



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:07 PM BST

PDB ID : 2WIK  
Title : NONAGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA6  
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Deposited on : 2009-05-12  
Resolution : 2.10 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

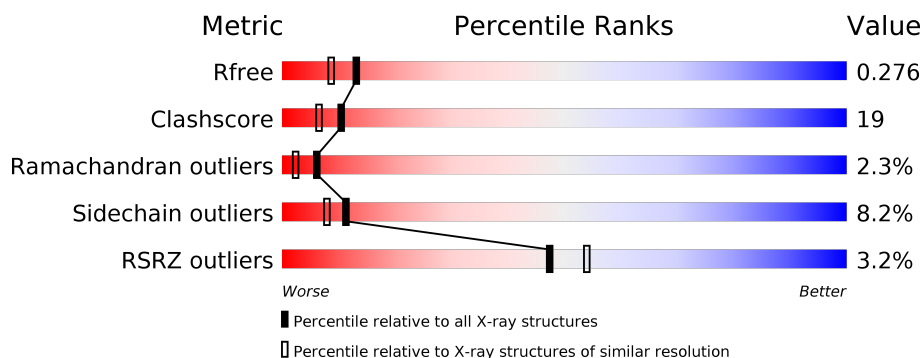
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>8%</div> </div> </div>
2	B	3	<div> <div>100%</div> </div>
2	D	3	<div> <div>100%</div> </div>
3	C	2	<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
8	NAG	A	615	X	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4754 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.

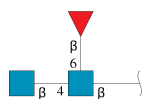
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4205	2713	709	768	15	0	2	0

There are 3 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

- 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.



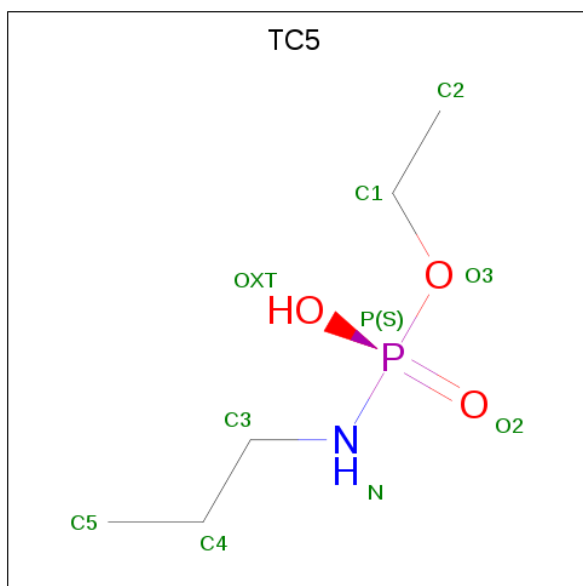
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

- 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 PROPYLAMIDOPHOSPHATE (three-letter code: TC5) (formula:  $C_5H_{14}NO_3P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			9	5	1	2	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (three-letter code: 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 SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

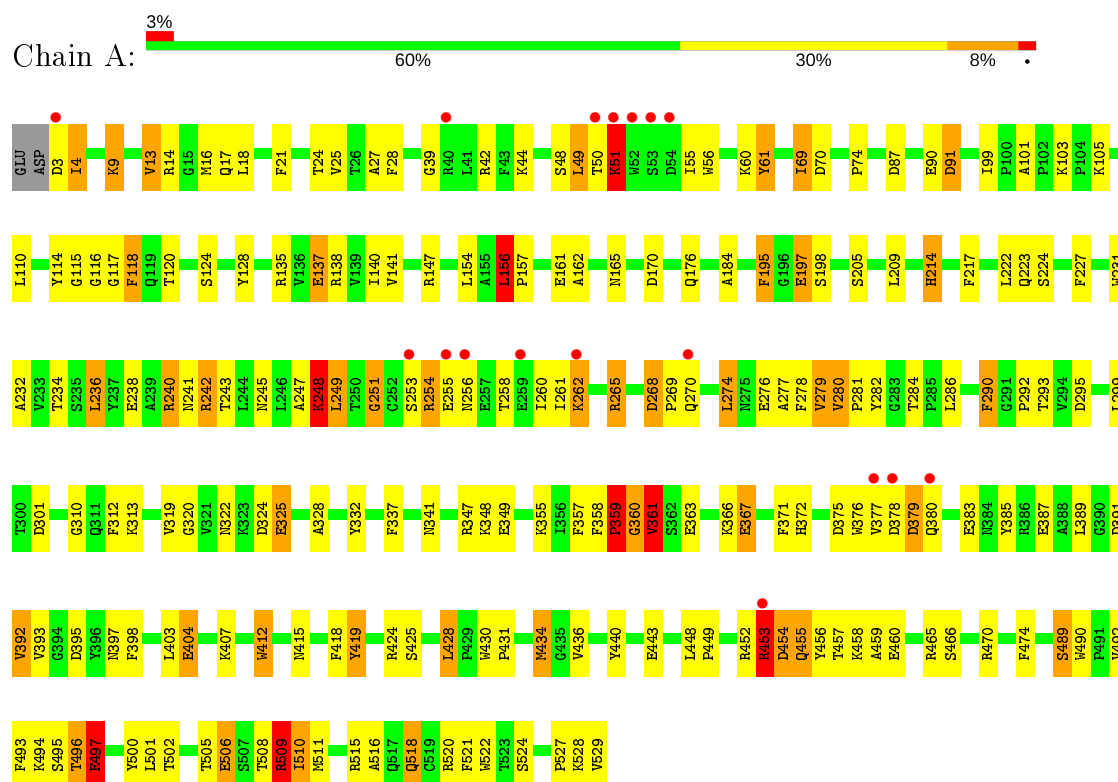
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	384	Total	O	0	0
			384	384		

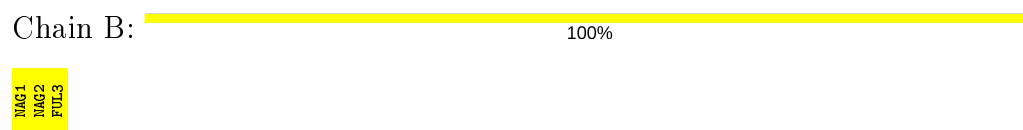
### 3 Residue-property plots

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.

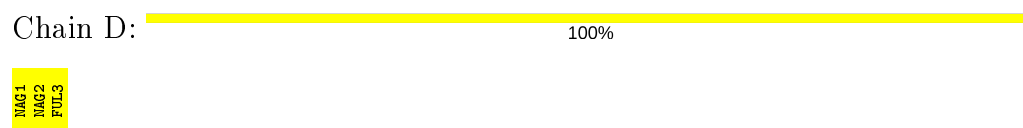
#### • Molecule 1: CHOLINESTERASE



#### • 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

Chain C:

100%

MA61  
FOI2

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.24Å 155.24Å 127.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 2.10 55.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.05-2.10) 99.7 (55.05-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.213 , 0.276 0.214 , 0.276	Depositor DCC
$R_{free}$ test set	1358 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 73.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, CL, NA, TC5, SO4, FUL

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	1.59	45/4330 (1.0%)	1.36	36/5879 (0.6%)

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

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLU	CG-CD	10.03	1.67	1.51
1	A	398	PHE	CE2-CZ	9.74	1.55	1.37
1	A	419	TYR	CD1-CE1	8.64	1.52	1.39
1	A	371	PHE	CE1-CZ	8.53	1.53	1.37
1	A	118	PHE	CE2-CZ	7.85	1.52	1.37
1	A	197	GLU	CB-CG	7.45	1.66	1.52
1	A	255	GLU	CG-CD	7.17	1.62	1.51
1	A	404	GLU	CG-CD	7.00	1.62	1.51
1	A	255	GLU	CB-CG	6.97	1.65	1.52
1	A	231	TRP	CE3-CZ3	6.77	1.50	1.38
1	A	371	PHE	CD2-CE2	6.64	1.52	1.39
1	A	114	TYR	CE2-CZ	-6.47	1.30	1.38
1	A	90	GLU	CG-CD	-6.46	1.42	1.51
1	A	61	TYR	CD1-CE1	6.42	1.49	1.39
1	A	443	GLU	CD-OE1	6.40	1.32	1.25
1	A	268	ASP	CB-CG	6.39	1.65	1.51
1	A	419	TYR	CZ-OH	6.25	1.48	1.37
1	A	419	TYR	CD2-CE2	6.23	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	VAL	CB-CG2	-6.13	1.40	1.52
1	A	128	TYR	CD1-CE1	6.11	1.48	1.39
1	A	56	TRP	CB-CG	-5.92	1.39	1.50
1	A	474	PHE	CE2-CZ	5.88	1.48	1.37
1	A	501	LEU	C-O	5.85	1.34	1.23
1	A	490	TRP	CE3-CZ3	5.84	1.48	1.38
1	A	440	TYR	CE1-CZ	5.75	1.46	1.38
1	A	521	PHE	CE1-CZ	5.74	1.48	1.37
1	A	60	LYS	CD-CE	5.61	1.65	1.51
1	A	510	ILE	C-O	5.49	1.33	1.23
1	A	349	GLU	CB-CG	5.46	1.62	1.52
1	A	497	GLU	CD-OE2	5.38	1.31	1.25
1	A	392	VAL	CB-CG1	-5.33	1.41	1.52
1	A	115	GLY	CA-C	5.21	1.60	1.51
1	A	290	PHE	CE1-CZ	5.18	1.47	1.37
1	A	137	GLU	CD-OE2	5.17	1.31	1.25
1	A	337	PHE	CD1-CE1	5.15	1.49	1.39
1	A	232	ALA	CA-CB	-5.14	1.41	1.52
1	A	419	TYR	CB-CG	5.09	1.59	1.51
1	A	363	GLU	CG-CD	5.08	1.59	1.51
1	A	404	GLU	CD-OE1	5.08	1.31	1.25
1	A	436	VAL	CB-CG2	5.06	1.63	1.52
1	A	418	PHE	CG-CD2	5.06	1.46	1.38
1	A	332	TYR	CE1-CZ	5.04	1.45	1.38
1	A	516	ALA	CA-CB	5.01	1.62	1.52
1	A	521	PHE	CG-CD1	5.01	1.46	1.38
1	A	456	TYR	CD1-CE1	5.01	1.46	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	509	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	170	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	520	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	A	242	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	501	LEU	CB-CG-CD1	-7.71	97.89	111.00
1	A	424	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	395	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	A	359	PRO	C-N-CA	-7.08	107.43	122.30
1	A	434	MET	CG-SD-CE	6.72	110.96	100.20
1	A	91	ASP	CB-CG-OD1	6.57	124.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	156	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	A	515	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	509	ARG	CG-CD-NE	6.11	124.63	111.80
1	A	49	LEU	CA-CB-CG	-5.75	102.09	115.30
1	A	319	VAL	CG1-CB-CG2	-5.68	101.82	110.90
1	A	14	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	44	LYS	CD-CE-NZ	-5.60	98.83	111.70
1	A	147	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	424	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	509	ARG	CD-NE-CZ	5.51	131.32	123.60
1	A	103	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	A	470	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	91	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	301	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	466	SER	CA-CB-OG	-5.28	96.94	111.20
1	A	520	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	87	ASP	CB-CA-C	-5.24	99.92	110.40
1	A	325	GLU	C-N-CA	-5.23	111.31	122.30
1	A	135	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	156	LEU	N-CA-C	-5.19	96.99	111.00
1	A	412	TRP	C-N-CA	-5.15	111.48	122.30
1	A	360	GLY	C-N-CA	5.12	134.51	121.70
1	A	324	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	389	LEU	CB-CG-CD1	5.03	119.55	111.00

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	4205	0	4104	158	1
2	B	38	0	34	0	0
2	D	38	0	34	0	0
3	C	24	0	22	0	0
4	A	9	0	13	2	0
5	A	3	0	0	1	0
6	A	10	0	0	1	0
7	A	1	0	0	0	0
8	A	42	0	39	1	0
9	A	384	0	0	37	0
All	All	4754	0	4246	160	1

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 19.

All (160) 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:495:SER:HA	9:A:2002:HOH:O	1.36	1.21
1:A:176:GLN:HB3	9:A:2007:HOH:O	1.01	1.16
1:A:50:THR:HG21	9:A:2276:HOH:O	1.41	1.16
1:A:4:ILE:N	1:A:4:ILE:HD12	1.51	1.14
1:A:4:ILE:H	1:A:4:ILE:HD12	0.92	1.07
1:A:4:ILE:CD1	1:A:4:ILE:H	1.69	1.06
1:A:518:GLN:H	1:A:518:GLN:NE2	1.66	0.93
4:A:601:TC5:H32C	4:A:601:TC5:H11C	1.52	0.92
1:A:48:SER:HA	9:A:2238:HOH:O	1.69	0.91
1:A:50:THR:O	1:A:51:LYS:HB3	1.71	0.91
1:A:495:SER:CA	9:A:2002:HOH:O	2.02	0.90
1:A:4:ILE:N	1:A:4:ILE:CD1	2.22	0.89
1:A:3:ASP:N	9:A:2001:HOH:O	2.04	0.88
1:A:496:THR:N	9:A:2002:HOH:O	2.05	0.86
1:A:518:GLN:H	1:A:518:GLN:HE21	0.87	0.86
1:A:518:GLN:HE21	1:A:518:GLN:N	1.72	0.85
1:A:494:LYS:HB2	9:A:2095:HOH:O	1.76	0.85
1:A:156:LEU:CD2	1:A:261:ILE:HD11	2.08	0.82
1:A:453:ARG:HG3	9:A:2349:HOH:O	1.80	0.82
1:A:372[A]:HIS:CE1	9:A:2113:HOH:O	2.32	0.81
1:A:377:VAL:O	1:A:377:VAL:HG23	1.78	0.81
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:HB2	9:A:2105:HOH:O	1.81	0.81
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.64	0.80
1:A:495:SER:O	1:A:496:THR:HG23	1.83	0.79
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.17	0.79
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.66	0.77
1:A:4:ILE:HG22	9:A:2171:HOH:O	1.84	0.76
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.20	0.76
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.68	0.74
1:A:453:ARG:HE	1:A:453:ARG:HA	1.53	0.74
1:A:489:SER:HB2	9:A:2133:HOH:O	1.90	0.72
1:A:377:VAL:O	1:A:377:VAL:CG2	2.39	0.70
1:A:522:TRP:O	1:A:527:PRO:HD3	1.93	0.69
1:A:270:GLN:O	1:A:274:LEU:HB2	1.93	0.68
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.29	0.68
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.08	0.67
1:A:284:THR:HG22	1:A:359:PRO:HG2	1.75	0.67
1:A:380:GLN:HB2	5:A:605:CL:CL	2.32	0.66
1:A:214:HIS:HB2	9:A:2136:HOH:O	1.95	0.66
1:A:509:ARG:HD3	9:A:2298:HOH:O	1.95	0.65
1:A:358:PHE:N	1:A:359:PRO:HD3	2.11	0.64
1:A:48:SER:CA	9:A:2238:HOH:O	2.36	0.64
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.80	0.63
1:A:157:PRO:HD2	1:A:240:ARG:CD	2.29	0.63
1:A:425:SER:O	9:A:2003:HOH:O	2.16	0.63
1:A:284:THR:CG2	1:A:359:PRO:HG2	2.28	0.63
1:A:454:ASP:O	1:A:455:GLN:HB2	1.98	0.63
1:A:227:PHE:CD2	1:A:227:PHE:C	2.72	0.62
1:A:105:LYS:HG3	9:A:2014:HOH:O	1.99	0.61
1:A:403:LEU:O	1:A:407:LYS:HG3	2.01	0.61
1:A:55:ILE:HD11	9:A:2360:HOH:O	2.01	0.60
1:A:355:LYS:HG2	1:A:366:LYS:HE3	1.83	0.60
1:A:49:LEU:HD12	1:A:50:THR:H	1.67	0.60
1:A:262:LYS:HG2	1:A:265:ARG:HH22	1.65	0.60
1:A:105:LYS:NZ	9:A:2014:HOH:O	2.34	0.59
1:A:425:SER:HB3	1:A:428:LEU:HD23	1.84	0.59
1:A:69:ILE:HG22	1:A:70:ASP:N	2.17	0.59
1:A:361:VAL:O	1:A:366:LYS:NZ	2.36	0.59
1:A:510:ILE:HD13	1:A:510:ILE:N	2.15	0.58
1:A:277:ALA:CB	9:A:2105:HOH:O	2.47	0.58
1:A:156:LEU:HD23	1:A:261:ILE:HD11	1.83	0.58
1:A:39:GLY:O	1:A:265:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLU:HG2	9:A:2167:HOH:O	2.05	0.57
1:A:176:GLN:NE2	9:A:2016:HOH:O	2.38	0.57
1:A:372[A]:HIS:HE1	1:A:518:GLN:HA	1.70	0.57
1:A:276:GLU:O	1:A:279:VAL:HG22	2.04	0.57
4:A:601:TC5:H32C	4:A:601:TC5:C1	2.32	0.57
1:A:378:ASP:O	1:A:380:GLN:N	2.37	0.56
1:A:116:GLY:HA3	1:A:120:THR:O	2.06	0.56
1:A:4:ILE:HG12	1:A:17:GLN:OE1	2.06	0.56
1:A:378:ASP:C	1:A:380:GLN:H	2.10	0.55
1:A:256:ASN:OD1	8:A:615:NAG:H3	2.07	0.55
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.06	0.55
1:A:357:PHE:C	1:A:359:PRO:HD3	2.27	0.55
1:A:509:ARG:HG2	9:A:2298:HOH:O	2.06	0.55
1:A:253:SER:O	1:A:254:ARG:HD3	2.06	0.55
1:A:17:GLN:HE21	1:A:24:THR:HG21	1.72	0.55
1:A:69:ILE:CG2	1:A:70:ASP:N	2.70	0.54
1:A:278:PHE:C	1:A:280:VAL:H	2.11	0.54
1:A:251:GLY:HA2	9:A:2230:HOH:O	2.07	0.53
1:A:383:GLU:CD	1:A:383:GLU:H	2.11	0.53
1:A:453:ARG:HE	1:A:453:ARG:CA	2.19	0.53
1:A:234:THR:O	1:A:293:THR:HG22	2.08	0.53
1:A:502:THR:OG1	1:A:509:ARG:NH1	2.42	0.53
1:A:214:HIS:HE1	9:A:2264:HOH:O	1.92	0.53
1:A:137:GLU:OE2	1:A:465:ARG:NH1	2.40	0.52
1:A:280:VAL:HG13	1:A:282:TYR:O	2.10	0.52
1:A:495:SER:O	1:A:496:THR:CG2	2.57	0.52
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.45	0.51
1:A:176:GLN:CG	9:A:2007:HOH:O	2.44	0.51
1:A:198:SER:HA	1:A:224:SER:O	2.10	0.50
1:A:385:TYR:HD2	9:A:2201:HOH:O	1.94	0.50
1:A:262:LYS:O	1:A:262:LYS:HD2	2.12	0.50
1:A:74:PRO:HA	9:A:2179:HOH:O	2.11	0.50
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.94	0.50
1:A:280:VAL:CG1	1:A:282:TYR:O	2.60	0.50
1:A:372[A]:HIS:CE1	1:A:518:GLN:HA	2.47	0.50
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.93	0.49
1:A:452:ARG:C	1:A:454:ASP:H	2.16	0.49
1:A:240:ARG:O	1:A:241:ASN:C	2.51	0.49
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.48	0.48
1:A:393:VAL:O	1:A:397:ASN:HB2	2.13	0.48
1:A:502:THR:O	1:A:508:THR:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:OG	1:A:325:GLU:OE2	2.22	0.48
1:A:347:ARG:HD2	1:A:385:TYR:OH	2.14	0.48
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.49	0.48
1:A:3:ASP:HA	1:A:4:ILE:HD12	1.96	0.47
1:A:495:SER:C	9:A:2002:HOH:O	2.33	0.47
1:A:238:GLU:O	1:A:242:ARG:HG3	2.15	0.47
1:A:448:LEU:N	1:A:449:PRO:CD	2.78	0.47
1:A:295:ASP:OD1	1:A:295:ASP:N	2.44	0.47
1:A:245:ASN:O	1:A:249:LEU:HD12	2.16	0.46
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.51	0.46
1:A:48:SER:CB	9:A:2238:HOH:O	2.61	0.46
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.51	0.46
1:A:117:GLY:O	1:A:118:PHE:HB2	2.16	0.45
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.97	0.45
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.46	0.45
1:A:524:SER:O	1:A:528:LYS:HE3	2.16	0.45
1:A:458:LYS:HD2	1:A:458:LYS:HA	1.58	0.45
1:A:322:ASN:O	1:A:325:GLU:HG2	2.16	0.45
1:A:176:GLN:CB	9:A:2007:HOH:O	1.87	0.45
1:A:17:GLN:NE2	1:A:24:THR:HG21	2.32	0.45
1:A:452:ARG:O	1:A:454:ASP:N	2.50	0.45
1:A:18:LEU:HD11	1:A:27:ALA:HB2	1.98	0.44
1:A:157:PRO:HG2	1:A:236:LEU:HG	2.00	0.44
1:A:25:VAL:HG13	1:A:99:ILE:O	2.18	0.43
1:A:248:LYS:O	1:A:251:GLY:N	2.52	0.43
1:A:262:LYS:C	1:A:262:LYS:HD2	2.39	0.43
1:A:279:VAL:HG21	1:A:290:PHE:CE2	2.54	0.43
1:A:348:LYS:HB3	9:A:2144:HOH:O	2.18	0.43
1:A:13:VAL:HG23	1:A:28:PHE:HD2	1.84	0.43
1:A:49:LEU:HD12	1:A:50:THR:N	2.33	0.42
1:A:247:ALA:O	1:A:248:LYS:C	2.57	0.42
1:A:21:PHE:N	9:A:2005:HOH:O	2.23	0.42
1:A:217:PHE:O	1:A:313:LYS:HE2	2.20	0.42
1:A:415:ASN:HB2	6:A:606:SO4:O3	2.20	0.42
1:A:497:GLU:HG3	1:A:497:GLU:H	1.34	0.42
1:A:509:ARG:CG	9:A:2298:HOH:O	2.66	0.42
1:A:197:GLU:HA	1:A:223:GLN:O	2.20	0.42
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.20	0.41
1:A:28:PHE:N	1:A:28:PHE:CD1	2.88	0.41
1:A:341:ASN:C	1:A:341:ASN:OD1	2.59	0.41
1:A:391:ASP:O	1:A:392:VAL:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ALA:HB1	1:A:505:THR:HB	2.00	0.41
1:A:110:LEU:HB3	1:A:195:PHE:CE1	2.56	0.41
1:A:328:ALA:HA	1:A:434:MET:CE	2.51	0.41
1:A:509:ARG:CD	9:A:2298:HOH:O	2.63	0.41
1:A:378:ASP:CG	1:A:379:ASP:H	2.24	0.41
1:A:347:ARG:HB2	1:A:385:TYR:OH	2.21	0.41
1:A:518:GLN:NE2	1:A:518:GLN:N	2.47	0.41
1:A:407:LYS:HG2	1:A:493:PHE:HE1	1.85	0.41
1:A:140:ILE:HG22	1:A:141:VAL:N	2.36	0.41
1:A:157:PRO:HD2	1:A:240:ARG:HD3	2.04	0.40
1:A:24:THR:O	1:A:101:ALA:HB3	2.21	0.40
1:A:184:ALA:N	9:A:2023:HOH:O	2.45	0.40
1:A:268:ASP:HA	1:A:269:PRO:HD2	1.84	0.40
1:A:39:GLY:O	1:A:265:ARG:CD	2.69	0.40
1:A:495:SER:O	1:A:496:THR:CB	2.70	0.40

All (1) 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:367:GLU:OE1	1:A:367:GLU:OE1[5_555]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	527/529 (100%)	475 (90%)	40 (8%)	12 (2%)	<b>6</b> <b>2</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	379	ASP
1	A	496	THR
1	A	249	LEU
1	A	453	ARG
1	A	506	GLU
1	A	281	PRO
1	A	9	LYS
1	A	361	VAL
1	A	279	VAL
1	A	251	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	452/454 (100%)	415 (92%)	37 (8%)	11 8

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	13	VAL
1	A	16	MET
1	A	51	LYS
1	A	69	ILE
1	A	91	ASP
1	A	138	ARG
1	A	156	LEU
1	A	195	PHE
1	A	214	HIS
1	A	236	LEU
1	A	240	ARG
1	A	248	LYS
1	A	254	ARG

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Mol	Chain	Res	Type
1	A	262	LYS
1	A	265	ARG
1	A	274	LEU
1	A	280	VAL
1	A	286	LEU
1	A	299	LEU
1	A	359	PRO
1	A	361	VAL
1	A	375	ASP
1	A	376	TRP
1	A	387	GLU
1	A	428	LEU
1	A	453	ARG
1	A	454	ASP
1	A	455	GLN
1	A	489	SER
1	A	492	VAL
1	A	497	GLU
1	A	506	GLU
1	A	509	ARG
1	A	518	GLN
1	A	529	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	289	ASN
1	A	380	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	1.23	1 (7%)	17,19,21	3.08	10 (58%)
2	NAG	B	2	2	14,14,15	0.74	0	17,19,21	3.07	8 (47%)
2	FUL	B	3	2	10,10,11	1.38	2 (20%)	14,14,16	3.57	5 (35%)
3	NAG	C	1	1,3	14,14,15	1.81	5 (35%)	17,19,21	2.76	8 (47%)
3	FUL	C	2	3	10,10,11	0.79	0	14,14,16	3.50	7 (50%)
2	NAG	D	1	1,2	14,14,15	1.03	0	17,19,21	2.74	8 (47%)
2	NAG	D	2	2	14,14,15	1.51	3 (21%)	17,19,21	1.85	4 (23%)
2	FUL	D	3	2	10,10,11	0.89	0	14,14,16	4.37	7 (50%)

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	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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUL	D	3	2	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	4.11	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.93	1.56	1.52
2	B	1	NAG	C2-N2	-2.71	1.41	1.46
3	C	1	NAG	C3-C2	2.64	1.58	1.52
2	B	3	FUL	C4-C5	2.59	1.58	1.52
3	C	1	NAG	O5-C1	2.33	1.47	1.43
2	D	2	NAG	C4-C5	2.22	1.57	1.53
2	B	3	FUL	C6-C5	2.21	1.56	1.51
2	D	2	NAG	O7-C7	2.10	1.28	1.23
3	C	1	NAG	C4-C5	2.09	1.57	1.53
3	C	1	NAG	C6-C5	2.03	1.58	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	FUL	C1-C2-C3	-12.84	93.88	109.67
3	C	2	FUL	C1-C2-C3	-9.85	97.56	109.67
2	B	2	NAG	C3-C4-C5	-7.84	96.26	110.24
2	B	3	FUL	C1-C2-C3	-7.28	100.72	109.67
2	B	3	FUL	C3-C4-C5	6.40	119.74	109.77
2	B	1	NAG	O5-C1-C2	-6.05	101.73	111.29
2	B	3	FUL	C1-O5-C5	-5.88	99.44	112.78
2	B	2	NAG	O6-C6-C5	-5.77	91.49	111.29
3	C	1	NAG	O5-C5-C6	5.76	116.23	107.20
2	D	3	FUL	C3-C4-C5	5.45	118.25	109.77
2	B	1	NAG	C3-C4-C5	-5.42	100.57	110.24
2	D	3	FUL	C1-O5-C5	-5.41	100.51	112.78
2	B	3	FUL	C6-C5-C4	5.30	122.87	113.07
2	D	1	NAG	C1-O5-C5	5.04	119.02	112.19
2	D	1	NAG	O5-C1-C2	-4.88	103.58	111.29
3	C	1	NAG	C3-C4-C5	-4.69	101.87	110.24
2	B	1	NAG	C8-C7-N2	4.64	123.95	116.10
2	D	1	NAG	O3-C3-C4	-4.57	99.78	110.35
2	B	2	NAG	C4-C3-C2	-4.46	104.48	111.02
3	C	2	FUL	C1-O5-C5	-4.42	102.75	112.78
2	B	1	NAG	O4-C4-C3	-4.31	100.38	110.35
3	C	1	NAG	O4-C4-C5	4.30	119.97	109.30
2	D	3	FUL	O3-C3-C4	4.20	120.06	110.35
3	C	1	NAG	O5-C1-C2	-3.90	105.13	111.29
2	D	1	NAG	C3-C4-C5	-3.90	103.28	110.24
3	C	2	FUL	C3-C4-C5	3.70	115.53	109.77
2	B	2	NAG	O4-C4-C5	3.57	118.16	109.30
2	D	2	NAG	C1-O5-C5	3.56	117.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUL	O5-C5-C6	3.54	114.94	107.33
2	D	1	NAG	O7-C7-C8	-3.51	115.54	122.06
2	D	2	NAG	O4-C4-C5	3.45	117.87	109.30
3	C	1	NAG	O3-C3-C2	3.42	116.54	109.47
2	D	1	NAG	O7-C7-N2	3.34	128.10	121.95
2	B	1	NAG	C2-N2-C7	3.16	127.40	122.90
3	C	2	FUL	O5-C5-C6	2.98	113.74	107.33
3	C	1	NAG	O7-C7-C8	-2.92	116.64	122.06
2	D	2	NAG	C2-N2-C7	2.91	127.05	122.90
2	D	3	FUL	O2-C2-C1	2.83	114.95	109.15
2	D	3	FUL	O4-C4-C5	-2.81	103.44	109.67
2	B	1	NAG	O3-C3-C4	-2.69	104.13	110.35
2	D	1	NAG	C4-C3-C2	2.65	114.90	111.02
2	B	2	NAG	O4-C4-C3	2.64	116.45	110.35
3	C	2	FUL	C2-C3-C4	-2.63	106.35	110.89
3	C	2	FUL	O2-C2-C1	2.48	114.22	109.15
3	C	1	NAG	C6-C5-C4	2.46	118.76	113.00
2	D	2	NAG	O3-C3-C2	2.44	114.52	109.47
2	D	3	FUL	C2-C3-C4	-2.44	106.67	110.89
2	B	1	NAG	O7-C7-N2	-2.42	117.50	121.95
2	B	2	NAG	O5-C5-C4	2.39	116.65	110.83
2	B	1	NAG	O4-C4-C5	2.39	115.23	109.30
2	B	1	NAG	O6-C6-C5	2.33	119.30	111.29
3	C	2	FUL	O5-C1-C2	-2.24	107.31	110.77
2	D	1	NAG	C2-N2-C7	2.23	126.08	122.90
3	C	1	NAG	C8-C7-N2	2.22	119.86	116.10
2	B	2	NAG	C2-N2-C7	2.14	125.95	122.90
2	B	2	NAG	O3-C3-C2	2.13	113.88	109.47
2	B	1	NAG	C1-C2-N2	2.04	113.98	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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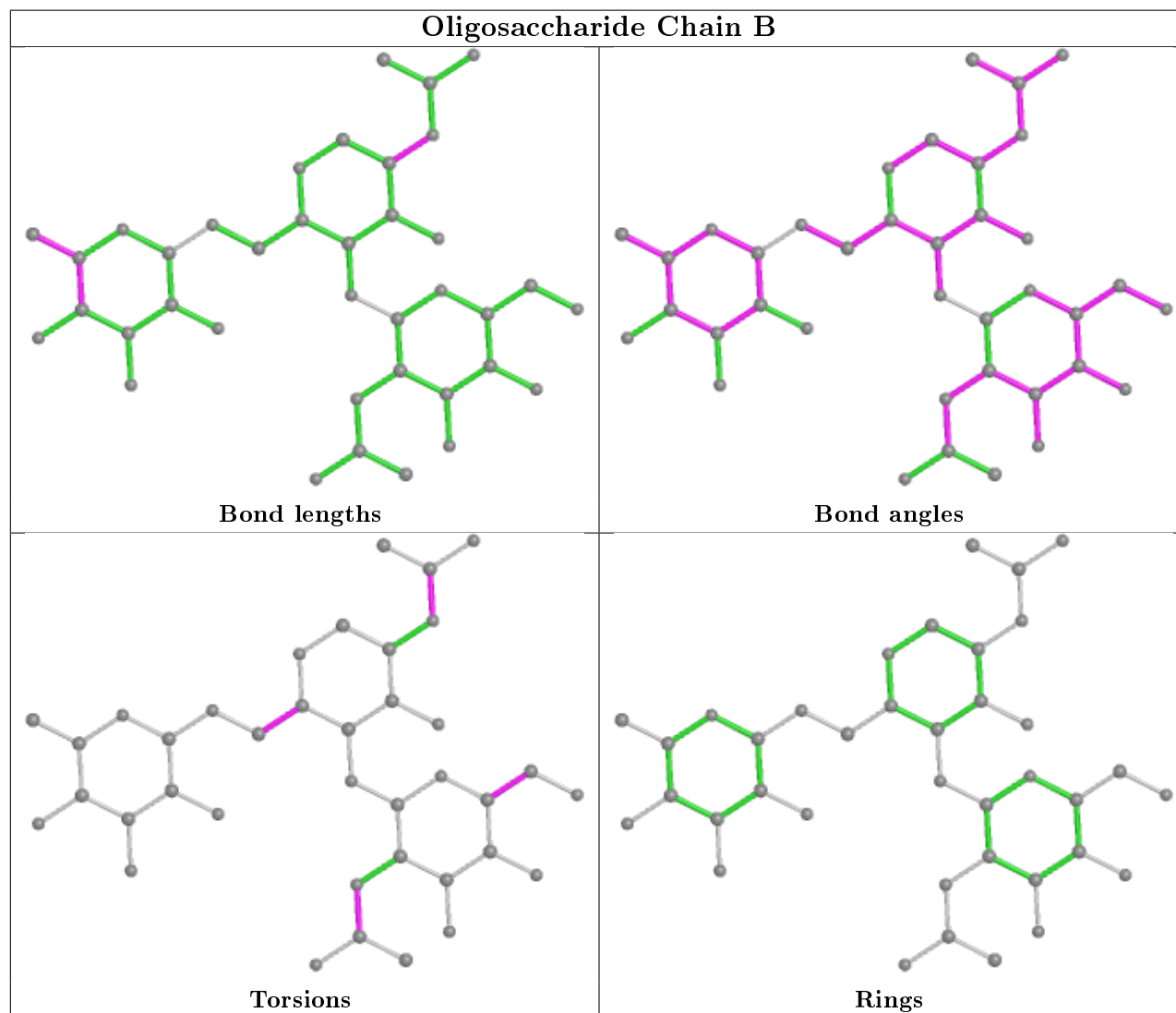
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Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

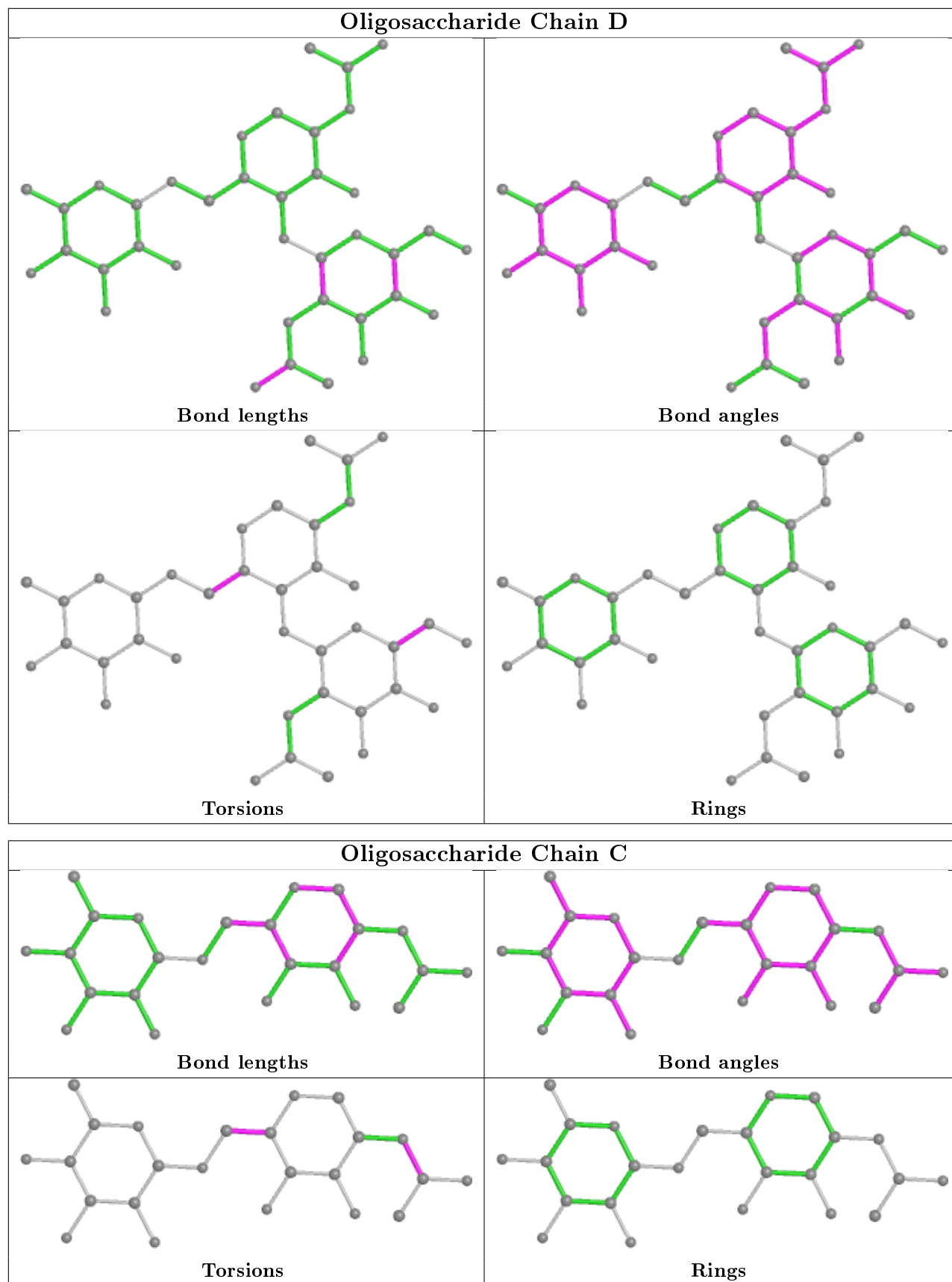
There are no ring outliers.

No monomer is involved in short contacts.

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 10 ligands modelled in this entry, 4 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
6	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.49	0
8	NAG	A	613	1	14,14,15	0.86	0	17,19,21	2.30	8 (47%)
6	SO4	A	606	-	4,4,4	0.20	0	6,6,6	0.58	0
4	TC5	A	601	1	5,8,9	0.94	0	3,8,11	2.26	1 (33%)
8	NAG	A	614	1	14,14,15	1.66	4 (28%)	17,19,21	2.81	8 (47%)
8	NAG	A	615	1	14,14,15	1.08	0	17,19,21	2.14	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TC5	A	601	1	-	1/3/7/9	-
8	NAG	A	613	1	-	4/6/23/26	0/1/1/1
8	NAG	A	614	1	-	0/6/23/26	0/1/1/1
8	NAG	A	615	1	1/1/5/7	6/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	614	NAG	C3-C2	3.80	1.60	1.52
8	A	614	NAG	C2-N2	2.40	1.50	1.46
8	A	614	NAG	C1-C2	2.35	1.55	1.52
8	A	614	NAG	C4-C3	2.02	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	614	NAG	O7-C7-C8	-5.81	111.27	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	615	NAG	C1-O5-C5	5.51	119.66	112.19
8	A	614	NAG	C8-C7-N2	4.98	124.53	116.10
8	A	614	NAG	C2-N2-C7	-4.57	116.39	122.90
8	A	613	NAG	C8-C7-N2	4.46	123.66	116.10
8	A	613	NAG	O5-C1-C2	-4.10	104.81	111.29
4	A	601	TC5	C4-C3-N	-3.72	101.54	112.89
8	A	614	NAG	C1-O5-C5	-3.34	107.66	112.19
8	A	613	NAG	C1-O5-C5	3.25	116.60	112.19
8	A	615	NAG	O7-C7-C8	-3.01	116.46	122.06
8	A	614	NAG	C3-C4-C5	2.94	115.49	110.24
8	A	613	NAG	O5-C5-C6	2.84	111.65	107.20
8	A	614	NAG	O5-C1-C2	-2.65	107.11	111.29
8	A	614	NAG	C4-C3-C2	2.64	114.88	111.02
8	A	615	NAG	C2-N2-C7	2.48	126.43	122.90
8	A	615	NAG	C3-C4-C5	2.44	114.59	110.24
8	A	615	NAG	O5-C5-C4	2.42	116.72	110.83
8	A	613	NAG	C6-C5-C4	2.31	118.42	113.00
8	A	613	NAG	O7-C7-N2	-2.25	117.81	121.95
8	A	613	NAG	C4-C3-C2	-2.23	107.74	111.02
8	A	613	NAG	O3-C3-C4	2.09	115.19	110.35
8	A	614	NAG	O3-C3-C2	2.08	113.77	109.47
8	A	615	NAG	O5-C1-C2	-2.05	108.05	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	615	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	TC5	N-C3-C4-C5
8	A	615	NAG	C3-C2-N2-C7
8	A	615	NAG	C8-C7-N2-C2
8	A	615	NAG	O7-C7-N2-C2
8	A	613	NAG	C4-C5-C6-O6
8	A	613	NAG	O5-C5-C6-O6
8	A	615	NAG	O5-C5-C6-O6
8	A	613	NAG	C8-C7-N2-C2
8	A	613	NAG	O7-C7-N2-C2
8	A	615	NAG	C4-C5-C6-O6
8	A	615	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	SO4	1	0
4	A	601	TC5	2	0
8	A	615	NAG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	527/529 (99%)	-0.14	17 (3%)	47 54	17, 32, 59, 80	11 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ARG	3.1
1	A	380	GLN	3.1
1	A	51	LYS	3.0
1	A	453	ARG	2.8
1	A	378	ASP	2.8
1	A	3	ASP	2.6
1	A	377	VAL	2.5
1	A	255	GLU	2.5
1	A	253	SER	2.4
1	A	50	THR	2.4
1	A	256	ASN	2.4
1	A	54	ASP	2.3
1	A	52	TRP	2.3
1	A	53	SER	2.2
1	A	270	GLN	2.2
1	A	259	GLU	2.1
1	A	262	LYS	2.1

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

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

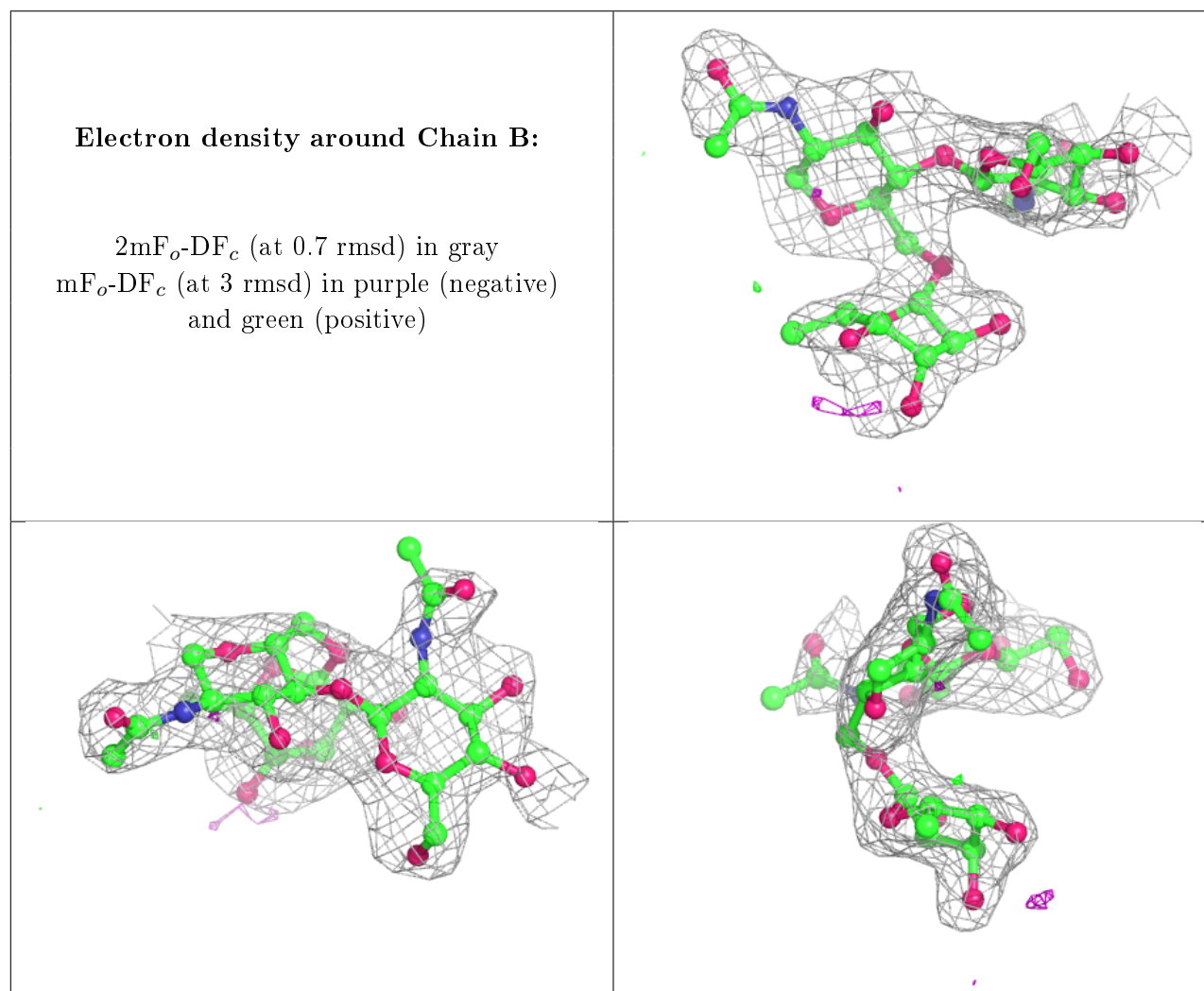
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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.

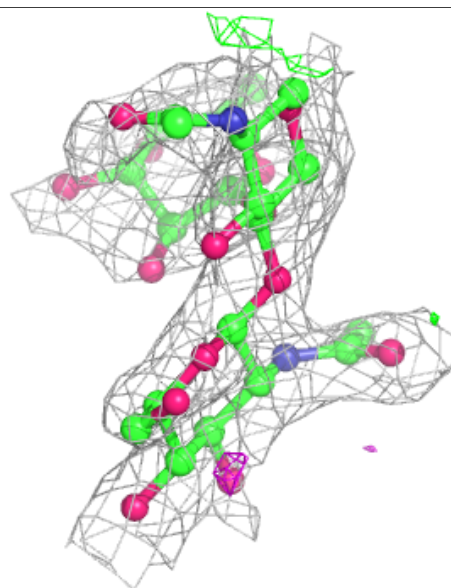
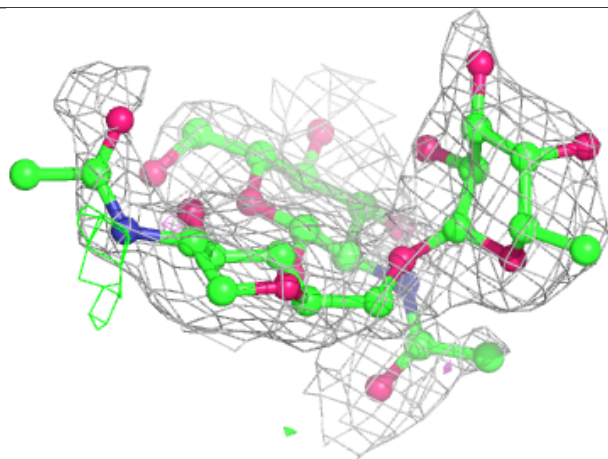
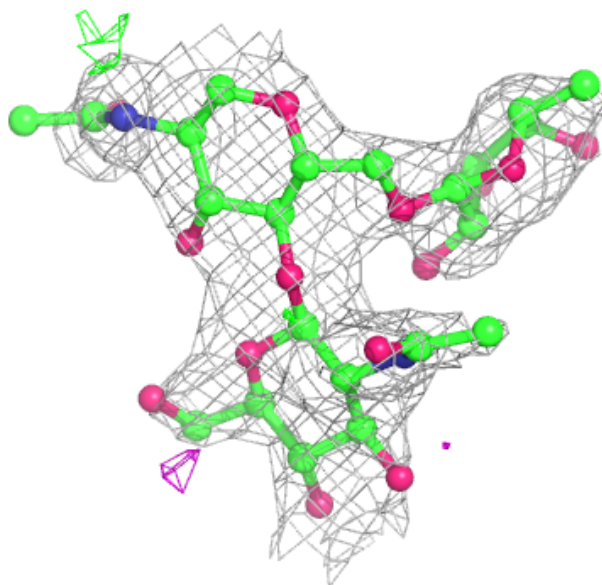
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	2	14/15	0.71	0.28	70,79,81,82	0
3	NAG	C	1	14/15	0.77	0.23	59,66,68,69	0
3	FUL	C	2	10/11	0.78	0.24	39,44,49,50	10
2	NAG	B	2	14/15	0.85	0.21	65,72,75,75	0
2	FUL	B	3	10/11	0.86	0.15	72,76,78,79	0
2	FUL	D	3	10/11	0.88	0.20	64,70,74,77	0
2	NAG	D	1	14/15	0.90	0.20	70,74,83,84	0
2	NAG	B	1	14/15	0.96	0.11	43,47,61,69	0

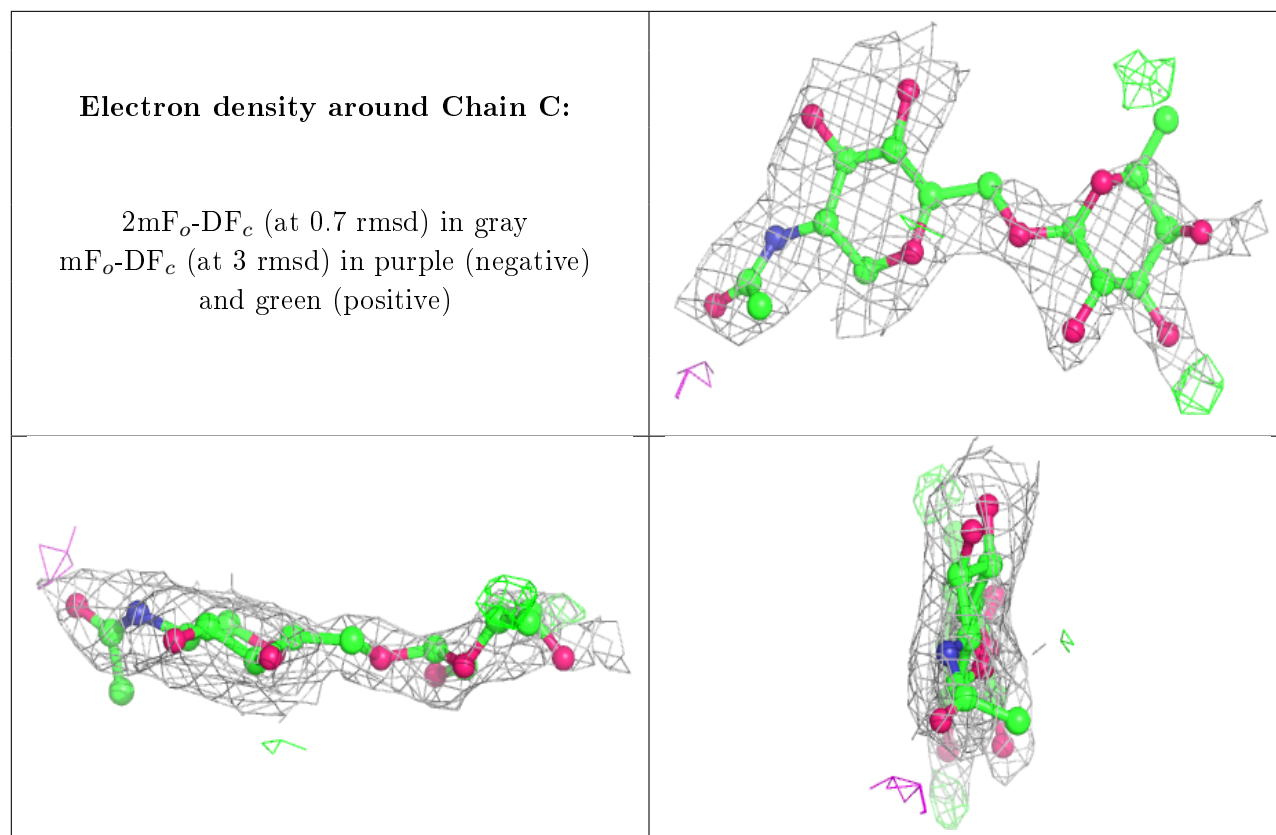
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
8	NAG	A	615	14/15	0.65	0.45	89,91,97,98	0
8	NAG	A	614	14/15	0.71	0.22	53,73,80,81	0
8	NAG	A	613	14/15	0.73	0.32	81,87,89,90	0
5	CL	A	605	1/1	0.76	0.12	81,81,81,81	0
5	CL	A	607	1/1	0.91	0.14	73,73,73,73	0
6	SO4	A	603	5/5	0.94	0.12	51,57,59,60	5
5	CL	A	602	1/1	0.95	0.16	51,51,51,51	0
7	NA	A	604	1/1	0.96	0.11	43,43,43,43	1
6	SO4	A	606	5/5	0.97	0.11	39,41,45,48	5
4	TC5	A	601	9/10	0.98	0.14	27,32,45,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.