



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:29 AM UTC

PDB ID : 6C2W / pdb_00006c2w
Title : Crystal structure of human prothrombin mutant S101C/A470C
Authors : Chinnaraj, M.; Chen, Z.; Pelc, L.; Grese, Z.; Bystranowska, D.; Di Cera, E.; Pozzi, N.
Deposited on : 2018-01-09
Resolution : 4.12 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

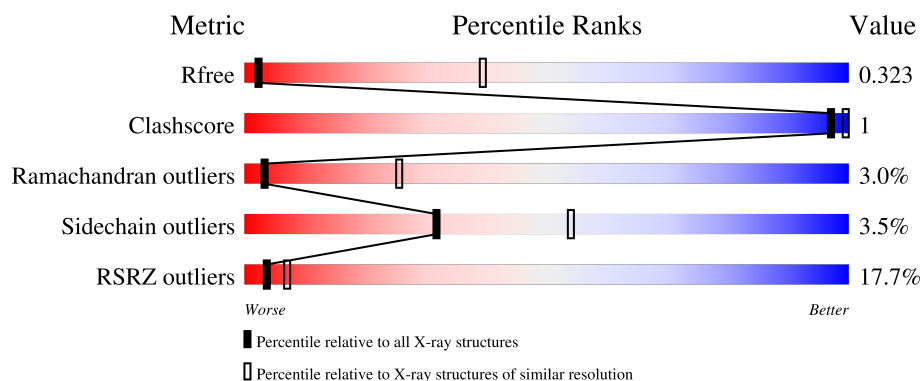
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.12 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	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	582	14% 90% 9% .
1	B	582	21% 90% 9% ..
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9278 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4594	2861	801	897	35			
1	B	575	Total	C	N	O	S	0	0	0
			4594	2861	801	897	35			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	CYS	SER	engineered mutation	UNP P00734
A	122	MET	THR	variant	UNP P00734
A	470	CYS	ALA	engineered mutation	UNP P00734
A	580	TYR	-	expression tag	UNP P00734
A	581	LEU	-	expression tag	UNP P00734
A	582	GLU	-	expression tag	UNP P00734
B	101	CYS	SER	engineered mutation	UNP P00734
B	122	MET	THR	variant	UNP P00734
B	470	CYS	ALA	engineered mutation	UNP P00734
B	580	TYR	-	expression tag	UNP P00734
B	581	LEU	-	expression tag	UNP P00734
B	582	GLU	-	expression tag	UNP P00734

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			25	14	1	10			

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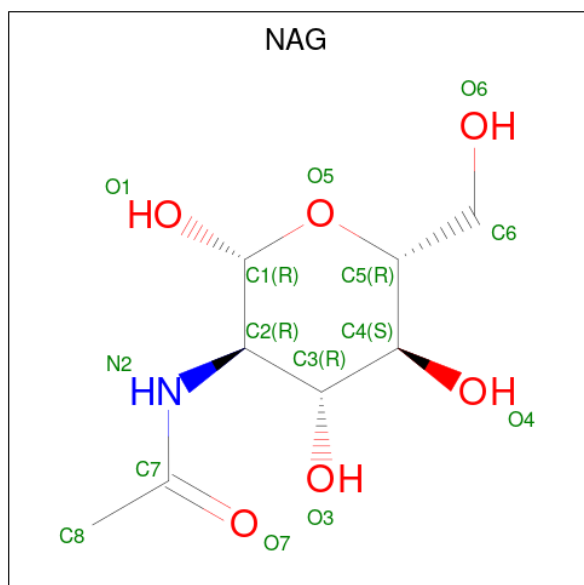
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Mg	0	0
			6	6		
3	B	6	Total	Mg	0	0
			6	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

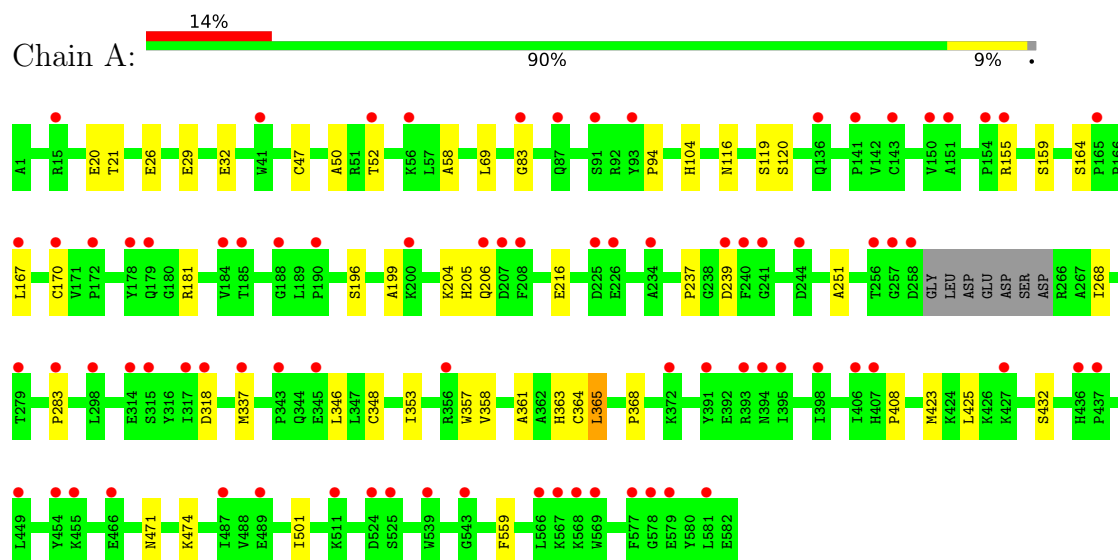


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

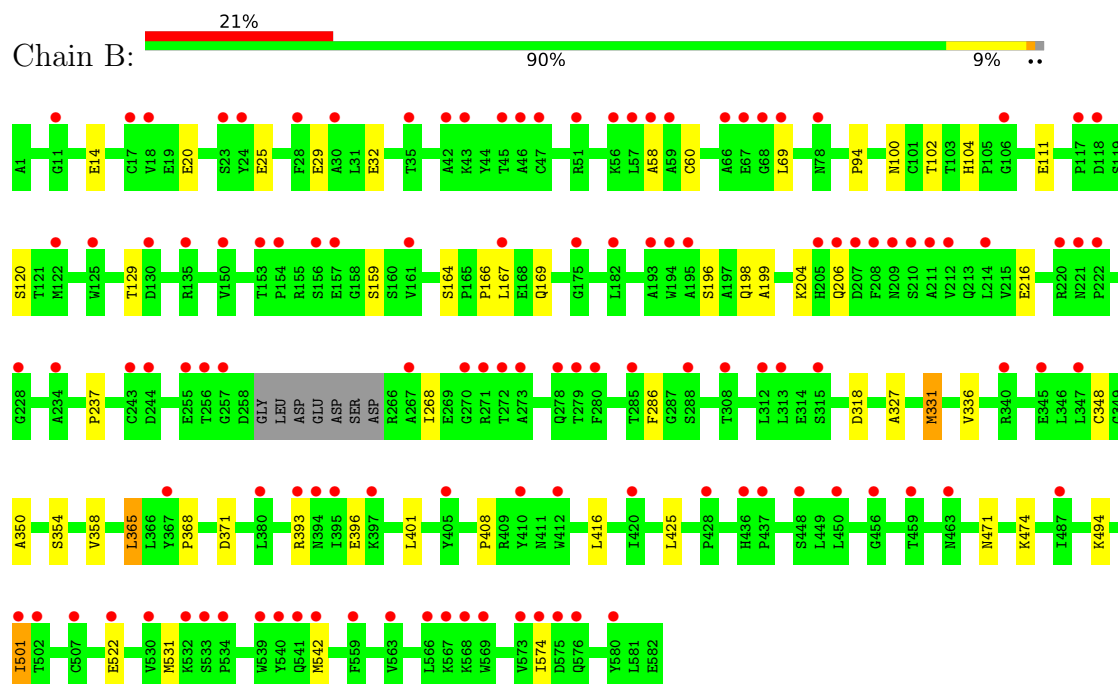
3 Residue-property plots [i](#)

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: Prothrombin



• Molecule 1: Prothrombin



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
BMA2

- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50%  50%

MAG1
BMA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 85.07Å 153.80Å 105.35° 90.00° 90.05°	Depositor
Resolution (Å)	30.32 – 4.12 30.32 – 4.12	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.32-4.12) 96.3 (30.32-4.12)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.11Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.278 , 0.333 0.289 , 0.323	Depositor DCC
R_{free} test set	1508 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	171.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l 0.046 for -h,k,-k-l 0.029 for -h,-k,k+l	Xtriage
Reported twinning fraction	0.290 for H, K, L 0.231 for h,-k,-l 0.214 for -H, -K, K+L 0.265 for -H, K, -K-L	Depositor
Outliers	0 of 30926 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	9278	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: NAG, CGU, BMA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	0/4576	0.80	2/6190 (0.0%)
1	B	0.64	0/4576	0.78	1/6190 (0.0%)
All	All	0.66	0/9152	0.79	3/12380 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	PRO	N-CA-C	6.29	118.37	110.70
1	A	368	PRO	N-CA-C	6.00	118.01	110.70
1	A	170	CYS	N-CA-C	5.40	117.05	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4594	0	4330	8	0
1	B	4594	0	4330	9	0
2	C	25	0	22	0	0
2	D	25	0	22	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	B	14	0	13	0	0
All	All	9278	0	8730	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LYS:HA	1:B:501:ILE:HD11	1.86	0.57
1:B:69:LEU:HD13	1:B:120:SER:HB3	1.87	0.56
1:A:353:ILE:HD11	1:A:357:TRP:HB3	1.89	0.54
1:B:358:VAL:HG21	1:B:425:LEU:HD21	1.90	0.53
1:B:100:ASN:HD21	1:B:102:THR:HB	1.77	0.49
1:B:336:VAL:HB	1:B:350:ALA:HB3	1.97	0.47
1:A:361:ALA:HB3	1:A:364:CYS:SG	2.55	0.46
1:A:47:CYS:HB3	1:A:50:ALA:HB3	1.99	0.45
1:B:327:ALA:HB1	1:B:331:MET:HE2	1.98	0.45
1:A:69:LEU:HD13	1:A:120:SER:HB3	1.99	0.44
1:A:337:MET:HE2	1:A:346:LEU:HD22	2.00	0.43
1:A:358:VAL:HB	1:A:423:MET:HB2	2.00	0.43
1:B:401:LEU:HD23	1:B:425:LEU:HD23	2.02	0.42
1:B:531:MET:HE3	1:B:542:MET:HB2	2.00	0.42
1:A:361:ALA:HB1	1:A:363:HIS:CE1	2.55	0.42
1:A:358:VAL:HG21	1:A:425:LEU:HD21	2.02	0.41
1:B:286:PHE:HB2	1:B:574:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

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	561/582 (96%)	451 (80%)	92 (16%)	18 (3%)	3	24
1	B	561/582 (96%)	449 (80%)	96 (17%)	16 (3%)	3	26
All	All	1122/1164 (96%)	900 (80%)	188 (17%)	34 (3%)	3	25

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	SER
1	A	237	PRO
1	B	237	PRO
1	A	58	ALA
1	A	83	GLY
1	A	199	ALA
1	A	318	ASP
1	B	164	SER
1	B	199	ALA
1	A	159	SER
1	A	251	ALA
1	A	283	PRO
1	B	58	ALA
1	B	159	SER
1	B	169	GLN
1	B	216	GLU
1	B	318	ASP
1	A	216	GLU
1	A	471	ASN
1	B	94	PRO
1	B	166	PRO
1	B	365	LEU
1	B	416	LEU
1	B	471	ASN
1	A	119	SER
1	A	155	ARG
1	A	181	ARG
1	A	196	SER
1	A	365	LEU
1	A	408	PRO
1	B	196	SER
1	B	371	ASP
1	B	408	PRO
1	A	94	PRO

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	484/490 (99%)	468 (97%)	16 (3%)	33	55
1	B	484/490 (99%)	466 (96%)	18 (4%)	30	52
All	All	968/980 (99%)	934 (96%)	34 (4%)	32	54

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	52	THR
1	A	104	HIS
1	A	116	ASN
1	A	167	LEU
1	A	204	LYS
1	A	205	HIS
1	A	206	GLN
1	A	239	ASP
1	A	268	ILE
1	A	348	CYS
1	A	365	LEU
1	A	432	SER
1	A	474	LYS
1	A	501	ILE
1	A	559	PHE
1	B	60	CYS
1	B	104	HIS
1	B	111	GLU
1	B	129	THR
1	B	167	LEU
1	B	198	GLN
1	B	204	LYS
1	B	206	GLN
1	B	268	ILE
1	B	331	MET
1	B	348	CYS

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Mol	Chain	Res	Type
1	B	354	SER
1	B	365	LEU
1	B	393	ARG
1	B	396	GLU
1	B	474	LYS
1	B	501	ILE
1	B	522	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	72	ASN
1	A	147	GLN
1	A	278	GLN
1	A	411	ASN
1	A	541	GLN
1	A	571	GLN
1	B	100	ASN
1	B	110	GLN
1	B	145	GLN
1	B	246	ASN
1	B	411	ASN
1	B	436	HIS
1	B	476	GLN
1	B	571	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](#)

20 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CGU	B	19	1,3	9,11,12	0.94	0	10,14,16	1.09	0
1	CGU	A	26	1,3	9,11,12	1.03	0	10,14,16	1.11	1 (10%)
1	CGU	B	32	1	9,11,12	1.07	0	10,14,16	1.37	1 (10%)
1	CGU	A	6	1	9,11,12	1.01	0	10,14,16	1.13	0
1	CGU	A	29	1,3	9,11,12	1.07	0	10,14,16	1.52	1 (10%)
1	CGU	B	6	1	9,11,12	1.03	0	10,14,16	0.67	0
1	CGU	A	25	1	9,11,12	1.02	0	10,14,16	0.86	0
1	CGU	B	29	1,3	9,11,12	1.08	0	10,14,16	1.14	1 (10%)
1	CGU	B	26	1,3	9,11,12	1.11	0	10,14,16	1.02	0
1	CGU	B	20	1	9,11,12	0.97	0	10,14,16	1.48	1 (10%)
1	CGU	A	19	1,3	9,11,12	1.09	0	10,14,16	1.07	0
1	CGU	A	20	1	9,11,12	1.08	0	10,14,16	1.49	1 (10%)
1	CGU	B	14	1	9,11,12	1.02	0	10,14,16	0.90	1 (10%)
1	CGU	B	7	1	9,11,12	1.06	0	10,14,16	0.51	0
1	CGU	B	25	1	9,11,12	1.00	0	10,14,16	1.44	2 (20%)
1	CGU	A	7	1	9,11,12	1.05	0	10,14,16	0.79	0
1	CGU	A	32	1,3	9,11,12	1.08	0	10,14,16	1.22	1 (10%)
1	CGU	A	16	1,3	9,11,12	1.03	0	10,14,16	0.80	0
1	CGU	B	16	1,3	9,11,12	0.98	0	10,14,16	0.90	0
1	CGU	A	14	1,3	9,11,12	0.94	0	10,14,16	1.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	B	19	1,3	-	2/13/14/16	-
1	CGU	A	26	1,3	-	0/13/14/16	-
1	CGU	B	32	1	-	4/13/14/16	-
1	CGU	A	6	1	-	4/13/14/16	-
1	CGU	A	29	1,3	-	2/13/14/16	-
1	CGU	B	6	1	-	2/13/14/16	-
1	CGU	A	25	1	-	0/13/14/16	-
1	CGU	B	29	1,3	-	2/13/14/16	-
1	CGU	B	26	1,3	-	0/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	B	20	1	-	4/13/14/16	-
1	CGU	A	19	1,3	-	5/13/14/16	-
1	CGU	A	20	1	-	3/13/14/16	-
1	CGU	B	14	1	-	4/13/14/16	-
1	CGU	B	7	1	-	5/13/14/16	-
1	CGU	B	25	1	-	5/13/14/16	-
1	CGU	A	7	1	-	5/13/14/16	-
1	CGU	A	32	1,3	-	5/13/14/16	-
1	CGU	A	16	1,3	-	4/13/14/16	-
1	CGU	B	16	1,3	-	4/13/14/16	-
1	CGU	A	14	1,3	-	2/13/14/16	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	CGU	CB-CA-C	4.31	117.63	110.99
1	A	29	CGU	CB-CG-CD2	-3.96	105.07	113.11
1	B	20	CGU	CB-CA-C	3.87	116.94	110.99
1	B	32	CGU	CB-CG-CD1	-3.67	105.67	113.11
1	A	32	CGU	CB-CG-CD1	-3.24	106.54	113.11
1	B	29	CGU	CB-CG-CD2	-2.91	107.20	113.11
1	B	25	CGU	CB-CG-CD2	-2.87	107.29	113.11
1	A	26	CGU	CB-CG-CD2	-2.57	107.89	113.11
1	B	25	CGU	CB-CA-C	2.14	114.29	110.99
1	B	14	CGU	CB-CG-CD2	-2.14	108.77	113.11

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	6	CGU	CA-CB-CG-CD1
1	A	6	CGU	CA-CB-CG-CD2
1	A	6	CGU	OE11-CD1-CG-CD2
1	A	6	CGU	OE12-CD1-CG-CD2
1	A	7	CGU	N-CA-CB-CG
1	A	7	CGU	C-CA-CB-CG
1	A	7	CGU	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	A	7	CGU	CA-CB-CG-CD2
1	A	19	CGU	CA-CB-CG-CD1
1	A	19	CGU	CA-CB-CG-CD2
1	A	20	CGU	O-C-CA-CB
1	A	20	CGU	CA-CB-CG-CD1
1	A	20	CGU	CA-CB-CG-CD2
1	A	32	CGU	N-CA-CB-CG
1	B	6	CGU	CA-CB-CG-CD1
1	B	6	CGU	CA-CB-CG-CD2
1	B	7	CGU	C-CA-CB-CG
1	B	14	CGU	OE11-CD1-CG-CB
1	B	20	CGU	O-C-CA-CB
1	B	7	CGU	CA-CB-CG-CD1
1	B	32	CGU	N-CA-CB-CG
1	A	14	CGU	OE11-CD1-CG-CB
1	A	16	CGU	OE21-CD2-CG-CB
1	A	16	CGU	OE22-CD2-CG-CB
1	A	19	CGU	OE21-CD2-CG-CB
1	A	19	CGU	OE22-CD2-CG-CB
1	A	29	CGU	OE21-CD2-CG-CB
1	A	29	CGU	OE22-CD2-CG-CB
1	A	32	CGU	OE11-CD1-CG-CB
1	A	32	CGU	OE12-CD1-CG-CB
1	B	7	CGU	OE11-CD1-CG-CB
1	B	14	CGU	OE12-CD1-CG-CB
1	B	16	CGU	OE21-CD2-CG-CB
1	B	16	CGU	OE22-CD2-CG-CB
1	B	19	CGU	OE21-CD2-CG-CB
1	B	19	CGU	OE22-CD2-CG-CB
1	B	25	CGU	OE21-CD2-CG-CB
1	B	25	CGU	OE22-CD2-CG-CB
1	B	29	CGU	OE21-CD2-CG-CB
1	B	29	CGU	OE22-CD2-CG-CB
1	A	16	CGU	OE21-CD2-CG-CD1
1	A	16	CGU	OE22-CD2-CG-CD1
1	A	32	CGU	OE12-CD1-CG-CD2
1	B	14	CGU	OE11-CD1-CG-CD2
1	B	14	CGU	OE12-CD1-CG-CD2
1	B	25	CGU	OE11-CD1-CG-CD2
1	B	7	CGU	CA-CB-CG-CD2
1	A	14	CGU	OE12-CD1-CG-CB
1	B	7	CGU	OE12-CD1-CG-CB

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Mol	Chain	Res	Type	Atoms
1	B	20	CGU	OE21-CD2-CG-CB
1	B	25	CGU	OE11-CD1-CG-CB
1	B	25	CGU	OE12-CD1-CG-CB
1	B	32	CGU	OE12-CD1-CG-CB
1	A	7	CGU	OE11-CD1-CG-CD2
1	A	19	CGU	OE22-CD2-CG-CD1
1	A	32	CGU	OE11-CD1-CG-CD2
1	B	16	CGU	OE21-CD2-CG-CD1
1	B	16	CGU	OE22-CD2-CG-CD1
1	B	20	CGU	OE21-CD2-CG-CD1
1	B	20	CGU	OE22-CD2-CG-CD1
1	B	32	CGU	OE11-CD1-CG-CD2
1	B	32	CGU	OE12-CD1-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
2	BMA	C	2	2	11,11,12	0.59	0	15,15,17	1.01	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.68	0	17,19,21	0.85	0
2	BMA	D	2	2	11,11,12	0.60	0	15,15,17	0.89	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	BMA	C	2	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	BMA	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BMA	C2-C3-C4	2.25	114.83	110.86
2	C	1	NAG	C1-O5-C5	2.09	114.99	112.19
2	D	2	BMA	C1-C2-C3	2.02	112.58	109.64

There are no chirality outliers.

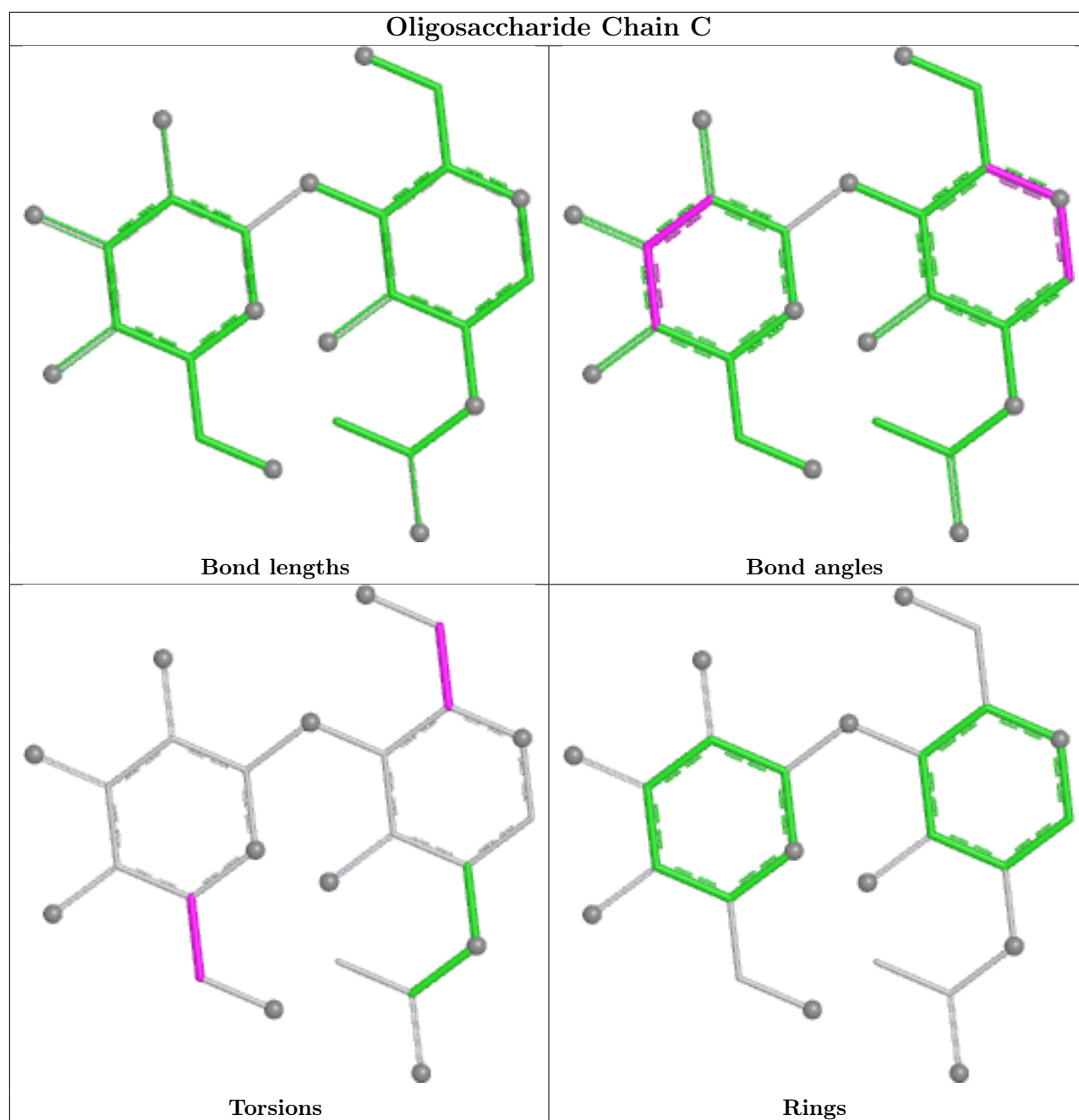
All (6) torsion outliers are listed below:

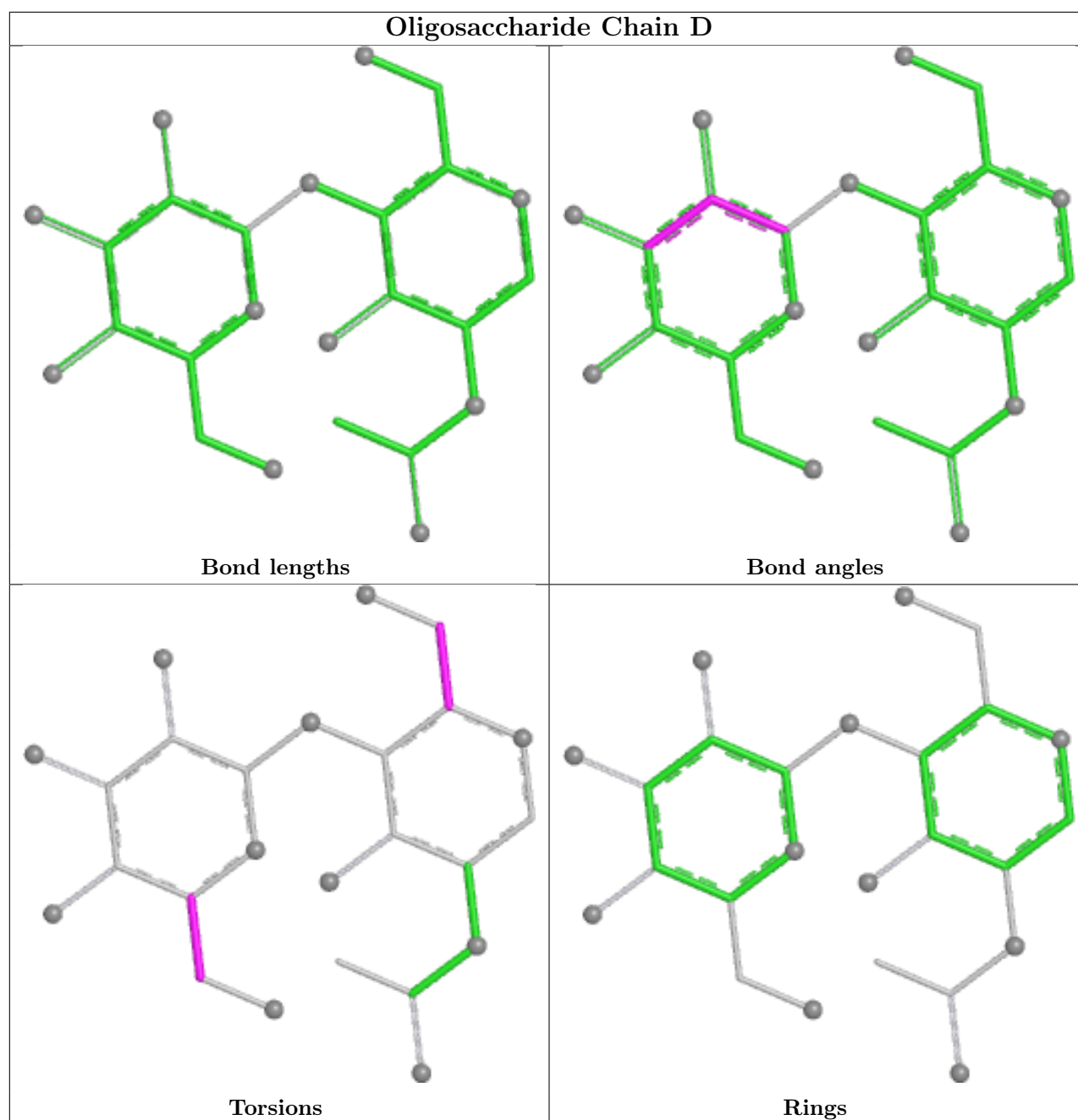
Mol	Chain	Res	Type	Atoms
2	C	2	BMA	O5-C5-C6-O6
2	D	2	BMA	O5-C5-C6-O6
2	C	2	BMA	C4-C5-C6-O6
2	D	2	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

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 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	609	1	14,14,15	0.70	1 (7%)	17,19,21	1.16	2 (11%)
4	NAG	B	609	1	14,14,15	0.53	0	17,19,21	0.83	1 (5%)

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	609	1	-	2/6/23/26	0/1/1/1
4	NAG	B	609	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	609	NAG	C1-C2	2.19	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	609	NAG	C4-C3-C2	2.40	114.54	111.02
4	A	609	NAG	C1-O5-C5	2.14	115.06	112.19
4	B	609	NAG	C4-C3-C2	2.03	114.00	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	NAG	C4-C5-C6-O6
4	A	609	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	565/582 (97%)	0.93	80 (14%) 6 10	102, 186, 247, 305	0
1	B	565/582 (97%)	1.26	120 (21%) 2 5	111, 200, 265, 336	0
All	All	1130/1164 (97%)	1.10	200 (17%) 4 7	102, 193, 256, 336	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	THR	10.6
1	B	68	GLY	8.9
1	A	579	GLU	8.6
1	A	318	ASP	7.5
1	A	568	LYS	6.2
1	B	315	SER	6.2
1	A	241	GLY	6.1
1	A	257	GLY	6.1
1	B	256	THR	6.0
1	B	279	THR	5.9
1	B	207	ASP	5.8
1	A	239	ASP	5.8
1	A	179	GLN	5.8
1	B	56	LYS	5.3
1	B	206	GLN	5.1
1	A	240	PHE	5.1
1	B	567	LYS	5.0
1	B	280	PHE	4.9
1	B	436	HIS	4.8
1	A	455	LYS	4.8
1	A	567	LYS	4.8
1	B	153	THR	4.7
1	B	532	LYS	4.7
1	B	69	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	454	TYR	4.6
1	B	244	ASP	4.5
1	A	398	ILE	4.5
1	B	156	SER	4.5
1	B	234	ALA	4.5
1	A	427	LYS	4.5
1	B	559	PHE	4.4
1	A	165	PRO	4.4
1	A	56	LYS	4.4
1	A	406	ILE	4.4
1	B	222	PRO	4.4
1	A	436	HIS	4.3
1	B	209	ASN	4.3
1	B	569	TRP	4.3
1	A	279	THR	4.2
1	B	394	ASN	4.2
1	A	394	ASN	4.1
1	A	83	GLY	4.1
1	B	542	MET	4.1
1	B	135	ARG	4.1
1	A	578	GLY	4.0
1	B	563	VAL	3.9
1	A	150	VAL	3.9
1	B	30	ALA	3.9
1	A	395	ILE	3.8
1	B	541	GLN	3.8
1	B	210	SER	3.8
1	B	66	ALA	3.8
1	A	581	LEU	3.8
1	B	23	SER	3.7
1	B	288	SER	3.7
1	A	317	ILE	3.6
1	A	315	SER	3.6
1	A	170	CYS	3.6
1	A	141	PRO	3.6
1	A	393	ARG	3.6
1	B	566	LEU	3.5
1	B	228	GLY	3.5
1	B	150	VAL	3.5
1	A	489	GLU	3.5
1	B	45	THR	3.5
1	B	393	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	397	LYS	3.4
1	A	206	GLN	3.3
1	B	285	THR	3.3
1	B	194	TRP	3.3
1	A	184	VAL	3.3
1	A	154	PRO	3.2
1	A	93	TYR	3.2
1	B	502	THR	3.1
1	B	568	LYS	3.1
1	B	43	LYS	3.1
1	A	372	LYS	3.1
1	B	576	GLN	3.1
1	B	257	GLY	3.1
1	B	539	TRP	3.1
1	B	573	VAL	3.1
1	B	278	GLN	3.0
1	A	178	TYR	3.0
1	A	298	LEU	3.0
1	B	211	ALA	3.0
1	B	487	ILE	3.0
1	B	106	GLY	3.0
1	B	367	TYR	3.0
1	B	28	PHE	3.0
1	B	501	ILE	2.9
1	B	428	PRO	2.9
1	B	122	MET	2.9
1	A	577	PHE	2.9
1	B	340	ARG	2.9
1	A	87	GLN	2.9
1	B	214	LEU	2.9
1	B	271	ARG	2.9
1	B	273	ALA	2.9
1	B	208	PHE	2.9
1	A	466	GLU	2.8
1	B	182	LEU	2.8
1	A	487	ILE	2.8
1	B	450	LEU	2.8
1	B	267	ALA	2.8
1	B	130	ASP	2.8
1	A	345	GLU	2.8
1	A	91	SER	2.7
1	B	272	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	2.7
1	A	539	TRP	2.7
1	A	41	TRP	2.7
1	B	420	ILE	2.7
1	A	511	LYS	2.7
1	A	172	PRO	2.7
1	B	380	LEU	2.6
1	B	175	GLY	2.6
1	B	51	ARG	2.6
1	A	524	ASP	2.6
1	B	395	ILE	2.6
1	B	410	TYR	2.6
1	B	405	TYR	2.6
1	B	243	CYS	2.6
1	B	212	VAL	2.6
1	B	57	LEU	2.5
1	A	525	SER	2.5
1	B	167	LEU	2.5
1	B	412	TRP	2.5
1	A	437	PRO	2.5
1	B	154	PRO	2.5
1	B	59	ALA	2.5
1	B	24	TYR	2.5
1	B	161	VAL	2.5
1	A	407	HIS	2.5
1	B	255	GLU	2.5
1	A	225	ASP	2.5
1	A	391	TYR	2.5
1	A	566	LEU	2.5
1	A	155	ARG	2.5
1	B	540	TYR	2.4
1	B	125	TRP	2.4
1	B	118	ASP	2.4
1	B	345	GLU	2.3
1	B	448	SER	2.3
1	A	151	ALA	2.3
1	B	17	CYS	2.3
1	B	47	CYS	2.3
1	B	220	ARG	2.3
1	A	167	LEU	2.3
1	A	143	CYS	2.3
1	A	569	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLU	2.3
1	B	533	SER	2.3
1	A	200	LYS	2.3
1	A	15	ARG	2.3
1	B	221	ASN	2.3
1	A	185	THR	2.3
1	B	522	GLU	2.2
1	B	507	CYS	2.2
1	B	574	ILE	2.2
1	A	188	GLY	2.2
1	B	11	GLY	2.2
1	B	312	LEU	2.2
1	A	337	MET	2.2
1	B	18	VAL	2.2
1	B	42	ALA	2.2
1	B	58	ALA	2.2
1	B	117	PRO	2.2
1	B	195	ALA	2.2
1	B	580	TYR	2.2
1	A	356	ARG	2.2
1	B	35	THR	2.2
1	A	52	THR	2.2
1	A	208	PHE	2.2
1	A	207	ASP	2.1
1	A	234	ALA	2.1
1	B	437	PRO	2.1
1	B	205	HIS	2.1
1	B	459	THR	2.1
1	A	136	GLN	2.1
1	A	314	GLU	2.1
1	B	313	LEU	2.1
1	B	530	VAL	2.1
1	B	78	ASN	2.1
1	B	193	ALA	2.1
1	B	347	LEU	2.1
1	A	543	GLY	2.1
1	A	343	PRO	2.1
1	B	534	PRO	2.1
1	B	575	ASP	2.1
1	A	226	GLU	2.1
1	A	258	ASP	2.0
1	B	270	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	308	THR	2.0
1	A	244	ASP	2.0
1	B	456	GLY	2.0
1	A	190	PRO	2.0
1	B	46	ALA	2.0
1	A	283	PRO	2.0
1	B	463	ASN	2.0
1	A	449	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

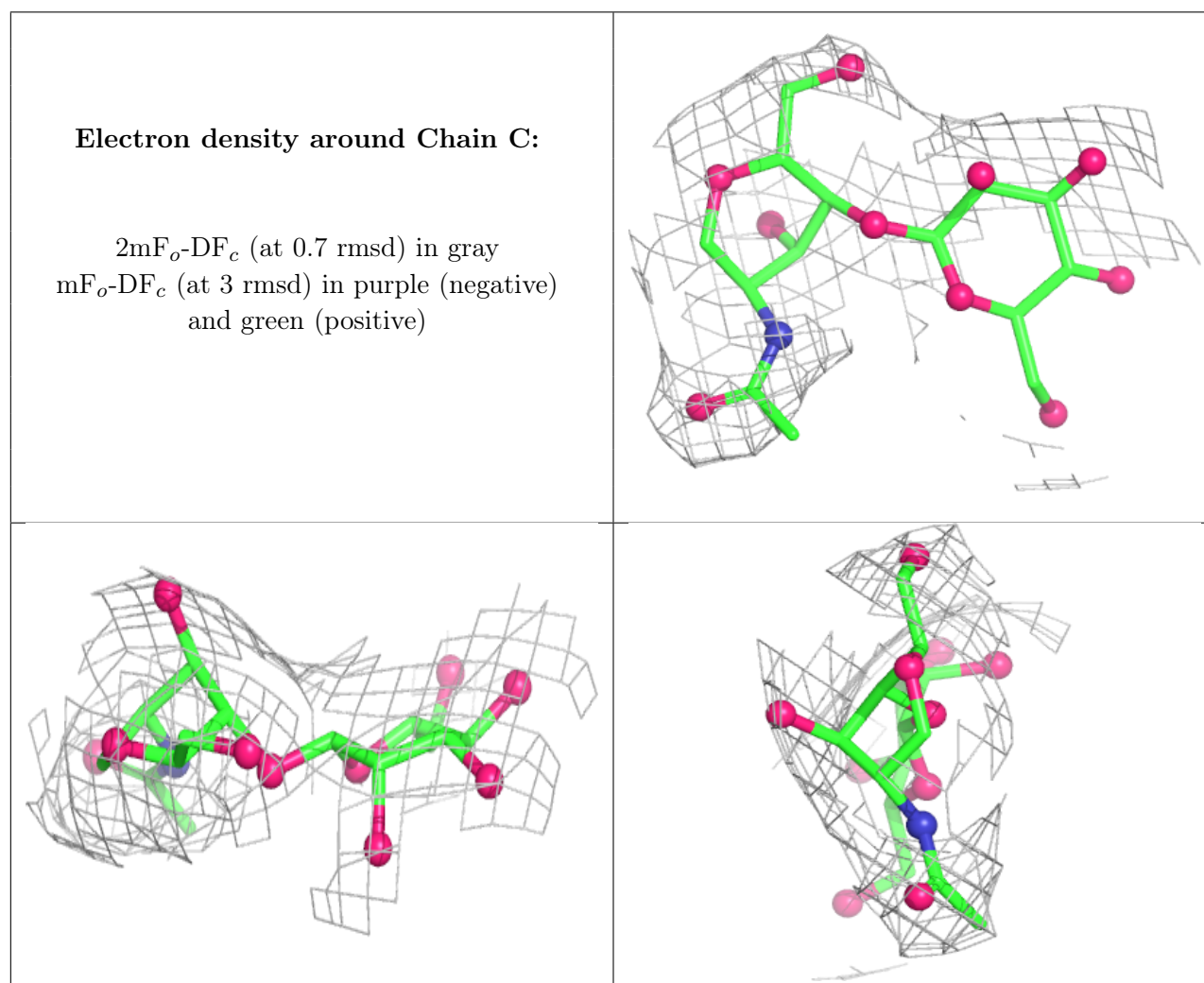
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CGU	B	14	12/13	0.75	0.20	128,171,178,188	0
1	CGU	B	25	12/13	0.77	0.18	135,158,163,166	0
1	CGU	B	32	12/13	0.77	0.13	133,151,195,199	0
1	CGU	B	6	12/13	0.78	0.11	119,156,167,169	0
1	CGU	A	6	12/13	0.78	0.13	129,145,175,181	0
1	CGU	A	25	12/13	0.82	0.22	139,169,178,180	0
1	CGU	B	16	12/13	0.83	0.17	216,227,233,235	0
1	CGU	B	19	12/13	0.83	0.21	97,157,178,182	0
1	CGU	B	20	12/13	0.85	0.18	158,178,182,188	0
1	CGU	B	7	12/13	0.85	0.17	147,173,179,180	0
1	CGU	B	29	12/13	0.85	0.18	206,227,242,251	0
1	CGU	A	14	12/13	0.85	0.17	115,146,168,174	0
1	CGU	A	20	12/13	0.86	0.16	186,201,204,205	0
1	CGU	A	26	12/13	0.87	0.15	110,133,152,157	0
1	CGU	A	32	12/13	0.89	0.08	110,144,171,180	0
1	CGU	A	19	12/13	0.91	0.17	96,131,184,190	0
1	CGU	A	16	12/13	0.91	0.16	113,133,157,161	0
1	CGU	B	26	12/13	0.92	0.11	111,151,158,160	0
1	CGU	A	7	12/13	0.93	0.09	168,177,190,191	0
1	CGU	A	29	12/13	0.94	0.15	174,198,208,216	0

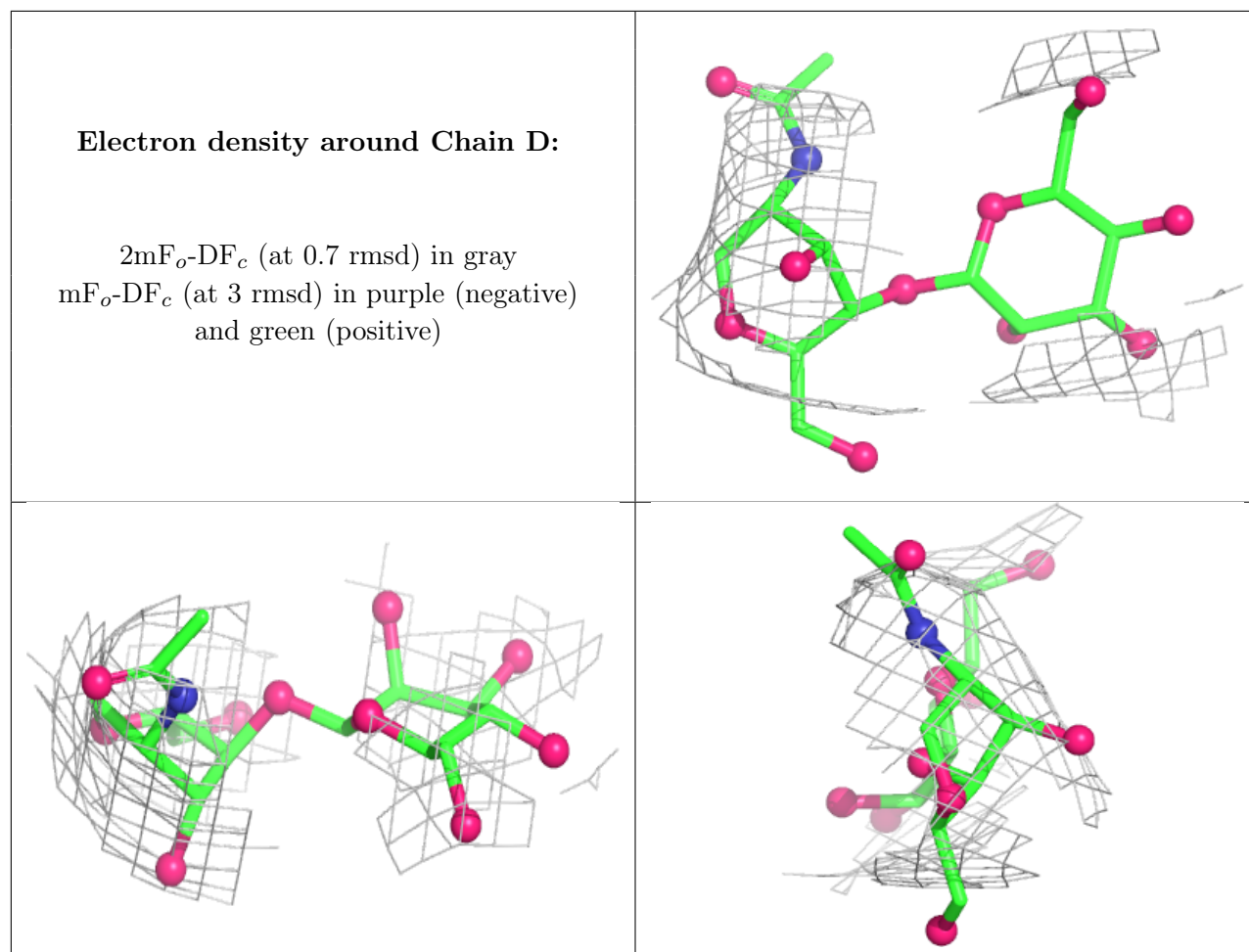
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	BMA	C	2	11/12	0.70	0.13	119,144,147,148	0
2	NAG	D	1	14/15	0.73	0.24	157,204,221,228	0
2	BMA	D	2	11/12	0.76	0.11	162,190,200,204	0
2	NAG	C	1	14/15	0.77	0.14	116,152,167,179	0

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





6.4 Ligands [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
3	MG	B	601	1/1	0.73	0.18	116,116,116,116	0
4	NAG	A	609	14/15	0.82	0.17	126,185,213,218	0
3	MG	B	606	1/1	0.87	0.11	43,43,43,43	0
3	MG	B	602	1/1	0.88	0.20	92,92,92,92	0
4	NAG	B	609	14/15	0.88	0.12	196,208,224,224	0
3	MG	A	605	1/1	0.89	0.10	90,90,90,90	0
3	MG	B	605	1/1	0.90	0.10	79,79,79,79	0
3	MG	A	601	1/1	0.91	0.24	133,133,133,133	0
3	MG	A	602	1/1	0.93	0.06	84,84,84,84	0
3	MG	A	606	1/1	0.95	0.20	57,57,57,57	0
3	MG	B	604	1/1	0.95	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	604	1/1	0.96	0.16	102,102,102,102	0
3	MG	A	603	1/1	0.97	0.14	92,92,92,92	0
3	MG	B	603	1/1	0.98	0.04	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.