HA	8:A:713:HOH:O	1.83	0.77
1:A:380:GLN:HE21	1:A:380:GLN:CA	1.97	0.75
1:A:282:TYR:CB	8:A:700:HOH:O	2.35	0.74
1:A:378:ASP:OD1	1:A:378:ASP:C	2.31	0.73
1:A:53:SER:O	8:A:729:HOH:O	2.06	0.72
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.72	0.70
1:A:495:SER:O	1:A:496:THR:OG1	2.08	0.68
1:A:378:ASP:O	1:A:380:GLN:NE2	2.27	0.68
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.75	0.68
1:A:227:PHE:CD2	1:A:227:PHE:C	2.72	0.67
1:A:375:ASP:HB2	8:A:720:HOH:O	1.95	0.66
1:A:496:THR:N	8:A:713:HOH:O	2.21	0.65
1:A:380:GLN:H	1:A:381:ARG:HB2	1.59	0.65
1:A:4:ILE:HG12	1:A:17:GLN:OE1	1.98	0.63
1:A:518:GLN:HE21	1:A:518:GLN:N	1.90	0.63
1:A:378:ASP:O	1:A:380:GLN:N	2.32	0.62
1:A:495:SER:CA	8:A:713:HOH:O	2.47	0.60
1:A:377:VAL:HG13	1:A:377:VAL:O	2.00	0.60
1:A:48:SER:CB	8:A:732:HOH:O	2.50	0.60
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.36	0.60
1:A:370:LEU:HD12	1:A:374:THR:HG21	1.83	0.59
1:A:54:ASP:HB2	8:A:729:HOH:O	2.01	0.59
1:A:383:GLU:O	1:A:387:GLU:HG2	2.04	0.57
1:A:522:TRP:O	1:A:527:PRO:HD3	2.04	0.56
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.21	0.56
1:A:495:SER:O	1:A:496:THR:CB	2.53	0.55
1:A:253:SER:O	1:A:254:ARG:HD3	2.06	0.55
1:A:454:ASP:O	1:A:455:GLN:HB2	2.06	0.55
1:A:380:GLN:N	1:A:381:ARG:HB2	2.23	0.53
1:A:267:LYS:HE3	1:A:271:GLU:OE1	2.08	0.53
1:A:48:SER:HA	8:A:732:HOH:O	2.10	0.52
1:A:219:ARG:HD3	1:A:316:GLN:OE1	2.10	0.51
1:A:48:SER:HB3	8:A:732:HOH:O	2.11	0.51
1:A:206:LEU:HD21	1:A:227:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PRO:HG3	2:D:1:NAG:H83	1.94	0.50
1:A:380:GLN:CA	1:A:380:GLN:NE2	2.71	0.50
1:A:74:PRO:HA	1:A:80:GLU:OE1	2.13	0.49
1:A:284:THR:C	1:A:286:LEU:H	2.19	0.49
1:A:126:HIS:HD2	8:A:752:HOH:O	1.94	0.49
1:A:383:GLU:O	1:A:387:GLU:CG	2.61	0.48
1:A:495:SER:O	1:A:496:THR:HG23	2.13	0.48
1:A:49:LEU:HD12	1:A:50:THR:H	1.79	0.48
1:A:56:TRP:C	1:A:56:TRP:CD1	2.92	0.47
1:A:112:TRP:HA	1:A:195:PHE:O	2.14	0.47
1:A:95:LEU:HD12	1:A:95:LEU:C	2.39	0.47
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.47
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.50	0.47
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.82	0.47
1:A:377:VAL:N	1:A:378:ASP:HA	2.30	0.47
1:A:472:ALA:O	1:A:476:LYS:HG3	2.15	0.46
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.66	0.46
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.50	0.46
1:A:25:VAL:HG13	1:A:99:ILE:O	2.15	0.46
1:A:63:ASN:HB3	1:A:89:SER:HB3	1.98	0.46
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.98	0.46
1:A:454:ASP:O	1:A:455:GLN:CB	2.63	0.45
1:A:191:SER:HB2	3:C:2:FUL:H3	1.98	0.45
1:A:177:TRP:O	1:A:181:ASN:HB2	2.17	0.45
1:A:270:GLN:O	1:A:274:LEU:HB2	2.17	0.45
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.98	0.45
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.99	0.44
1:A:276:GLU:O	1:A:279:VAL:HG22	2.16	0.44
1:A:495:SER:C	1:A:496:THR:HG23	2.41	0.44
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.65	0.44
1:A:338:SER:HB2	2:B:1:NAG:H62	1.99	0.44
1:A:284:THR:C	1:A:286:LEU:N	2.75	0.44
1:A:33:TYR:OH	1:A:145:ASN:O	2.31	0.44
1:A:4:ILE:N	1:A:4:ILE:CD1	2.61	0.43
1:A:317:ILE:HD12	1:A:319:VAL:HG21	1.99	0.43
1:A:240:ARG:O	1:A:241:ASN:C	2.62	0.43
1:A:50:THR:O	1:A:51:LYS:CB	2.67	0.43
1:A:317:ILE:HD12	1:A:319:VAL:CG2	2.49	0.43
1:A:102:PRO:O	1:A:103:LYS:C	2.62	0.43
1:A:502:THR:O	1:A:508:THR:HB	2.19	0.42
1:A:378:ASP:OD1	1:A:380:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.55	0.42
1:A:169:PHE:CZ	1:A:298:PHE:HB2	2.55	0.42
1:A:156:LEU:HD22	1:A:261:ILE:HD11	2.02	0.42
1:A:507:SER:O	1:A:507:SER:OG	2.38	0.41
1:A:101:ALA:HA	1:A:102:PRO:C	2.44	0.41
1:A:48:SER:CA	8:A:732:HOH:O	2.65	0.41
1:A:50:THR:O	1:A:51:LYS:HB3	2.21	0.41
1:A:117:GLY:O	1:A:118:PHE:HB2	2.21	0.41
1:A:254:ARG:HB2	1:A:260:ILE:CG1	2.50	0.41
1:A:197:GLU:HA	1:A:223:GLN:O	2.21	0.41
1:A:341:ASN:OD1	1:A:341:ASN:C	2.64	0.40
1:A:491:PRO:CD	1:A:510:ILE:HD12	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:CG	8:A:747:HOH:O[7_555]	2.10	0.10
1:A:379:ASP:OD2	8:A:747:HOH:O[7_555]	2.18	0.02

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	526/529 (99%)	494 (94%)	25 (5%)	7 (1%)	9 10

All (7) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	361	VAL
1	A	378	ASP
1	A	380	GLN
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	452/453 (100%)	422 (93%)	30 (7%)	15	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	THR
1	A	9	LYS
1	A	50	THR
1	A	51	LYS
1	A	161	GLU
1	A	195	PHE
1	A	236	LEU
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	280	VAL
1	A	286	LEU
1	A	287	SER
1	A	299	LEU
1	A	348	LYS
1	A	361	VAL
1	A	363	GLU
1	A	380	GLN
1	A	387	GLU
1	A	407	LYS
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	432	GLU
1	A	455	GLN
1	A	489	SER
1	A	495	SER
1	A	509	ARG
1	A	511	MET
1	A	518	GLN
1	A	529	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	214	HIS
1	A	289	ASN
1	A	311	GLN
1	A	351	GLN
1	A	380	GLN
1	A	455	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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEN	A	198	1	10,11,12	1.34	1 (10%)	7,15,17	2.83	4 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEN	A	198	1	-	4/10/14/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEN	P-N1	3.67	1.70	1.62

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEN	OG-CB-CA	4.94	112.96	108.14
1	A	198	SEN	O2-P-O3	3.87	119.04	109.86
1	A	198	SEN	OG-P-O3	-3.20	105.49	115.71
1	A	198	SEN	OG-P-N1	2.35	112.91	105.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEN	C1-N1-P-OG
1	A	198	SEN	N-CA-CB-OG
1	A	198	SEN	CB-OG-P-O3
1	A	198	SEN	C2-N1-P-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	0.95	1 (7%)	17,19,21	1.97	8 (47%)
2	NAG	B	2	2	14,14,15	0.74	0	17,19,21	0.87	0
2	FUL	B	3	2	10,10,11	0.89	0	14,14,16	2.24	6 (42%)
3	NAG	C	1	1,3	14,14,15	1.10	1 (7%)	17,19,21	2.26	9 (52%)
3	FUL	C	2	3	10,10,11	0.92	0	14,14,16	1.78	4 (28%)
2	NAG	D	1	1,2	14,14,15	0.62	0	17,19,21	1.96	5 (29%)
2	NAG	D	2	2	14,14,15	0.71	1 (7%)	17,19,21	2.78	8 (47%)
2	FUL	D	3	2	10,10,11	0.86	0	14,14,16	2.19	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsions 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	-	3/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	FUL	D	3	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	2.92	1.56	1.52
2	B	1	NAG	O5-C1	-2.10	1.40	1.43
2	D	2	NAG	C1-C2	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	-6.20	101.94	111.02
2	D	1	NAG	C1-O5-C5	5.61	119.70	112.19
2	D	3	FUL	C1-C2-C3	-4.94	102.45	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	4.55	118.28	112.19
2	D	3	FUL	C3-C4-C5	4.31	116.37	109.81
2	D	2	NAG	C3-C4-C5	-4.29	102.45	110.23
2	B	3	FUL	C3-C4-C5	4.19	116.17	109.81
3	C	1	NAG	O5-C5-C6	3.97	115.39	107.66
2	D	2	NAG	C1-C2-N2	3.95	116.66	110.43
2	B	3	FUL	C1-O5-C5	-3.59	104.50	112.97
2	B	3	FUL	O5-C1-C2	-3.59	102.23	110.79
3	C	2	FUL	C1-C2-C3	-3.59	104.42	109.64
2	B	1	NAG	O6-C6-C5	3.26	122.42	111.33
3	C	1	NAG	O4-C4-C5	3.20	117.21	109.32
2	B	1	NAG	C2-N2-C7	3.19	127.17	122.90
2	D	2	NAG	O3-C3-C2	3.07	115.78	109.40
2	D	3	FUL	C1-O5-C5	-3.04	105.80	112.97
2	B	3	FUL	C2-C3-C4	3.01	116.15	110.86
3	C	1	NAG	C8-C7-N2	3.00	121.09	116.12
3	C	1	NAG	C1-O5-C5	2.96	116.15	112.19
2	B	1	NAG	O5-C1-C2	-2.87	106.84	111.29
3	C	2	FUL	C3-C4-C5	2.78	114.04	109.81
3	C	1	NAG	C3-C4-C5	-2.62	105.48	110.23
3	C	1	NAG	O5-C1-C2	-2.57	107.31	111.29
3	C	2	FUL	O5-C1-C2	-2.56	104.68	110.79
2	D	2	NAG	O4-C4-C3	2.55	116.39	110.38
3	C	1	NAG	O3-C3-C2	2.53	114.66	109.40
2	D	2	NAG	O3-C3-C4	2.52	116.32	110.38
2	B	3	FUL	C1-C2-C3	-2.49	106.02	109.64
2	D	1	NAG	O5-C5-C6	-2.45	102.90	107.66
2	B	1	NAG	C3-C4-C5	-2.45	105.80	110.23
2	D	3	FUL	O2-C2-C1	2.45	114.82	109.22
2	D	1	NAG	O5-C1-C2	-2.31	107.72	111.29
2	D	1	NAG	O7-C7-C8	-2.25	118.04	122.05
3	C	2	FUL	C1-O5-C5	-2.25	107.66	112.97
2	B	1	NAG	C6-C5-C4	2.25	118.53	113.02
2	D	1	NAG	C8-C7-N2	2.23	119.82	116.12
2	B	1	NAG	O5-C5-C6	2.23	112.00	107.66
2	B	3	FUL	O5-C5-C6	2.11	111.99	107.40
3	C	1	NAG	O5-C5-C4	-2.09	105.74	110.83
2	D	2	NAG	O5-C5-C6	2.07	111.68	107.66
3	C	1	NAG	O6-C6-C5	2.03	118.24	111.33
2	B	1	NAG	C8-C7-N2	2.01	119.44	116.12
2	B	1	NAG	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

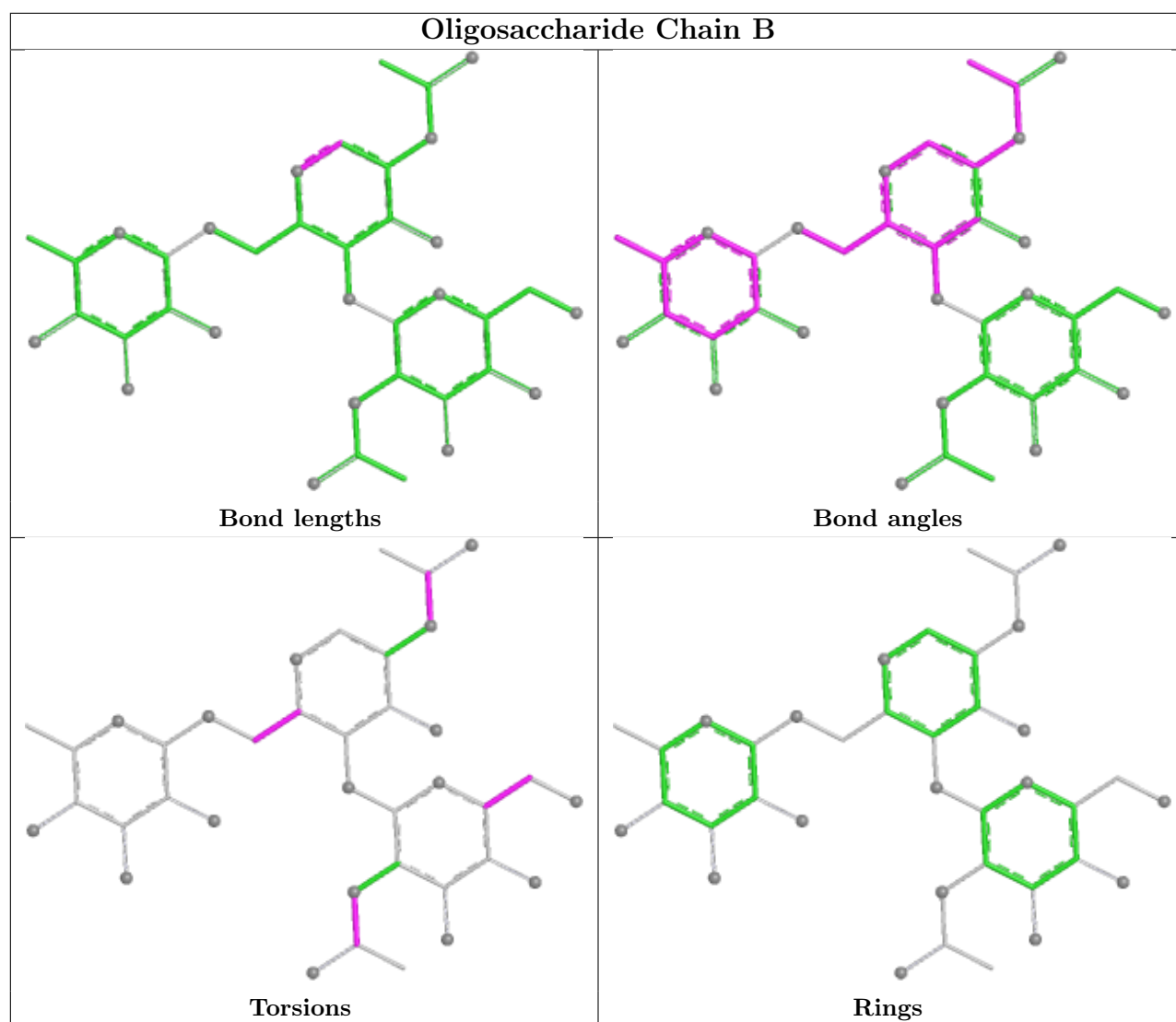
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6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

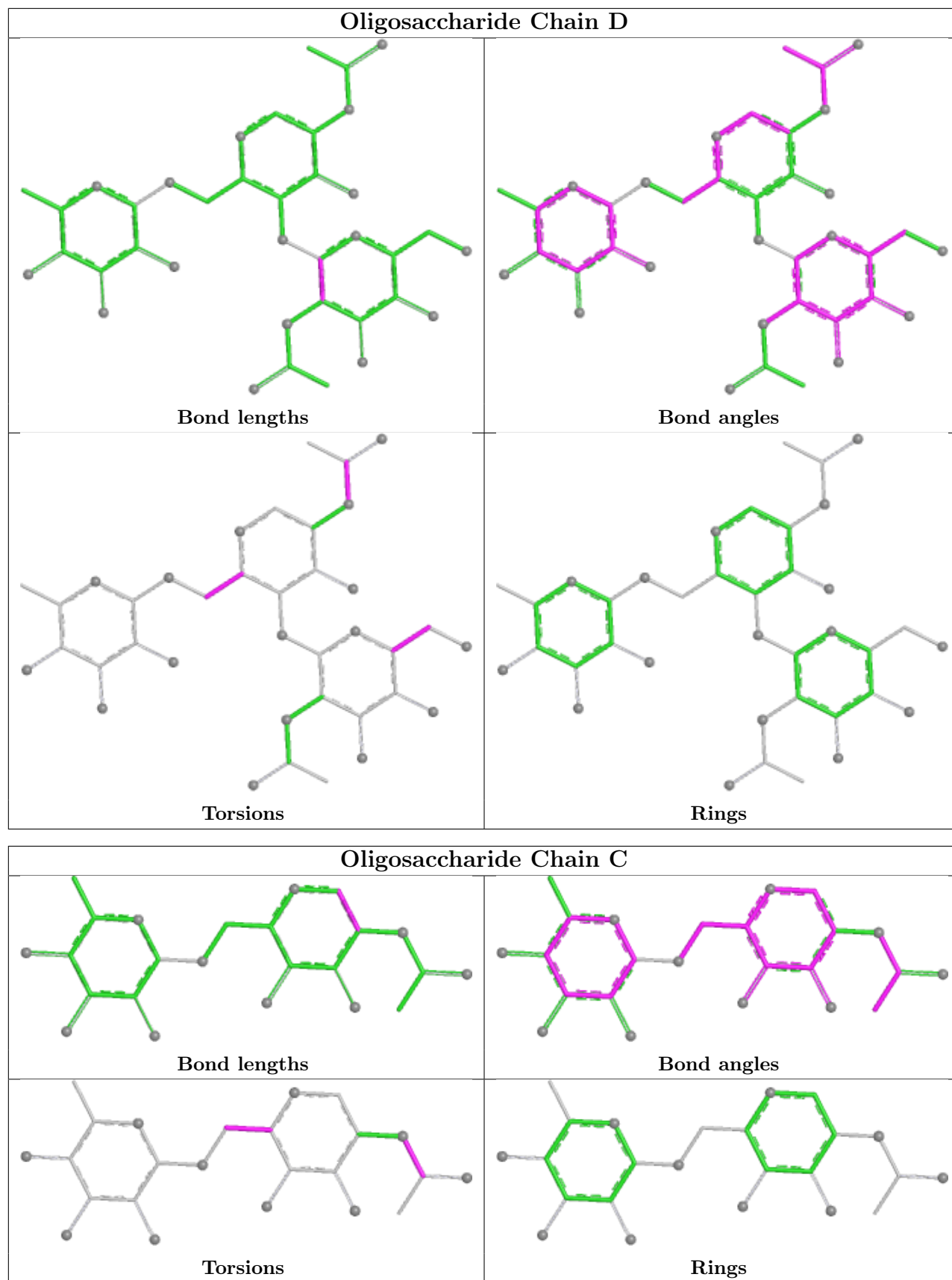
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	FUL	1	0
2	D	1	NAG	1	0
2	B	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	NAG	A	537	1	14,14,15	0.67	0	17,19,21	1.53	4 (23%)
4	NAG	A	536	1	14,14,15	0.82	0	17,19,21	1.26	2 (11%)
7	SO4	A	544	-	4,4,4	0.35	0	6,6,6	0.46	0
4	NAG	A	535	1	14,14,15	0.64	0	17,19,21	2.14	4 (23%)

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
4	NAG	A	537	1	-	2/6/23/26	0/1/1/1
4	NAG	A	536	1	-	0/6/23/26	0/1/1/1
4	NAG	A	535	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	535	NAG	O5-C1-C2	-5.76	102.38	111.29
4	A	537	NAG	C2-N2-C7	3.69	127.85	122.90
4	A	535	NAG	C2-N2-C7	-3.65	118.00	122.90
4	A	535	NAG	C1-O5-C5	3.02	116.24	112.19
4	A	535	NAG	C1-C2-N2	2.83	114.90	110.43
4	A	536	NAG	O5-C1-C2	-2.83	106.91	111.29
4	A	537	NAG	O5-C5-C6	2.52	112.57	107.66
4	A	536	NAG	O7-C7-C8	-2.27	118.01	122.05
4	A	537	NAG	C8-C7-N2	2.18	119.73	116.12
4	A	537	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	535	NAG	C8-C7-N2-C2
4	A	535	NAG	O7-C7-N2-C2
4	A	537	NAG	C8-C7-N2-C2
4	A	537	NAG	O7-C7-N2-C2
4	A	535	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	526/529 (99%)	-0.22	9 (1%) 69 71	19, 35, 61, 82	11 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	4.4
1	A	377	VAL	4.1
1	A	270	GLN	3.2
1	A	50	THR	3.0
1	A	259	GLU	2.6
1	A	237	TYR	2.6
1	A	379	ASP	2.3
1	A	378	ASP	2.1
1	A	4	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

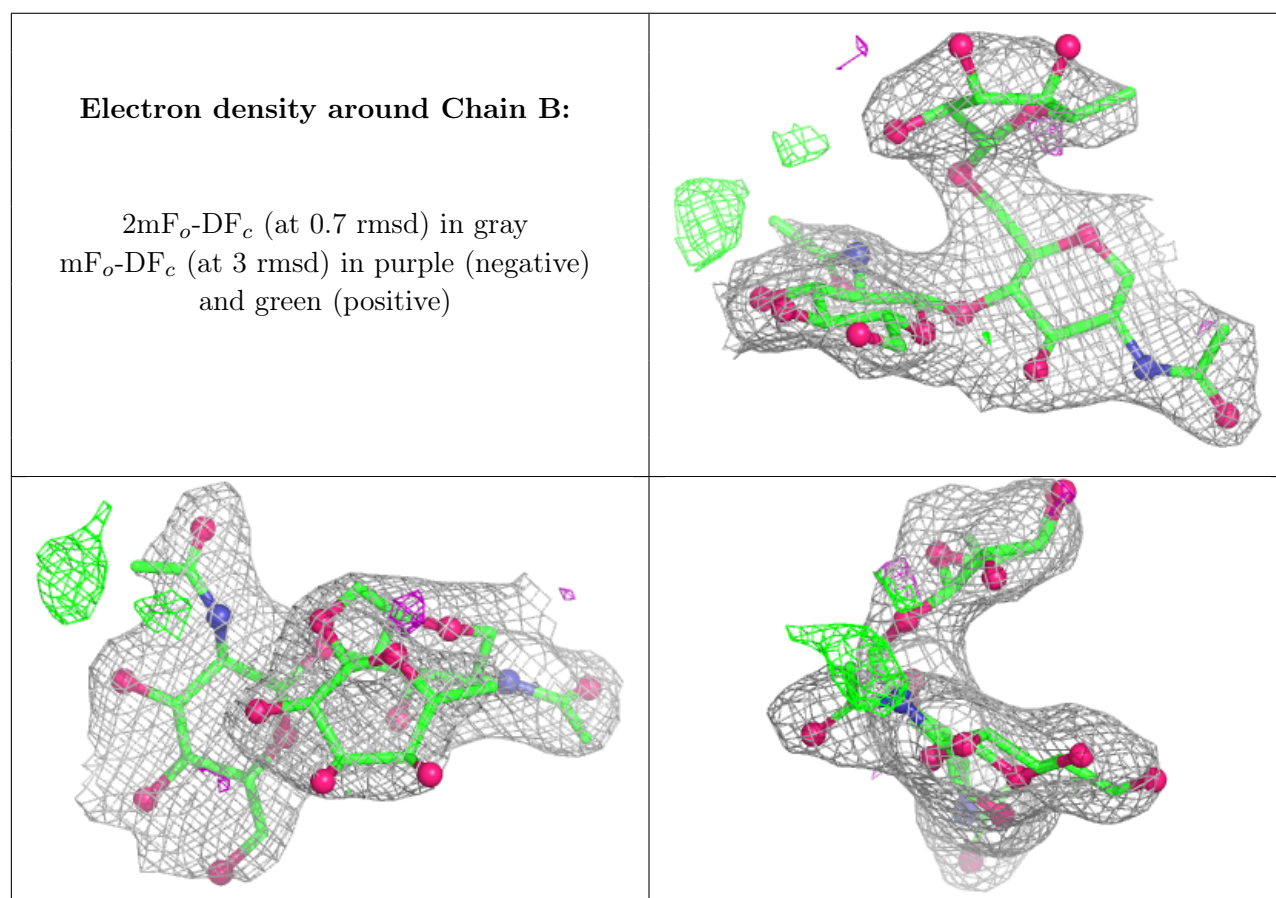
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEN	A	198	12/13	0.98	0.05	24,25,27,28	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

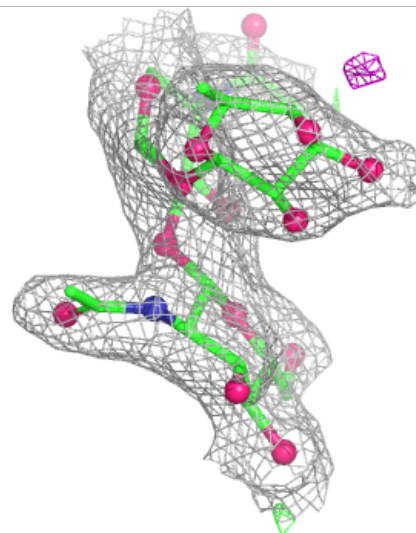
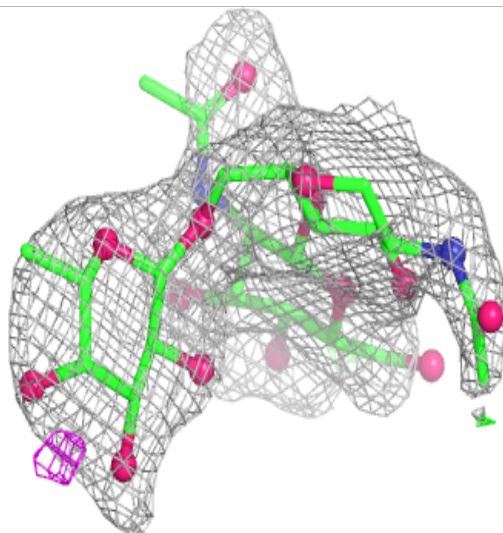
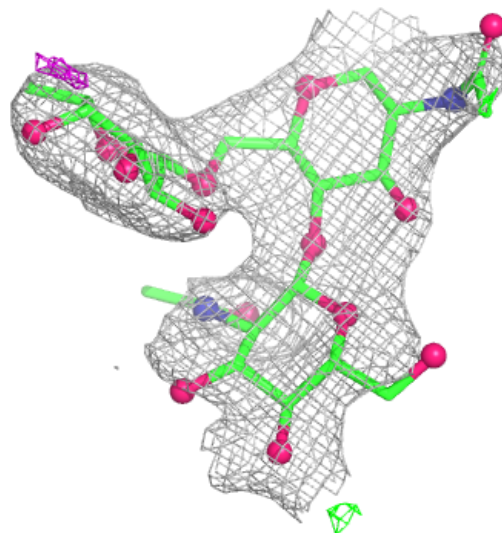
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.70	0.16	85,89,91,91	0
2	NAG	B	2	14/15	0.76	0.13	69,73,76,76	0
3	FUL	C	2	10/11	0.77	0.30	44,46,48,49	10
2	FUL	B	3	10/11	0.78	0.15	71,74,76,76	0
2	NAG	D	1	14/15	0.80	0.14	74,78,83,83	0
3	NAG	C	1	14/15	0.83	0.13	56,62,64,65	0
2	FUL	D	3	10/11	0.90	0.11	73,75,77,77	0
2	NAG	B	1	14/15	0.94	0.09	47,54,63,66	0

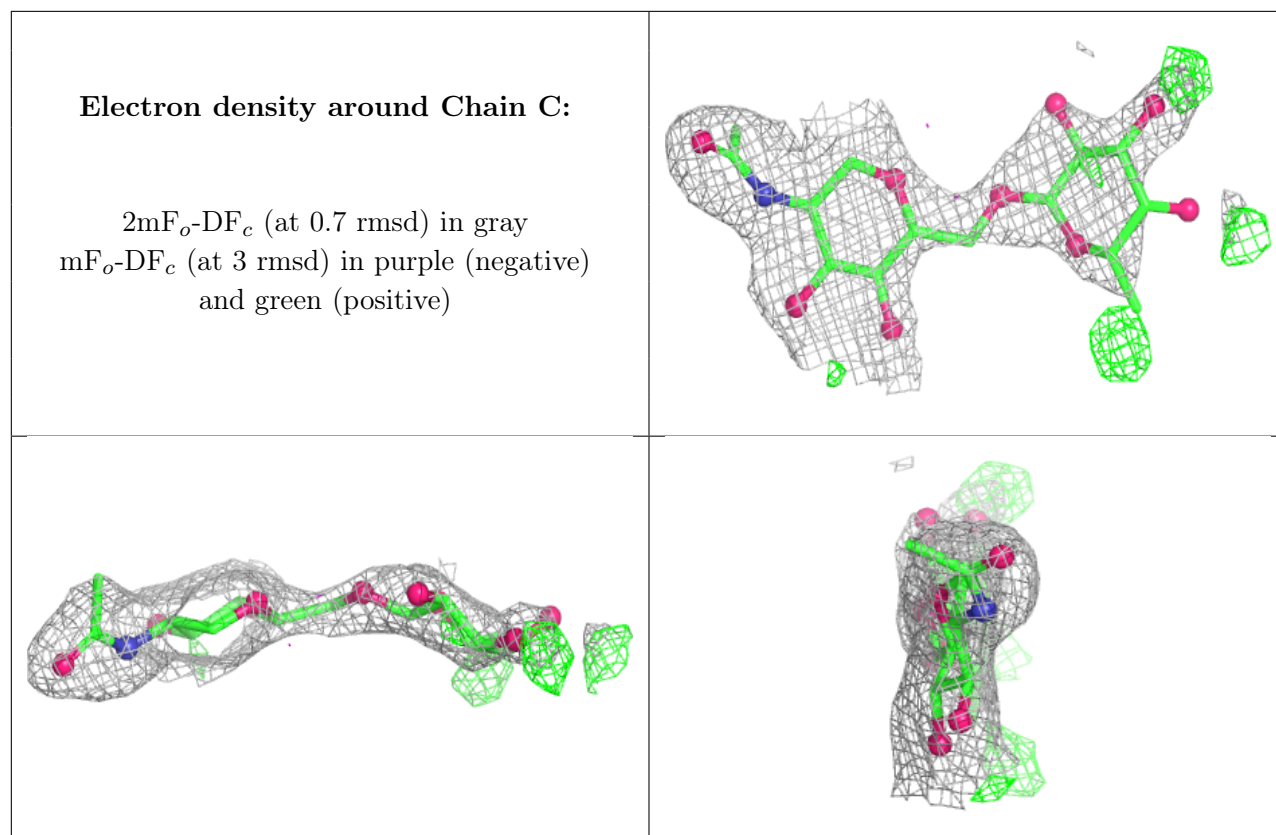
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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 [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
4	NAG	A	537	14/15	0.64	0.16	90,95,97,97	0
4	NAG	A	535	14/15	0.67	0.14	74,79,80,80	0
4	NAG	A	536	14/15	0.78	0.14	60,73,76,76	0
6	NA	A	543	1/1	0.89	0.22	57,57,57,57	1
5	CL	A	542	1/1	0.90	0.14	57,57,57,57	0
5	CL	A	541	1/1	0.96	0.15	63,63,63,63	0
7	SO4	A	544	5/5	0.96	0.07	40,42,46,47	5

6.5 Other polymers [i](#)

There are no such residues in this entry.