



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 2WIK / pdb_00002wik
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

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)
Xtrriage (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

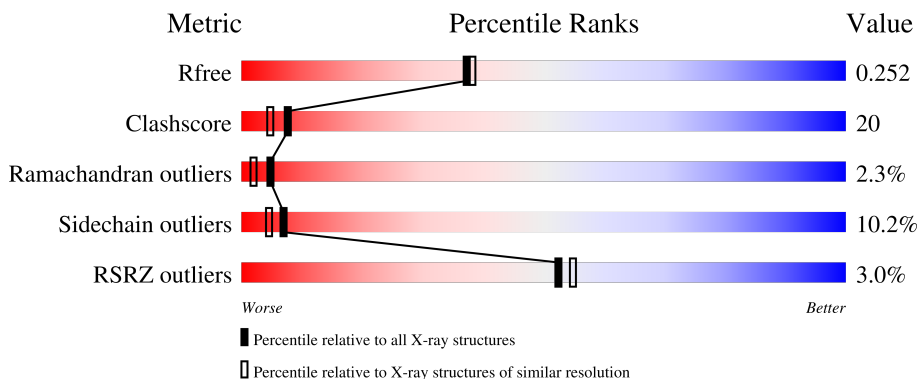
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	B	3	
2	D	3	
3	C	2	

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
6	SO4	A	606	-	-	X	-
8	NAG	A	615	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.

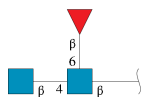
- Molecule 1 is a protein called CHOLINESTERASE.

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.



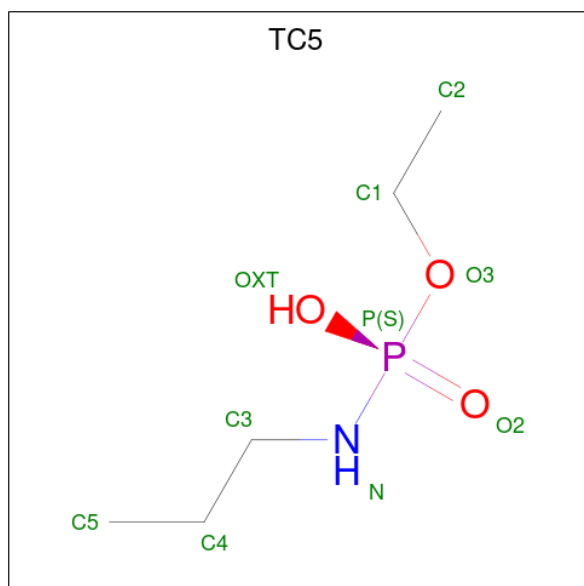
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

- 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
			Total	C	N	O			
3	C	2	24	14	1	9	0	0	0

- Molecule 4 is ETHYL HYDROGEN PROPYLAMIDOPHOSPHATE (CCD ID: TC5) (formula: $C_5H_{14}NO_3P$).



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

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

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

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



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- 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 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0

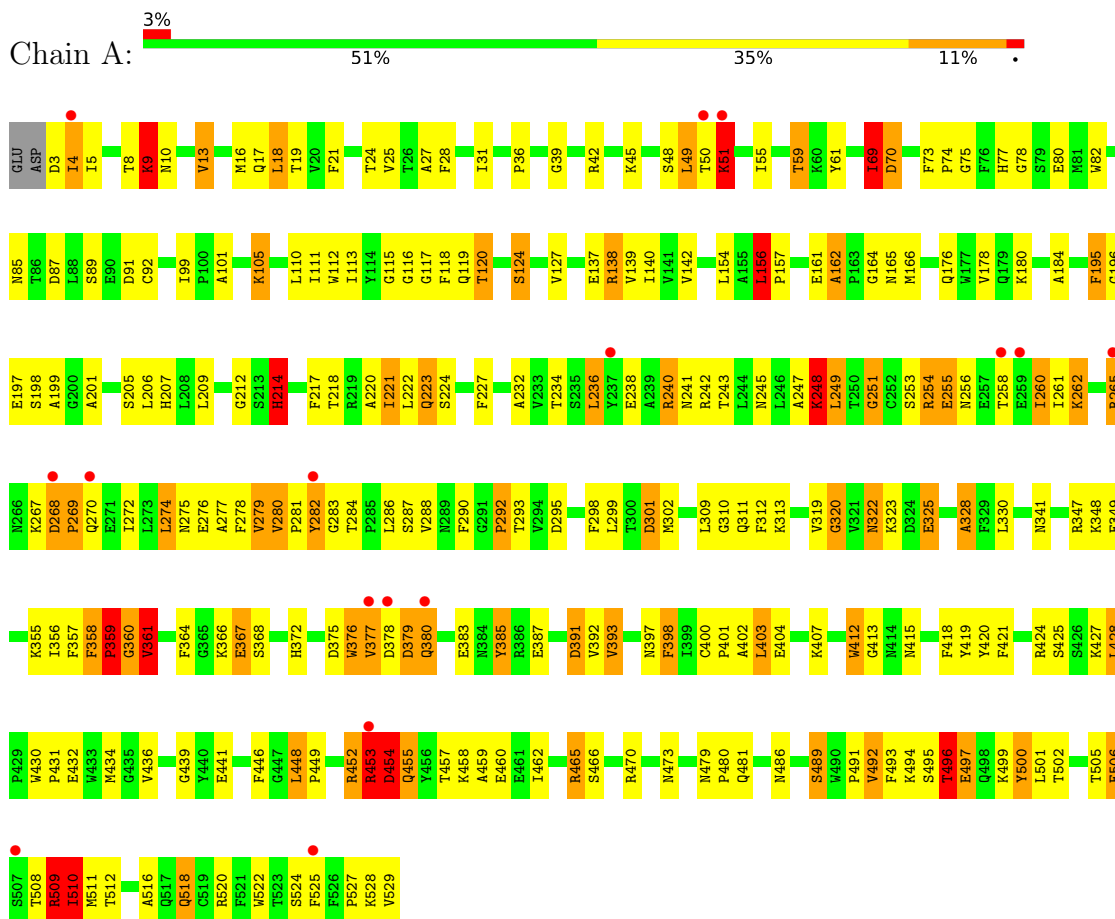
- Molecule 9 is water.

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

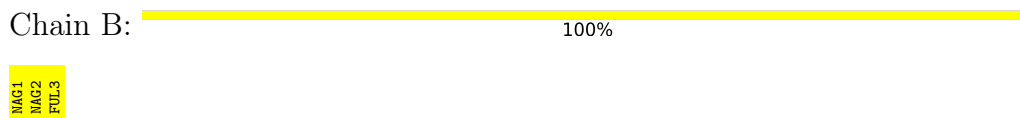
3 Residue-property plots [i](#)

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

Chain D:  100%

MAG1
MAG2
FUL3

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

Chain C:  100%

MAG1
FUL2

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 127.25Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.213 , 0.276 (Not available) , 0.252	Depositor DCC
R_{free} test set	1358 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4754	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TC5, NAG, NA, FUL, SO4, CL

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	1.86	74/4330 (1.7%)	1.74	82/5879 (1.4%)

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 (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PRO	CA-C	9.59	1.61	1.52
1	A	510	ILE	C-O	9.49	1.33	1.24
1	A	19	THR	CA-C	-8.87	1.41	1.52
1	A	501	LEU	C-O	8.64	1.34	1.24
1	A	112	TRP	N-CA	7.33	1.55	1.46
1	A	232	ALA	CA-CB	-7.26	1.41	1.53
1	A	113	ILE	CA-CB	7.19	1.62	1.53
1	A	301	ASP	C-O	-6.98	1.16	1.23
1	A	412	TRP	CA-C	-6.96	1.43	1.52
1	A	462	ILE	CA-CB	6.96	1.62	1.54
1	A	115	GLY	CA-C	6.94	1.60	1.51
1	A	368	SER	C-O	6.91	1.32	1.24
1	A	87	ASP	CA-C	-6.86	1.44	1.52
1	A	92	CYS	CA-C	6.76	1.61	1.52
1	A	85	ASN	N-CA	-6.68	1.38	1.46
1	A	178	VAL	CA-CB	6.63	1.62	1.54
1	A	470	ARG	N-CA	6.48	1.54	1.46
1	A	496	THR	CA-CB	6.36	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	ALA	CA-CB	6.21	1.62	1.53
1	A	70	ASP	CA-C	6.11	1.60	1.52
1	A	499	LYS	C-O	6.11	1.31	1.23
1	A	466	SER	CA-C	6.04	1.60	1.52
1	A	481	GLN	C-O	6.04	1.31	1.23
1	A	199	ALA	C-O	6.01	1.31	1.24
1	A	367	GLU	CG-CD	5.98	1.67	1.52
1	A	220	ALA	CA-CB	-5.97	1.43	1.53
1	A	402	ALA	N-CA	5.93	1.53	1.46
1	A	432	GLU	C-O	-5.92	1.17	1.24
1	A	439	GLY	C-O	-5.91	1.15	1.24
1	A	320	GLY	C-O	5.90	1.31	1.23
1	A	510	ILE	CA-CB	5.88	1.60	1.54
1	A	272	ILE	CA-CB	-5.86	1.47	1.54
1	A	328	ALA	C-O	5.80	1.31	1.24
1	A	398	PHE	CE2-CZ	5.74	1.55	1.38
1	A	349	GLU	C-O	5.71	1.30	1.24
1	A	201	ALA	N-CA	5.70	1.53	1.46
1	A	124	SER	C-O	-5.70	1.16	1.24
1	A	520	ARG	C-O	-5.69	1.17	1.24
1	A	142	VAL	C-O	5.67	1.29	1.24
1	A	82	TRP	C-O	5.62	1.31	1.24
1	A	462	ILE	CA-C	5.62	1.59	1.52
1	A	111	ILE	CA-CB	-5.61	1.47	1.54
1	A	466	SER	C-O	5.57	1.30	1.24
1	A	196	GLY	CA-C	-5.54	1.46	1.51
1	A	525	PHE	CA-C	5.53	1.59	1.52
1	A	319	VAL	CA-C	-5.51	1.46	1.52
1	A	288	VAL	N-CA	-5.49	1.40	1.46
1	A	436	VAL	C-O	5.48	1.30	1.24
1	A	500	TYR	N-CA	5.44	1.52	1.45
1	A	140	ILE	CA-CB	-5.43	1.47	1.54
1	A	364	PHE	N-CA	5.43	1.53	1.46
1	A	330	LEU	N-CA	5.42	1.53	1.46
1	A	269	PRO	C-O	5.40	1.30	1.24
1	A	82	TRP	N-CA	5.39	1.53	1.46
1	A	480	PRO	CA-C	-5.37	1.48	1.53
1	A	282	TYR	CA-C	5.37	1.60	1.53
1	A	512	THR	N-CA	5.36	1.52	1.46
1	A	441	GLU	C-O	-5.36	1.17	1.24
1	A	322	ASN	N-CA	-5.34	1.39	1.45
1	A	309	LEU	CA-C	-5.30	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	VAL	CA-CB	5.30	1.61	1.54
1	A	418	PHE	C-O	5.28	1.30	1.24
1	A	105	LYS	N-CA	-5.27	1.39	1.46
1	A	268	ASP	CB-CG	5.25	1.65	1.52
1	A	492	VAL	CA-CB	5.24	1.60	1.54
1	A	120	THR	C-O	5.23	1.30	1.23
1	A	413	GLY	C-O	-5.19	1.17	1.24
1	A	89	SER	C-O	-5.17	1.17	1.23
1	A	111	ILE	CA-C	-5.16	1.45	1.52
1	A	195	PHE	CA-C	-5.15	1.46	1.52
1	A	403	LEU	CA-CB	-5.12	1.45	1.53
1	A	413	GLY	N-CA	-5.06	1.40	1.45
1	A	292	PRO	CA-CB	5.05	1.60	1.53
1	A	322	ASN	CA-C	-5.05	1.46	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	PHE	CA-C-N	11.45	131.15	119.24
1	A	358	PHE	C-N-CA	11.45	131.15	119.24
1	A	412	TRP	CA-C-N	-11.15	111.48	123.30
1	A	412	TRP	C-N-CA	-11.15	111.48	123.30
1	A	525	PHE	N-CA-C	8.84	120.84	111.03
1	A	214	HIS	N-CA-C	-8.38	102.08	111.71
1	A	162	ALA	CA-C-N	-7.82	111.74	119.64
1	A	162	ALA	C-N-CA	-7.82	111.74	119.64
1	A	465	ARG	N-CA-C	-7.70	102.53	112.23
1	A	454	ASP	N-CA-C	7.68	121.96	112.59
1	A	255	GLU	N-CA-C	-7.57	103.11	113.18
1	A	356	ILE	CB-CA-C	-7.31	102.61	111.97
1	A	298	PHE	N-CA-C	-7.22	103.50	111.36
1	A	359	PRO	CA-C-N	-7.13	107.43	121.41
1	A	359	PRO	C-N-CA	-7.13	107.43	121.41
1	A	360	GLY	CA-C-N	7.12	134.51	121.70
1	A	360	GLY	C-N-CA	7.12	134.51	121.70
1	A	466	SER	CA-CB-OG	-7.08	96.94	111.10
1	A	323	LYS	N-CA-C	6.96	118.87	111.28
1	A	473	ASN	N-CA-C	6.96	118.86	111.28
1	A	119	GLN	N-CA-C	-6.90	105.13	113.97
1	A	380	GLN	N-CA-C	6.75	119.95	111.24
1	A	402	ALA	N-CA-C	-6.67	104.09	111.36
1	A	486	ASN	CB-CA-C	-6.57	102.57	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	THR	N-CA-C	-6.52	104.94	114.39
1	A	400	CYS	CA-C-N	-6.40	112.40	119.19
1	A	400	CYS	C-N-CA	-6.40	112.40	119.19
1	A	180	LYS	N-CA-C	6.19	119.67	111.75
1	A	364	PHE	N-CA-C	-6.04	104.78	111.36
1	A	207	HIS	N-CA-C	-6.02	104.64	112.23
1	A	31	ILE	CA-C-N	-5.96	114.47	120.31
1	A	31	ILE	C-N-CA	-5.96	114.47	120.31
1	A	19	THR	N-CA-C	-5.83	99.73	109.24
1	A	49	LEU	CA-C-N	5.83	128.02	120.44
1	A	49	LEU	C-N-CA	5.83	128.02	120.44
1	A	385	TYR	N-CA-C	5.79	118.37	111.71
1	A	439	GLY	N-CA-C	-5.79	107.10	115.27
1	A	45	LYS	CA-C-N	5.77	125.68	119.85
1	A	45	LYS	C-N-CA	5.77	125.68	119.85
1	A	509	ARG	CG-CD-NE	5.74	124.63	112.00
1	A	221	ILE	N-CA-C	5.72	116.17	108.17
1	A	283	GLY	O-C-N	-5.65	118.76	123.73
1	A	420	TYR	CB-CA-C	-5.63	102.50	111.17
1	A	424	ARG	N-CA-C	5.62	117.38	108.67
1	A	441	GLU	N-CA-C	-5.59	106.30	113.23
1	A	479	ASN	CA-C-N	-5.58	113.09	120.96
1	A	479	ASN	C-N-CA	-5.58	113.09	120.96
1	A	268	ASP	CA-C-N	5.56	126.79	119.84
1	A	268	ASP	C-N-CA	5.56	126.79	119.84
1	A	164	GLY	N-CA-C	-5.54	106.39	112.04
1	A	115	GLY	O-C-N	-5.53	116.96	122.82
1	A	69	ILE	CB-CA-C	-5.52	102.06	110.95
1	A	287	SER	N-CA-C	5.51	118.22	110.23
1	A	139	VAL	CB-CA-C	-5.49	103.91	111.49
1	A	275	ASN	N-CA-C	5.44	119.92	113.28
1	A	212	GLY	N-CA-C	-5.43	107.59	114.16
1	A	87	ASP	CB-CA-C	-5.42	99.92	109.62
1	A	446	PHE	CA-C-N	-5.42	113.81	122.10
1	A	446	PHE	C-N-CA	-5.42	113.81	122.10
1	A	325	GLU	CA-C-N	-5.41	111.31	120.79
1	A	325	GLU	C-N-CA	-5.41	111.31	120.79
1	A	127	VAL	N-CA-C	-5.41	105.72	113.07
1	A	138	ARG	CB-CA-C	-5.40	103.92	111.80
1	A	206	LEU	N-CA-C	-5.38	106.22	112.89
1	A	413	GLY	CA-C-O	-5.31	115.32	119.83
1	A	156	LEU	N-CA-C	-5.29	96.99	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	A	328	ALA	N-CA-C	-5.25	106.13	112.54
1	A	311	GLN	CB-CG-CD	-5.25	103.68	112.60
1	A	376	TRP	N-CA-C	5.22	117.21	109.69
1	A	491	PRO	CA-C-N	-5.19	113.17	120.75
1	A	491	PRO	C-N-CA	-5.19	113.17	120.75
1	A	223	GLN	N-CA-C	5.18	117.20	108.96
1	A	311	GLN	CB-CA-C	-5.16	102.64	111.31
1	A	465	ARG	CA-C-O	5.10	125.81	119.79
1	A	218	THR	N-CA-CB	-5.10	102.62	110.42
1	A	18	LEU	CA-C-N	-5.06	115.73	122.72
1	A	18	LEU	C-N-CA	-5.06	115.73	122.72
1	A	496	THR	N-CA-CB	5.06	119.04	110.49
1	A	391	ASP	N-CA-C	5.04	117.16	111.11
1	A	421	PHE	CA-C-N	-5.02	113.36	122.50
1	A	421	PHE	C-N-CA	-5.02	113.36	122.50

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 [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	4205	0	4104	171	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	2	0
7	A	1	0	0	0	0
8	A	42	0	39	1	0
9	A	384	0	0	38	0
All	All	4754	0	4246	173	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 20.

All (173) 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:HD12	1:A:4:ILE:N	1.51	1.14
1:A:4:ILE:HD12	1:A:4:ILE:H	0.92	1.07
1:A:4:ILE:H	1:A:4:ILE:CD1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.68	0.74
1:A:453:ARG:HA	1:A:453:ARG:HE	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:227:PHE:CD2	1:A:227:PHE:C	2.72	0.66
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: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:378:ASP:C	1:A:380:GLN:H	2.10	0.60
1:A:55:ILE:HD11	9:A:2360:HOH:O	2.01	0.60
1:A:49:LEU:HD12	1:A:50:THR:H	1.67	0.60
1:A:355:LYS:HG2	1:A:366:LYS:HE3	1.83	0.60
1:A:262:LYS:HG2	1:A:265:ARG:HH22	1.65	0.60
1:A:357:PHE:C	1:A:359:PRO:HD3	2.27	0.59
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:278:PHE:C	1:A:280:VAL:H	2.11	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:383:GLU:CD	1:A:383:GLU:H	2.11	0.58
1:A:39:GLY:O	1:A:265:ARG:HD3	2.04	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:452:ARG:C	1:A:454:ASP:H	2.16	0.54
1:A:240:ARG:O	1:A:241:ASN:C	2.51	0.53
1:A:251:GLY:HA2	9:A:2230:HOH:O	2.07	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:69:ILE:CG2	1:A:70:ASP:N	2.70	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:HD2	1:A:262:LYS:O	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: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
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.49	0.48
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:3:ASP:HA	1:A:4:ILE:HD12	1.96	0.47
1:A:262:LYS:HD2	1:A:262:LYS:C	2.39	0.47
1:A:238:GLU:O	1:A:242:ARG:HG3	2.15	0.47
1:A:295:ASP:OD1	1:A:295:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:N	1:A:449:PRO:CD	2.78	0.47
1:A:247:ALA:O	1:A:248:LYS:C	2.57	0.47
1:A:3:ASP:C	1:A:4:ILE:HD12	2.33	0.46
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:495:SER:C	9:A:2002:HOH:O	2.33	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:378:ASP:CG	1:A:379:ASP:H	2.24	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:341:ASN:OD1	1:A:341:ASN:C	2.59	0.45
1:A:391:ASP:O	1:A:392:VAL:C	2.58	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:HA	1:A:458:LYS:HD2	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:415:ASN:CG	6:A:606:SO4:O3	2.60	0.44
1:A:8:THR:O	1:A:9:LYS:C	2.60	0.44
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:75:GLY:H	1:A:80:GLU:CD	2.25	0.43
1:A:452:ARG:C	1:A:454:ASP:N	2.76	0.43
1:A:248:LYS:O	1:A:251:GLY:N	2.52	0.43
1:A:137:GLU:O	1:A:138:ARG:C	2.62	0.43
1:A:10:ASN:C	1:A:51:LYS:HE2	2.44	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:77:HIS:O	1:A:78:GLY:C	2.62	0.43
1:A:176:GLN:CD	9:A:2007:HOH:O	2.62	0.42
1:A:49:LEU:HD12	1:A:50:THR:N	2.33	0.42
1:A:278:PHE:C	1:A:280:VAL:N	2.77	0.42
1:A:165:ASN:O	1:A:166:MET:C	2.60	0.42
1:A:21:PHE:N	9:A:2005:HOH:O	2.23	0.42
1:A:398:PHE:C	1:A:401:PRO:HD2	2.45	0.42
1:A:217:PHE:O	1:A:313:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:HB2	6:A:606:SO4:O3	2.20	0.42
1:A:497:GLU:H	1:A:497:GLU:HG3	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:459:ALA:HB1	1:A:505:THR:HB	2.00	0.41
1:A:73:PHE:O	1:A:74:PRO:C	2.62	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:C	1:A:380:GLN:N	2.78	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: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:301:ASP:O	1:A:302:MET:C	2.63	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%)	5 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
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 [i](#)

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%)	406 (90%)	46 (10%)	7 4

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	ILE
1	A	9	LYS
1	A	13	VAL
1	A	16	MET
1	A	51	LYS
1	A	59	THR
1	A	69	ILE
1	A	91	ASP

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	214	HIS
1	A	221	ILE
1	A	236	LEU
1	A	240	ARG
1	A	248	LYS
1	A	254	ARG
1	A	255	GLU
1	A	260	ILE
1	A	262	LYS
1	A	265	ARG
1	A	267	LYS
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	377	VAL
1	A	387	GLU
1	A	427	LYS
1	A	428	LEU
1	A	448	LEU
1	A	452	ARG
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	510	ILE
1	A	518	GLN
1	A	529	VAL

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	63	ASN

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Mol	Chain	Res	Type
1	A	68	ASN
1	A	77	HIS
1	A	289	ASN
1	A	311	GLN
1	A	380	GLN
1	A	518	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	2,1	14,14,15	1.21	1 (7%)	17,19,21	3.11	11 (64%)
2	NAG	B	2	2	14,14,15	0.73	0	17,19,21	3.05	8 (47%)
2	FUL	B	3	2	10,10,11	1.37	2 (20%)	14,14,16	3.40	5 (35%)
3	NAG	C	1	3,1	14,14,15	1.88	5 (35%)	17,19,21	2.61	8 (47%)
3	FUL	C	2	3	10,10,11	0.79	0	14,14,16	3.13	6 (42%)
2	NAG	D	1	2,1	14,14,15	1.05	0	17,19,21	2.78	8 (47%)
2	NAG	D	2	2	14,14,15	1.56	3 (21%)	17,19,21	1.88	4 (23%)
2	FUL	D	3	2	10,10,11	0.91	0	14,14,16	3.93	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	2,1	-	5/6/23/26	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	-	5/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	2,1	-	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	4.50	1.58	1.52
2	D	2	NAG	C1-C2	3.21	1.56	1.52
2	B	1	NAG	C2-N2	-2.75	1.41	1.46
3	C	1	NAG	C3-C2	2.68	1.58	1.52
2	B	3	FUL	C4-C5	2.62	1.58	1.52
3	C	1	NAG	O5-C1	2.23	1.47	1.43
2	B	3	FUL	C6-C5	2.21	1.56	1.51
2	D	2	NAG	C4-C5	2.20	1.57	1.53
2	D	2	NAG	O7-C7	2.12	1.28	1.23
3	C	1	NAG	C4-C5	2.07	1.57	1.53
3	C	1	NAG	C6-C5	2.04	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	-10.82	93.88	109.64
3	C	2	FUL	C1-C2-C3	-8.30	97.56	109.64
2	B	2	NAG	C3-C4-C5	-7.71	96.26	110.23
2	B	3	FUL	C3-C4-C5	6.53	119.74	109.81
2	B	1	NAG	O5-C1-C2	-6.18	101.73	111.29
2	B	3	FUL	C1-C2-C3	-6.13	100.72	109.64
2	B	2	NAG	O6-C6-C5	-5.83	91.49	111.33
2	B	3	FUL	C1-O5-C5	-5.73	99.44	112.97
2	D	3	FUL	C3-C4-C5	5.55	118.25	109.81
2	B	3	FUL	C6-C5-C4	5.35	122.87	113.08
2	B	1	NAG	C3-C4-C5	-5.33	100.57	110.23
2	D	3	FUL	C1-O5-C5	-5.28	100.51	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	5.10	119.02	112.19
2	D	1	NAG	O5-C1-C2	-4.99	103.58	111.29
2	B	1	NAG	C8-C7-N2	4.72	123.95	116.12
3	C	1	NAG	C3-C4-C5	-4.61	101.87	110.23
2	D	1	NAG	O3-C3-C4	-4.49	99.78	110.38
2	B	2	NAG	C4-C3-C2	-4.46	104.48	111.02
3	C	1	NAG	O5-C5-C6	4.40	116.23	107.66
3	C	2	FUL	C1-O5-C5	-4.33	102.75	112.97
3	C	1	NAG	O4-C4-C5	4.32	119.97	109.32
2	B	1	NAG	O4-C4-C3	-4.24	100.38	110.38
2	D	3	FUL	O3-C3-C4	4.11	120.06	110.38
3	C	1	NAG	O5-C1-C2	-3.98	105.13	111.29
2	D	1	NAG	C3-C4-C5	-3.83	103.28	110.23
3	C	2	FUL	C3-C4-C5	3.76	115.53	109.81
2	D	1	NAG	O7-C7-C8	-3.66	115.54	122.05
2	D	2	NAG	C1-O5-C5	3.61	117.02	112.19
2	B	2	NAG	O4-C4-C5	3.59	118.16	109.32
2	B	3	FUL	O5-C5-C6	3.47	114.94	107.40
2	D	2	NAG	O4-C4-C5	3.47	117.87	109.32
2	D	1	NAG	O7-C7-N2	3.46	128.10	121.98
3	C	1	NAG	O3-C3-C2	3.44	116.54	109.40
2	B	1	NAG	C2-N2-C7	3.36	127.40	122.90
2	D	2	NAG	C2-N2-C7	3.10	127.05	122.90
3	C	1	NAG	O7-C7-C8	-3.04	116.64	122.05
3	C	2	FUL	O5-C5-C6	2.92	113.74	107.40
2	D	3	FUL	O4-C4-C5	-2.85	103.44	109.74
2	B	1	NAG	O3-C3-C4	-2.65	104.13	110.38
2	D	1	NAG	C4-C3-C2	2.65	114.90	111.02
2	B	2	NAG	O4-C4-C3	2.58	116.45	110.38
3	C	2	FUL	C2-C3-C4	-2.56	106.35	110.86
2	B	1	NAG	O7-C7-N2	-2.54	117.50	121.98
2	D	3	FUL	O2-C2-C1	2.50	114.95	109.22
2	D	2	NAG	O3-C3-C2	2.47	114.52	109.40
2	B	1	NAG	O4-C4-C5	2.40	115.23	109.32
2	B	2	NAG	O5-C5-C4	2.39	116.65	110.83
2	D	3	FUL	C2-C3-C4	-2.38	106.67	110.86
2	D	1	NAG	C2-N2-C7	2.37	126.08	122.90
3	C	1	NAG	C6-C5-C4	2.34	118.76	113.02
2	B	1	NAG	O6-C6-C5	2.34	119.30	111.33
2	B	2	NAG	C2-N2-C7	2.28	125.95	122.90
3	C	1	NAG	C8-C7-N2	2.25	119.86	116.12
2	B	1	NAG	C1-C2-N2	2.25	113.98	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FUL	O2-C2-C1	2.18	114.22	109.22
2	B	2	NAG	O3-C3-C2	2.16	113.88	109.40
2	B	1	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

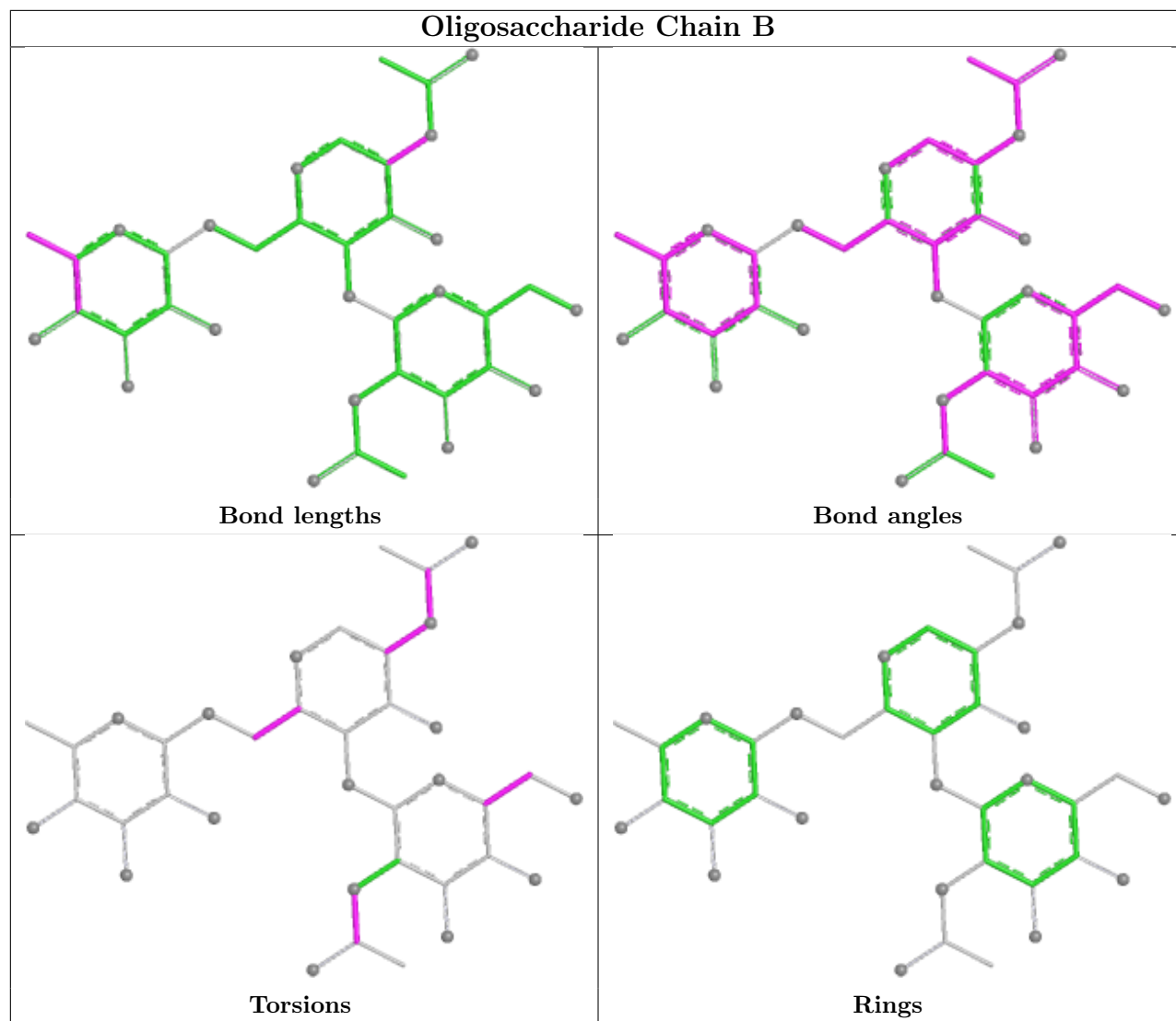
All (18) torsion outliers are listed below:

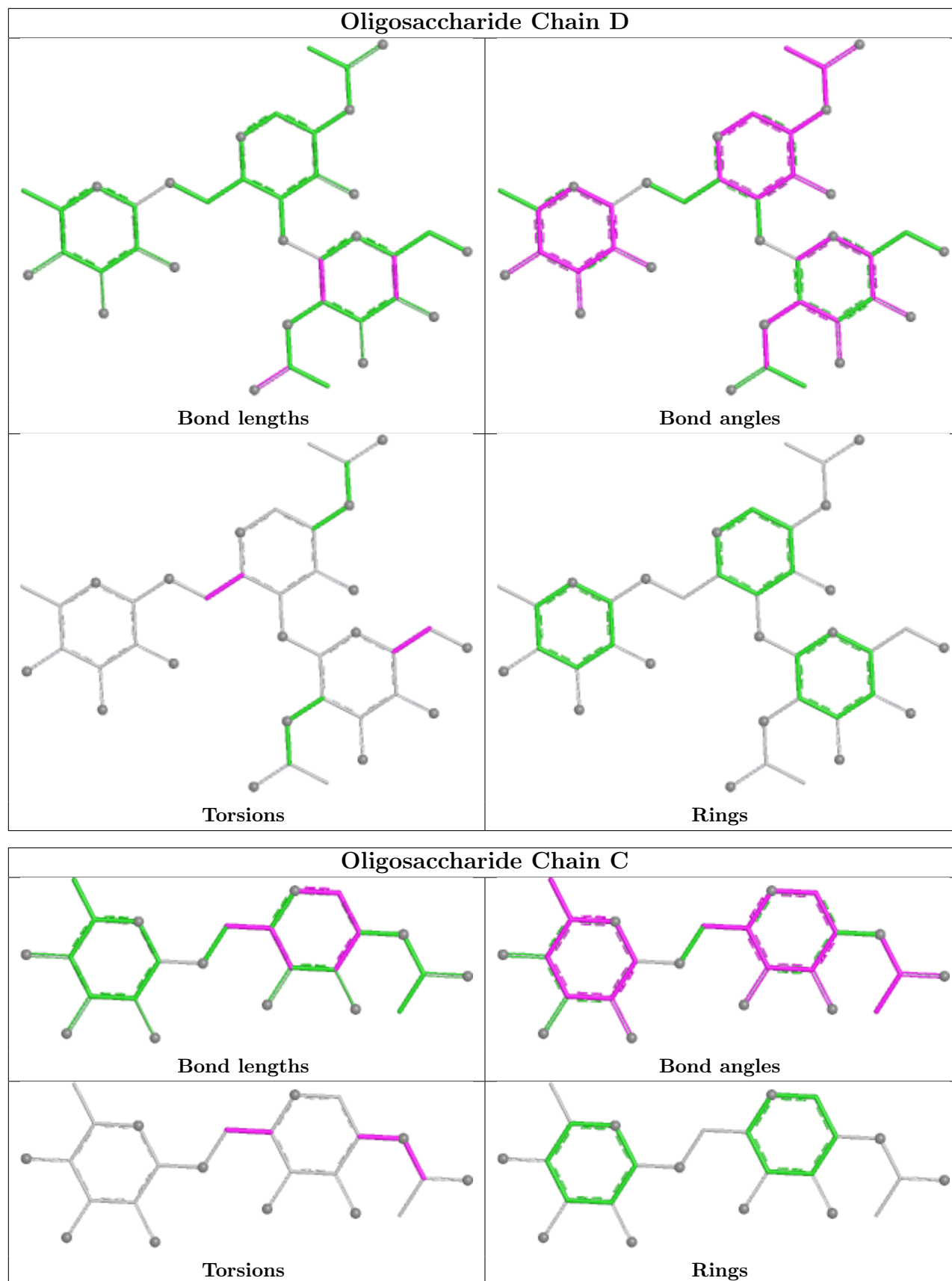
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6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

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 [i](#)

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	0.24	0	6,6,6	0.44	0
4	TC5	A	601	1	5,8,9	0.99	0	3,8,11	2.27	1 (33%)
8	NAG	A	613	1	14,14,15	0.86	0	17,19,21	2.27	8 (47%)
8	NAG	A	614	1	14,14,15	1.71	3 (21%)	17,19,21	2.86	8 (47%)
6	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.62	0
8	NAG	A	615	1	14,14,15	1.11	0	17,19,21	2.16	7 (41%)

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	615	1	1/1/5/7	6/6/23/26	0/1/1/1
8	NAG	A	614	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	614	NAG	C3-C2	3.85	1.60	1.52
8	A	614	NAG	C1-C2	2.57	1.55	1.52
8	A	614	NAG	C2-N2	2.50	1.50	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	614	NAG	O7-C7-C8	-6.06	111.27	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	615	NAG	C1-O5-C5	5.57	119.66	112.19
8	A	614	NAG	C8-C7-N2	5.07	124.53	116.12
8	A	614	NAG	C2-N2-C7	-4.86	116.39	122.90
8	A	613	NAG	C8-C7-N2	4.55	123.66	116.12
8	A	613	NAG	O5-C1-C2	-4.19	104.81	111.29
4	A	601	TC5	C4-C3-N	-3.74	101.54	112.97
8	A	614	NAG	C1-O5-C5	-3.37	107.66	112.19
8	A	613	NAG	C1-O5-C5	3.29	116.60	112.19
8	A	615	NAG	O7-C7-C8	-3.14	116.46	122.05
8	A	614	NAG	C3-C4-C5	2.90	115.49	110.23
8	A	614	NAG	O5-C1-C2	-2.70	107.11	111.29
8	A	614	NAG	C4-C3-C2	2.64	114.88	111.02
8	A	615	NAG	C2-N2-C7	2.63	126.43	122.90
8	A	615	NAG	O5-C5-C4	2.42	116.72	110.83
8	A	615	NAG	C3-C4-C5	2.40	114.59	110.23
8	A	613	NAG	O7-C7-N2	-2.36	117.81	121.98
8	A	613	NAG	C4-C3-C2	-2.23	107.74	111.02
8	A	613	NAG	C6-C5-C4	2.20	118.42	113.02
8	A	615	NAG	C1-C2-N2	2.12	113.77	110.43
8	A	614	NAG	O3-C3-C2	2.10	113.77	109.40
8	A	615	NAG	O5-C1-C2	-2.10	108.05	111.29
8	A	613	NAG	O5-C5-C6	2.05	111.65	107.66
8	A	613	NAG	O3-C3-C4	2.04	115.19	110.38

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	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	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	A	615	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	TC5	2	0
6	A	606	SO4	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, 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%)	0.05	16 (3%) 52 55	16, 32, 58, 80	13 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	4.4
1	A	377	VAL	4.2
1	A	237	TYR	3.4
1	A	282	TYR	3.0
1	A	380	GLN	2.8
1	A	270	GLN	2.7
1	A	525	PHE	2.4
1	A	268	ASP	2.3
1	A	4	ILE	2.3
1	A	259	GLU	2.2
1	A	265	ARG	2.2
1	A	453	ARG	2.1
1	A	51	LYS	2.1
1	A	378	ASP	2.1
1	A	507	SER	2.1
1	A	50	THR	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.

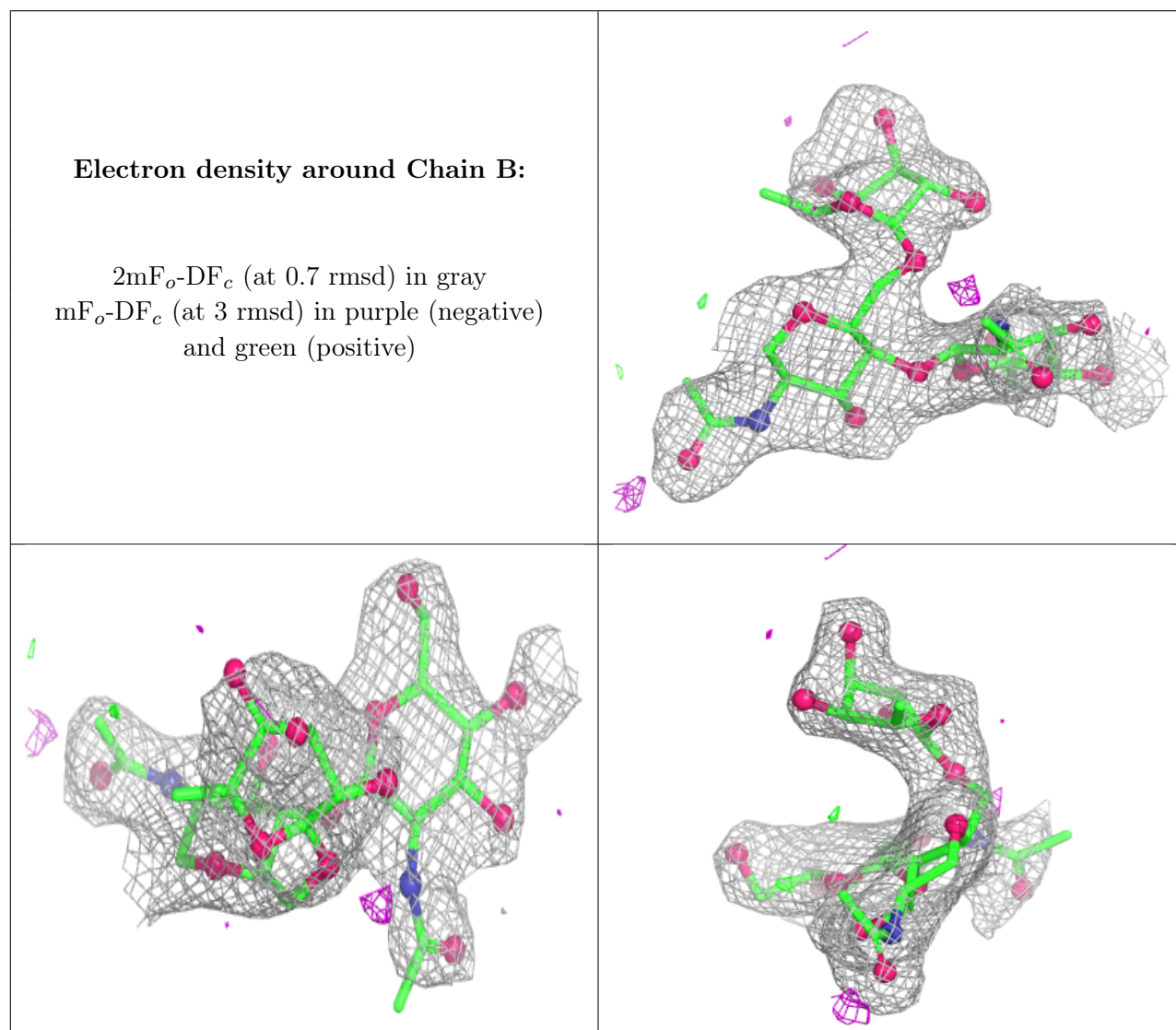
6.3 Carbohydrates [i](#)

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.

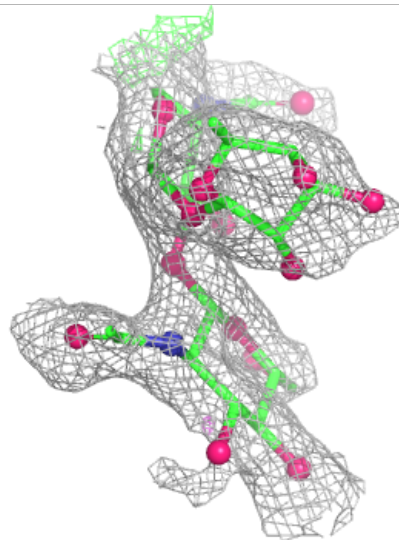
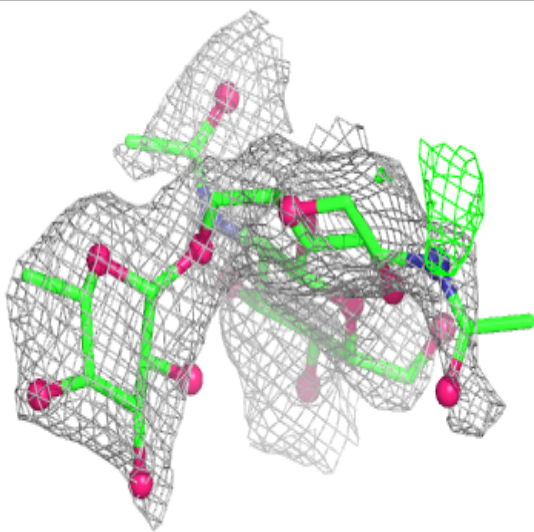
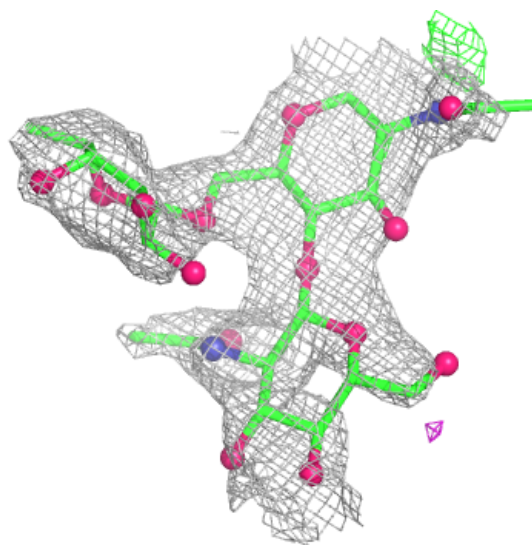
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.71	0.17	70,79,81,82	0
2	FUL	B	3	10/11	0.76	0.16	72,76,78,79	0
2	NAG	B	2	14/15	0.78	0.15	65,72,75,75	0
3	FUL	C	2	10/11	0.79	0.27	39,44,49,50	10
2	NAG	D	1	14/15	0.81	0.17	70,74,83,84	0
3	NAG	C	1	14/15	0.83	0.15	59,66,68,69	0
2	FUL	D	3	10/11	0.89	0.14	64,70,74,77	0
2	NAG	B	1	14/15	0.94	0.10	43,47,61,69	0

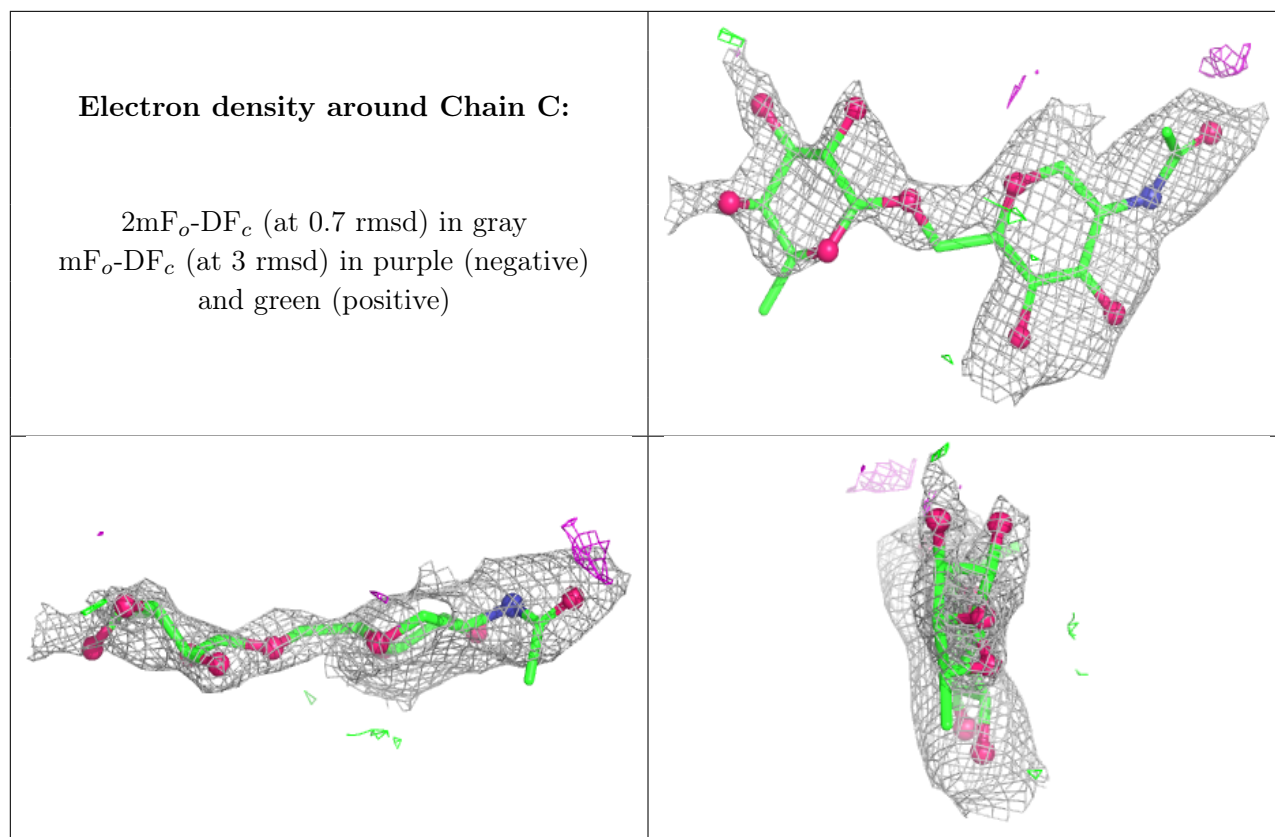
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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, 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	613	14/15	0.58	0.17	81,87,89,90	0
8	NAG	A	615	14/15	0.65	0.16	89,91,97,98	0
8	NAG	A	614	14/15	0.82	0.13	53,73,80,81	0
5	CL	A	605	1/1	0.88	0.18	81,81,81,81	0
6	SO4	A	603	5/5	0.90	0.11	51,57,59,60	5
5	CL	A	607	1/1	0.91	0.13	73,73,73,73	0
6	SO4	A	606	5/5	0.94	0.11	39,41,45,48	5
4	TC5	A	601	9/10	0.96	0.10	27,32,45,51	0
5	CL	A	602	1/1	0.96	0.08	51,51,51,51	0
7	NA	A	604	1/1	0.96	0.16	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.