



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:07 AM UTC

PDB ID : 2C6G / pdb_00002c6g
Title : Membrane-bound glutamate carboxypeptidase II (GCPII) with bound glutamate
Authors : Mesters, J.R.; Barinka, C.; Li, W.; Tsukamoto, T.; Majer, P.; Slusher, B.S.; Konvalinka, J.; Hilgenfeld, R.
Deposited on : 2005-11-09
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

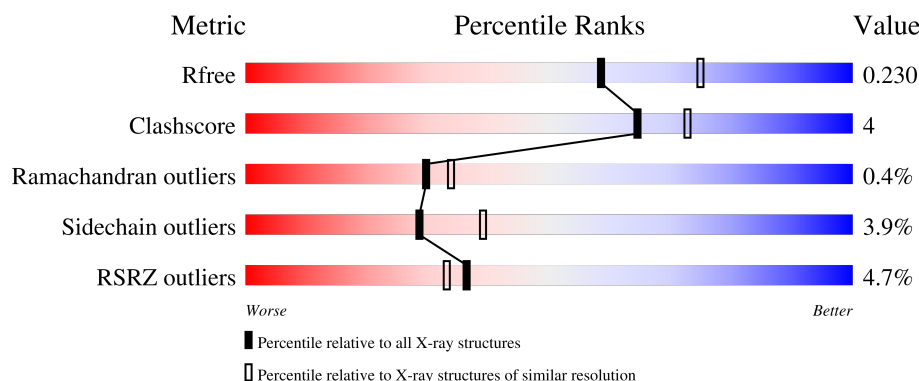
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	707	5% 83% 11% ...
2	B	2	100%
2	C	2	100%
3	D	4	75% 25%

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
8	NAG	A	1759	X	-	-	-

2 Entry composition [i](#)

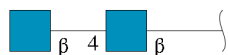
There are 9 unique types of molecules in this entry. The entry contains 5571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5266	3394	872	983	17			

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



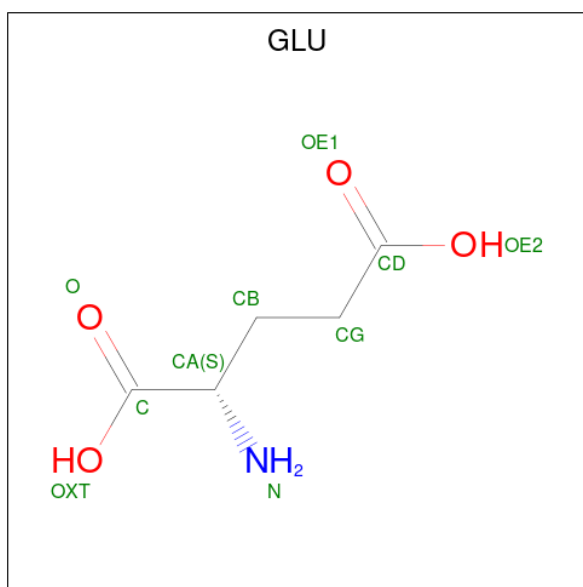
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

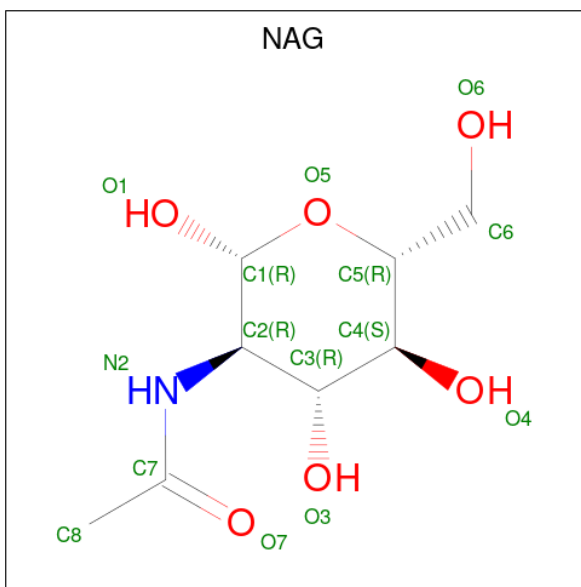
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

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

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



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

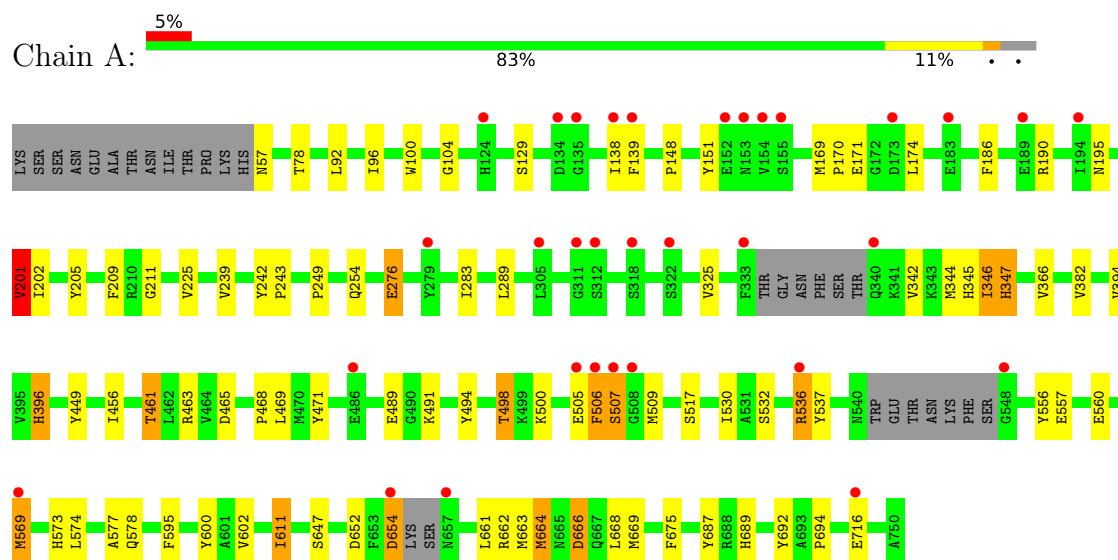
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	143	Total	O	0	0
			143	143		

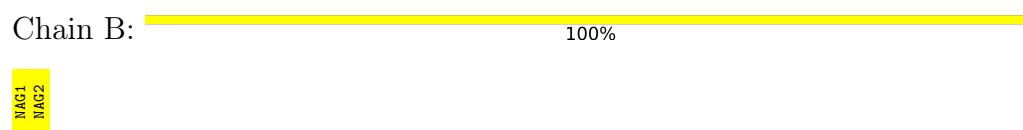
3 Residue-property plots

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.

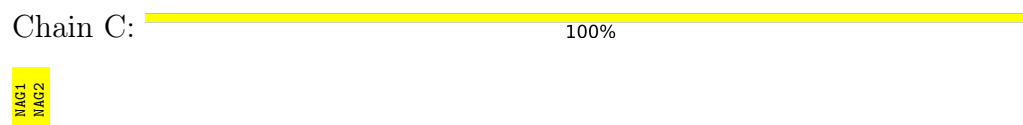
• Molecule 1: GLUTAMATE CARBOXYPEPTIDASE II



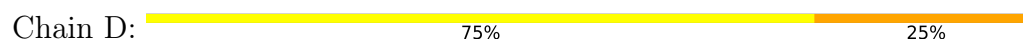
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.44Å 130.43Å 159.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20 100.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (100.00-2.20) 95.6 (100.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.186 , 0.228 0.193 , 0.230	Depositor DCC
R_{free} test set	1324 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5571	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, BMA, NAG, CA, MAN

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	1.20	10/5412 (0.2%)	1.11	16/7354 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	MET	SD-CE	-10.86	1.52	1.79
1	A	569	MET	SD-CE	10.52	2.05	1.79
1	A	602	VAL	CA-CB	6.47	1.61	1.54
1	A	669	MET	SD-CE	-6.00	1.64	1.79
1	A	661	LEU	C-O	-5.76	1.17	1.24
1	A	530	ILE	CA-CB	-5.56	1.47	1.54
1	A	611	ILE	CA-CB	5.32	1.61	1.54
1	A	347	HIS	CA-C	5.27	1.58	1.52
1	A	346	ILE	CA-CB	5.24	1.61	1.54
1	A	491	LYS	CA-C	5.17	1.60	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ILE	N-CA-C	11.36	125.63	108.71
1	A	507	SER	N-CA-C	-7.05	95.77	110.80
1	A	652	ASP	CB-CA-C	-6.95	102.68	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	ASP	N-CA-C	6.69	121.82	112.72
1	A	347	HIS	N-CA-C	-6.65	104.32	114.16
1	A	661	LEU	N-CA-C	-6.52	102.83	111.24
1	A	666	ASP	N-CA-C	-6.29	104.51	111.36
1	A	346	ILE	N-CA-C	6.02	116.79	108.12
1	A	461	THR	N-CA-C	5.86	116.83	108.74
1	A	78	THR	N-CA-C	5.79	119.93	112.41
1	A	104	GLY	N-CA-C	5.75	123.06	114.95
1	A	202	ILE	N-CA-CB	-5.17	102.58	110.86
1	A	138	ILE	N-CA-C	5.16	116.62	111.00
1	A	366	VAL	N-CA-C	5.09	116.51	111.67
1	A	201	VAL	CB-CA-C	5.06	118.53	111.34
1	A	505	GLU	N-CA-C	5.01	121.48	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	VAL	Peptide
1	A	289	LEU	Peptide
1	A	346	ILE	Peptide
1	A	506	PHE	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	5266	0	4957	41	1
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	D	50	0	43	0	1
4	A	10	0	5	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	42	0	39	0	0
9	A	143	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5571	0	5094	41	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 4.

All (41) 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:569:MET:SD	1:A:569:MET:CE	2.05	1.42
1:A:494:TYR:O	1:A:498:THR:CG2	2.36	0.73
1:A:494:TYR:O	1:A:498:THR:HG22	1.92	0.69
1:A:100:TRP:HE1	1:A:396:HIS:HD2	1.43	0.65
1:A:169:MET:HE3	1:A:347:HIS:CE1	2.37	0.60
1:A:654:ASP:OD1	1:A:654:ASP:N	2.35	0.59
1:A:666:ASP:OD2	9:A:2106:HOH:O	2.15	0.59
1:A:169:MET:HA	1:A:344:MET:O	2.04	0.58
1:A:494:TYR:O	1:A:498:THR:HG23	2.03	0.57
1:A:716:GLU:H	1:A:716:GLU:CD	2.13	0.57
1:A:169:MET:HE3	1:A:347:HIS:NE2	2.23	0.54
1:A:249:PRO:HG2	1:A:556:TYR:CE2	2.44	0.53
1:A:100:TRP:HE1	1:A:396:HIS:CD2	2.25	0.52
1:A:242:TYR:CG	1:A:243:PRO:HA	2.44	0.52
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.43	0.52
1:A:129:SER:HA	1:A:139:PHE:O	2.10	0.52
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.47	0.49
1:A:662:ARG:HD2	9:A:2106:HOH:O	2.13	0.48
1:A:689:HIS:HB3	1:A:692:TYR:O	2.14	0.48
1:A:456:ILE:HD13	1:A:573:HIS:HE1	1.81	0.46
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.51	0.45
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.51	0.45
1:A:169:MET:HE2	1:A:345:HIS:HD2	1.82	0.45
1:A:201:VAL:HG23	1:A:225:VAL:HG13	2.00	0.44
1:A:169:MET:N	1:A:170:PRO:CD	2.81	0.43
1:A:675:PHE:CB	1:A:689:HIS:CE1	3.02	0.43
1:A:517:SER:HB2	1:A:694:PRO:HG3	2.01	0.43
1:A:186:PHE:O	1:A:190:ARG:HB2	2.19	0.42
1:A:611:ILE:HD12	1:A:611:ILE:HA	1.87	0.42
1:A:456:ILE:O	1:A:456:ILE:HG13	2.19	0.42
1:A:463:ARG:NE	1:A:536:ARG:NH2	2.68	0.41
1:A:171:GLU:HA	1:A:342:VAL:O	2.20	0.41
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:HB	1:A:500:LYS:HD3	2.01	0.41
1:A:675:PHE:HB3	1:A:689:HIS:CE1	2.55	0.41
1:A:469:LEU:O	1:A:595:PHE:HA	2.21	0.41
1:A:394:VAL:HG13	1:A:577:ALA:HB2	2.04	0.40
1:A:151:TYR:OH	1:A:560:GLU:OE1	2.37	0.40
1:A:449:TYR:O	1:A:532:SER:HA	2.21	0.40
1:A:574:LEU:O	1:A:578:GLN:HG3	2.21	0.40
1:A:92:LEU:O	1:A:96:ILE:HG12	2.22	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:276:GLU:OE2	3:D:3:BMA:O2[2_565]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	671/707 (95%)	636 (95%)	32 (5%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	PHE
1	A	507	SER
1	A	382	VAL

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	531/603 (88%)	510 (96%)	21 (4%)	28	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	174	LEU
1	A	195	ASN
1	A	239	VAL
1	A	276	GLU
1	A	283	ILE
1	A	325	VAL
1	A	396	HIS
1	A	465	ASP
1	A	489	GLU
1	A	498	THR
1	A	509	MET
1	A	536	ARG
1	A	537	TYR
1	A	557	GLU
1	A	600	TYR
1	A	647	SER
1	A	654	ASP
1	A	663	MET
1	A	664	MET
1	A	668	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	136	ASN
1	A	260	ASN
1	A	396	HIS

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Mol	Chain	Res	Type
1	A	573	HIS
1	A	578	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	2,1	14,14,15	0.63	0	17,19,21	1.67	4 (23%)
2	NAG	B	2	2	14,14,15	0.75	0	17,19,21	2.37	6 (35%)
2	NAG	C	1	2,1	14,14,15	1.12	1 (7%)	17,19,21	1.87	4 (23%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	1.02	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	1.63	2 (11%)
3	NAG	D	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.77	4 (23%)
3	BMA	D	3	3	11,11,12	0.83	0	15,15,17	1.84	3 (20%)
3	MAN	D	4	3	11,11,12	0.66	0	15,15,17	1.30	3 (20%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.77	1.39	1.43
3	D	2	NAG	C1-C2	2.06	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-C2-C3	5.18	117.19	109.64
3	D	1	NAG	C1-O5-C5	4.96	118.83	112.19
2	C	1	NAG	O5-C1-C2	-4.76	103.93	111.29
2	B	2	NAG	C8-C7-N2	4.73	123.97	116.12
2	B	2	NAG	C2-N2-C7	4.65	129.13	122.90
2	B	2	NAG	C4-C3-C2	4.22	117.21	111.02
3	D	2	NAG	C1-C2-N2	3.88	116.55	110.43
2	B	1	NAG	O4-C4-C3	-3.70	101.66	110.38
2	C	1	NAG	C1-O5-C5	3.66	117.09	112.19
2	B	1	NAG	O5-C5-C6	3.15	113.80	107.66
2	B	2	NAG	O3-C3-C2	-3.11	102.94	109.40
2	B	1	NAG	C1-O5-C5	3.04	116.26	112.19
3	D	2	NAG	C1-O5-C5	2.94	116.12	112.19
3	D	3	BMA	O3-C3-C2	-2.77	104.41	110.05
3	D	2	NAG	C4-C3-C2	-2.75	106.99	111.02
3	D	2	NAG	C8-C7-N2	2.74	120.65	116.12
2	B	1	NAG	O5-C1-C2	-2.71	107.10	111.29
3	D	4	MAN	C3-C4-C5	-2.70	105.34	110.23
3	D	4	MAN	O5-C5-C6	2.58	112.69	107.66
2	C	1	NAG	O4-C4-C5	2.51	115.52	109.32
2	B	2	NAG	O7-C7-C8	-2.50	117.60	122.05
3	D	4	MAN	C1-O5-C5	2.34	115.32	112.19
2	C	1	NAG	O4-C4-C3	-2.14	105.33	110.38
2	C	2	NAG	O4-C4-C5	2.12	114.55	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O5-C1-C2	-2.10	108.05	111.29
3	D	3	BMA	O2-C2-C3	-2.08	105.84	110.15
2	B	2	NAG	O7-C7-N2	-2.01	118.43	121.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

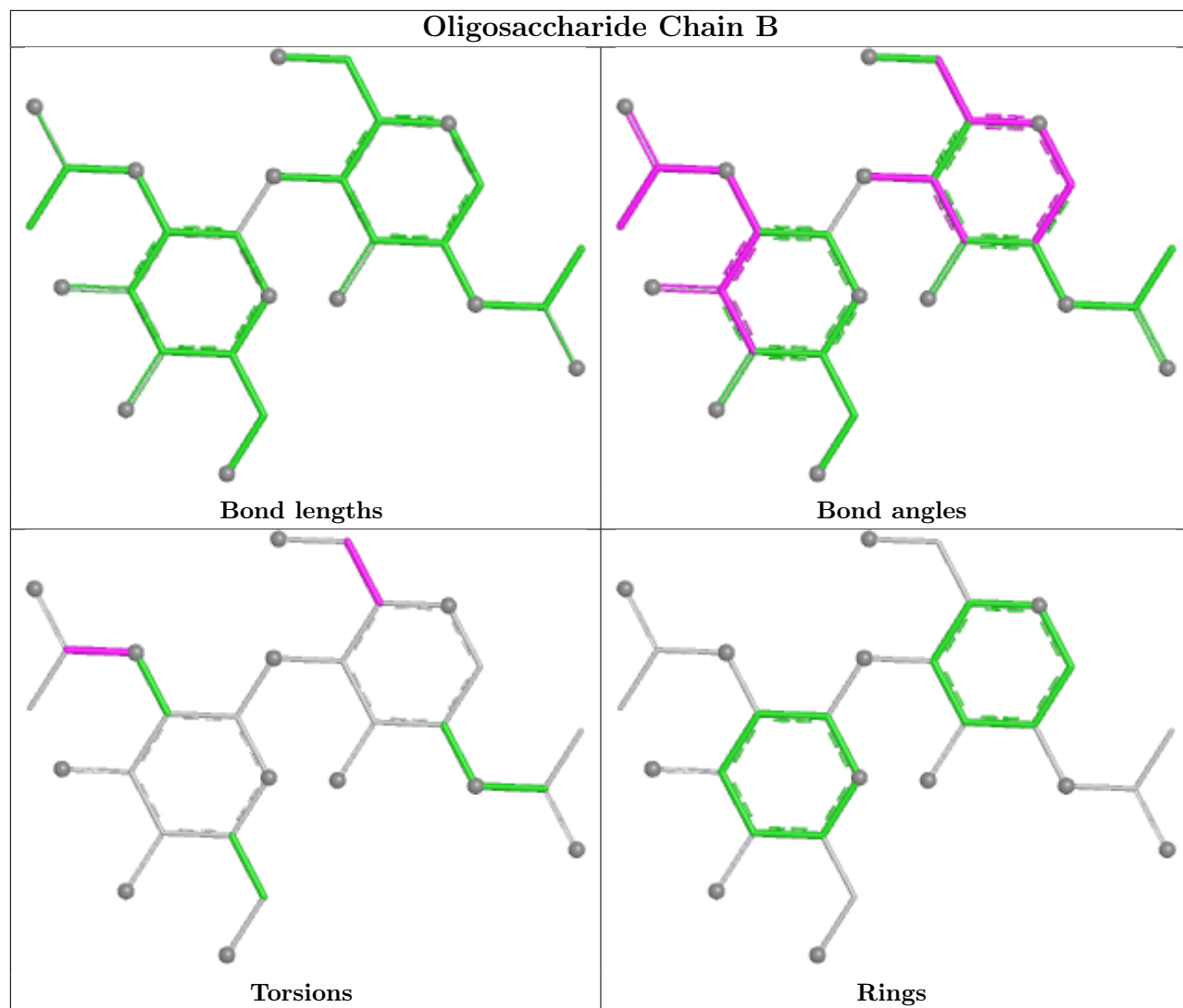
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

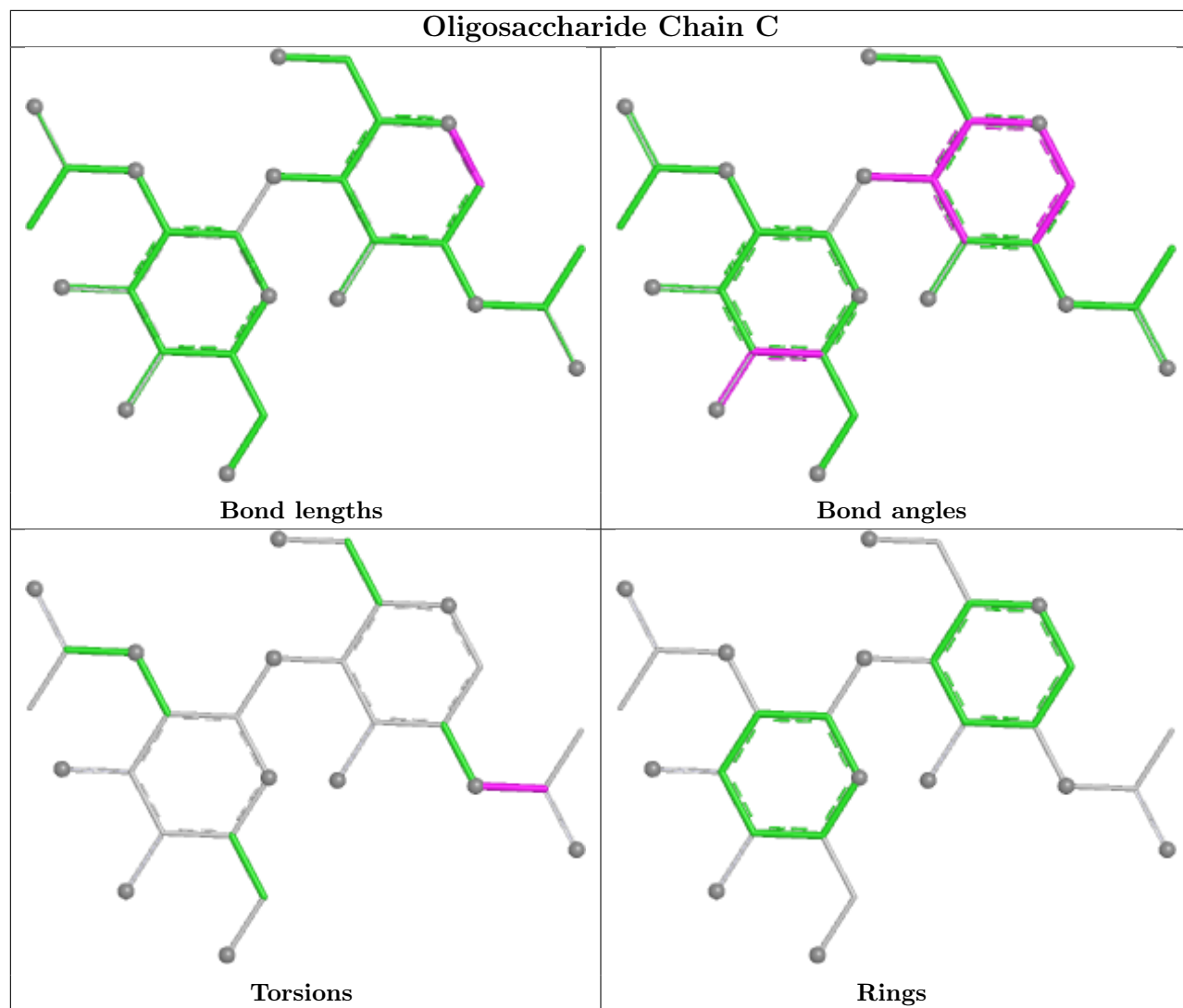
There are no ring outliers.

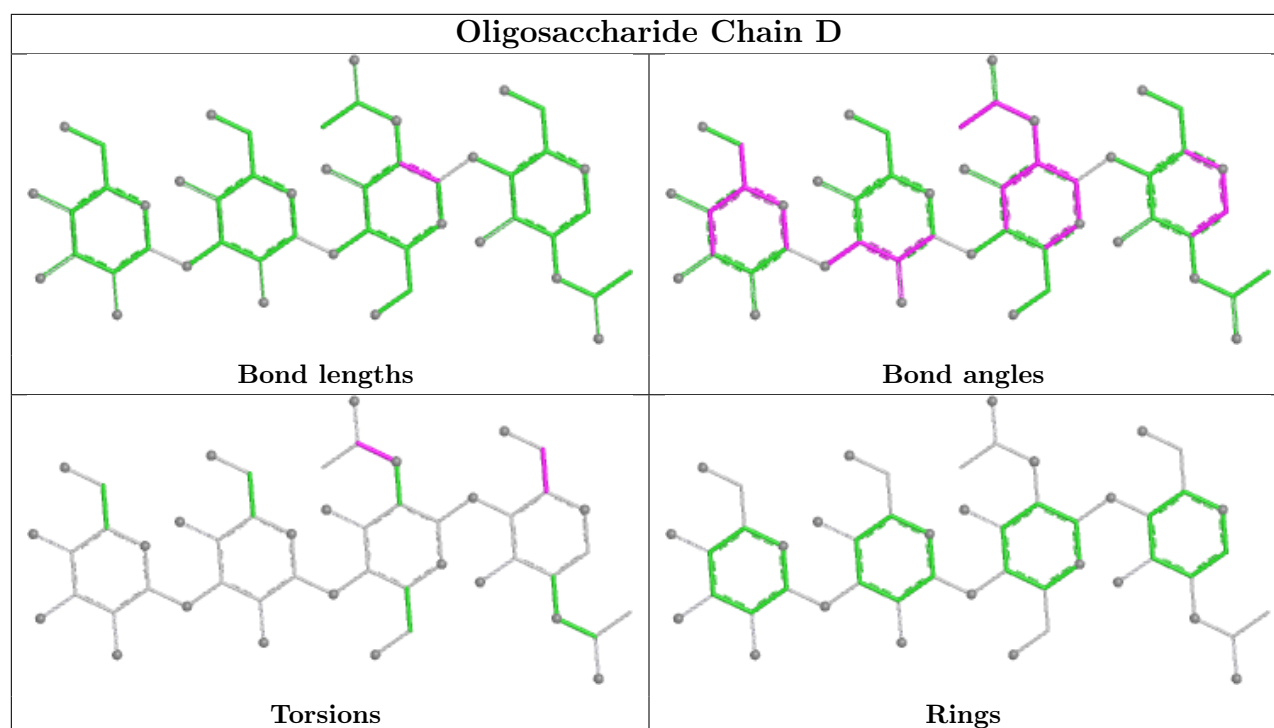
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	0	1

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1759	1	14,14,15	0.72	0	17,19,21	2.51	8 (47%)
4	GLU	A	1766	-	8,9,9	1.11	1 (12%)	8,11,11	1.20	1 (12%)
8	NAG	A	1757	1	14,14,15	0.77	0	17,19,21	2.40	7 (41%)
8	NAG	A	1758	1	14,14,15	1.05	1 (7%)	17,19,21	1.69	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1758	1	-	0/6/23/26	0/1/1/1
4	GLU	A	1766	-	-	0/9/9/9	-
8	NAG	A	1757	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1759	1	1/1/5/7	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1758	NAG	C4-C5	2.12	1.57	1.53
4	A	1766	GLU	OXT-C	-2.01	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1757	NAG	C1-O5-C5	6.91	121.44	112.19
8	A	1759	NAG	C1-O5-C5	6.32	120.65	112.19
8	A	1758	NAG	O5-C1-C2	-4.24	104.74	111.29
8	A	1759	NAG	O5-C1-C2	4.19	117.77	111.29
8	A	1759	NAG	C4-C3-C2	-3.87	105.34	111.02
8	A	1757	NAG	C3-C4-C5	3.65	116.85	110.23
8	A	1758	NAG	C1-O5-C5	2.99	116.19	112.19
8	A	1757	NAG	C4-C3-C2	2.76	115.07	111.02
4	A	1766	GLU	OXT-C-O	2.58	129.94	124.08
8	A	1757	NAG	O5-C5-C4	2.51	116.92	110.83
8	A	1759	NAG	C1-C2-N2	-2.49	106.51	110.43
8	A	1757	NAG	C8-C7-N2	2.45	120.18	116.12
8	A	1759	NAG	O7-C7-C8	-2.42	117.75	122.05
8	A	1757	NAG	O5-C1-C2	-2.38	107.61	111.29
8	A	1759	NAG	O5-C5-C4	2.26	116.33	110.83
8	A	1758	NAG	O7-C7-C8	-2.23	118.09	122.05
8	A	1759	NAG	O7-C7-N2	2.19	125.86	121.98
8	A	1757	NAG	O7-C7-C8	-2.11	118.29	122.05
8	A	1759	NAG	O5-C5-C6	2.07	111.69	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1759	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1759	NAG	C4-C5-C6-O6
8	A	1759	NAG	O5-C5-C6-O6
8	A	1757	NAG	C8-C7-N2-C2
8	A	1757	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	679/707 (96%)	0.17	32 (4%) 36 33	20, 36, 63, 75	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	GLY	4.9
1	A	340	GLN	4.6
1	A	194	ILE	4.0
1	A	139	PHE	3.5
1	A	312	SER	3.4
1	A	654	ASP	3.2
1	A	507	SER	3.1
1	A	124	HIS	3.1
1	A	138	ILE	3.1
1	A	506	PHE	2.9
1	A	152	GLU	2.9
1	A	154	VAL	2.8
1	A	279	TYR	2.8
1	A	508	GLY	2.8
1	A	505	GLU	2.7
1	A	153	ASN	2.6
1	A	189	GLU	2.6
1	A	311	GLY	2.6
1	A	569	MET	2.5
1	A	134	ASP	2.5
1	A	318	SER	2.4
1	A	657	ASN	2.4
1	A	155	SER	2.4
1	A	486	GLU	2.4
1	A	135	GLY	2.3
1	A	322	SER	2.2
1	A	536	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASP	2.1
1	A	333	PHE	2.1
1	A	305	LEU	2.1
1	A	183	GLU	2.0
1	A	716	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

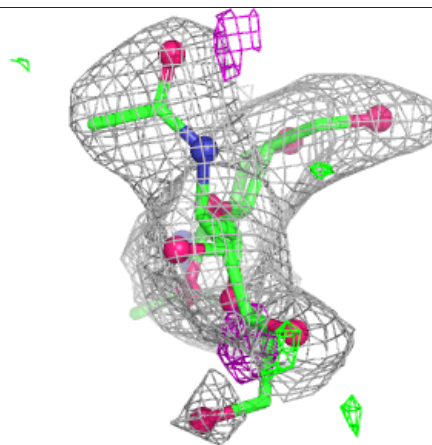
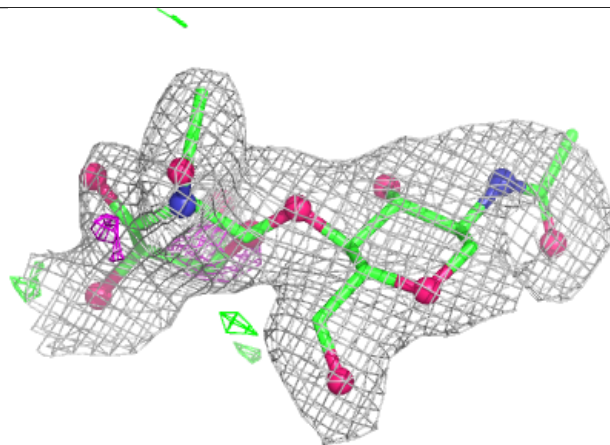
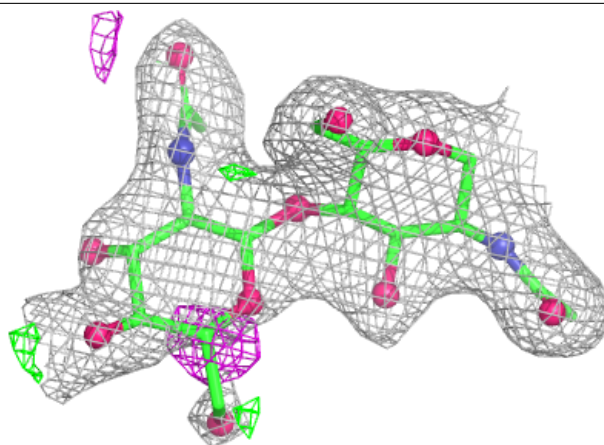
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.74	0.17	62,70,73,73	0
3	BMA	D	3	11/12	0.81	0.12	68,71,72,72	0
3	MAN	D	4	11/12	0.82	0.17	74,75,78,80	0
3	NAG	D	2	14/15	0.84	0.16	54,60,64,65	0
2	NAG	C	2	14/15	0.86	0.11	57,61,63,64	0
2	NAG	C	1	14/15	0.90	0.11	44,50,55,55	0
2	NAG	B	1	14/15	0.95	0.08	47,54,57,60	0
3	NAG	D	1	14/15	0.96	0.06	32,37,49,49	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.

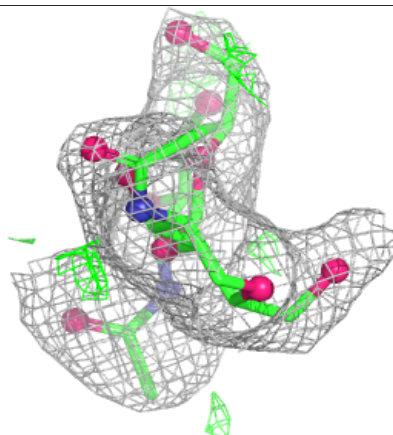
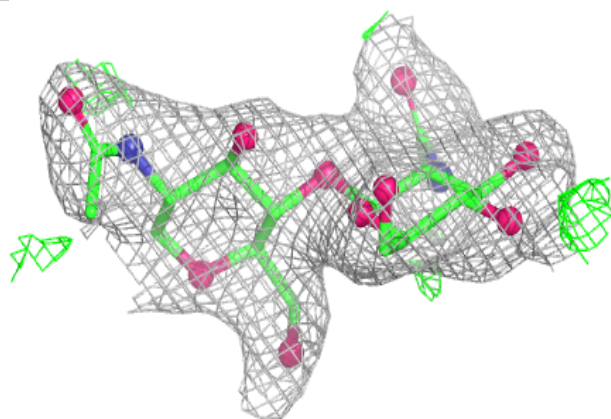
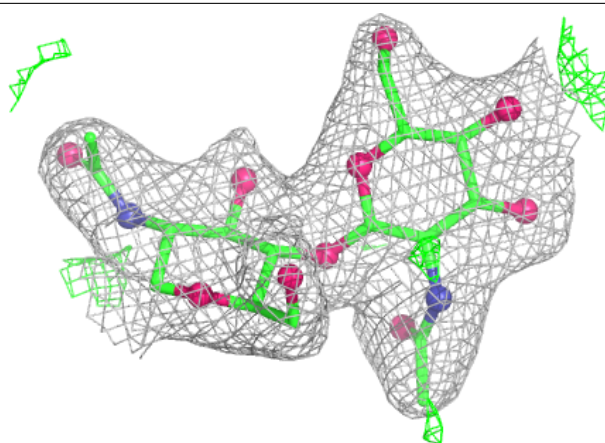
Electron density around Chain B:

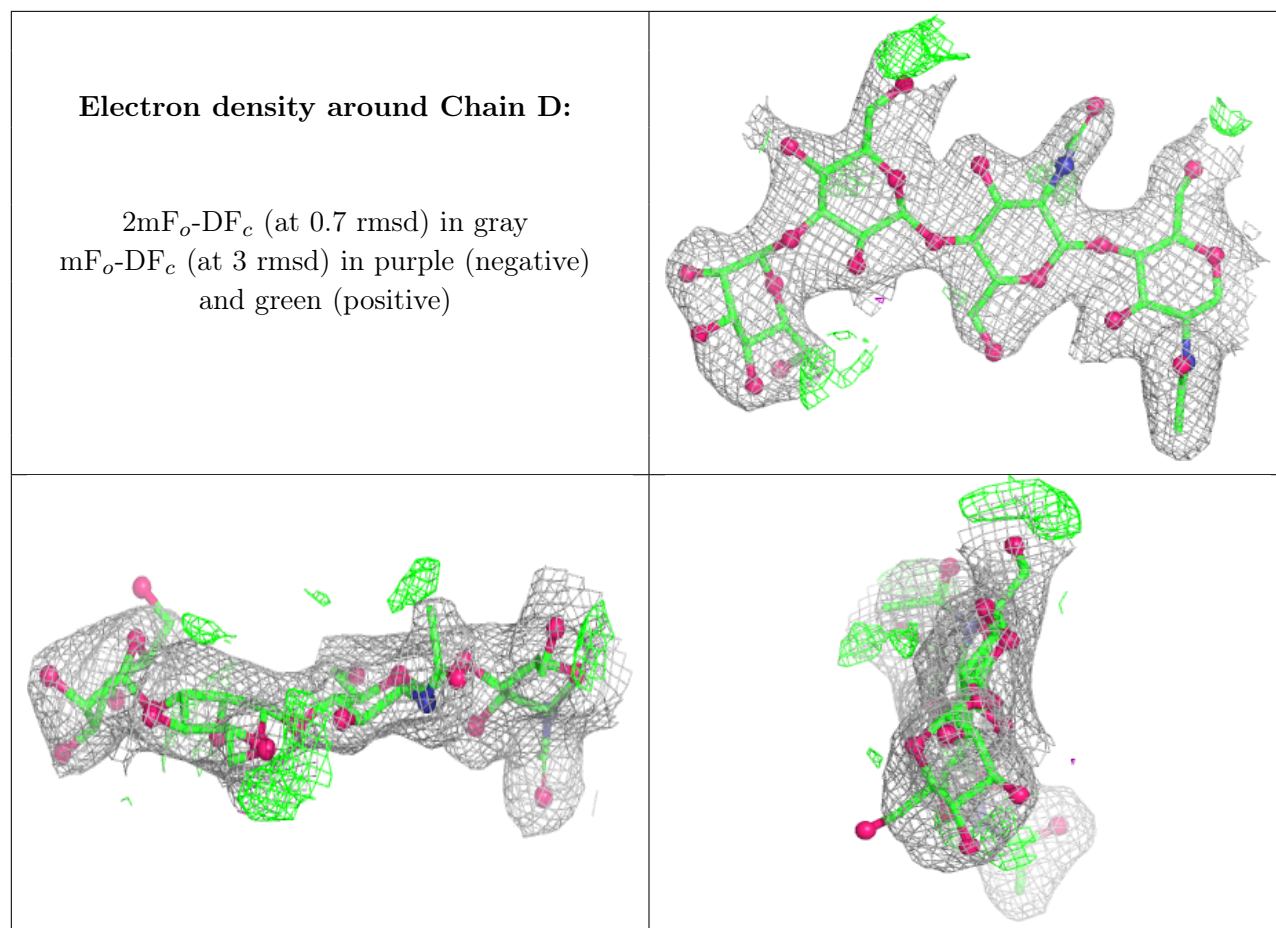
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

$2mF_o - DF_c$ (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	1757	14/15	0.70	0.19	73,77,82,83	0
8	NAG	A	1758	14/15	0.73	0.17	61,64,66,68	0
8	NAG	A	1759	14/15	0.87	0.14	44,58,68,70	0
4	GLU	A	1766	10/10	0.96	0.07	25,27,28,28	0
5	ZN	A	1751	1/1	0.99	0.02	27,27,27,27	0
5	ZN	A	1752	1/1	1.00	0.01	25,25,25,25	0
6	CA	A	1753	1/1	1.00	0.01	21,21,21,21	0
7	CL	A	1754	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.