



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:47 PM UTC

PDB ID : 2C6P / pdb_00002c6p
Title : Membrane-bound glutamate carboxypeptidase II (GCPII) in complex with phosphate anion
Authors : Mesters, J.R.; Barinka, C.; Li, W.; Tsukamoto, T.; Majer, P.; Slusher, B.S.; Konvalinka, J.; Hilgenfeld, R.
Deposited on : 2005-11-11
Resolution : 2.39 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

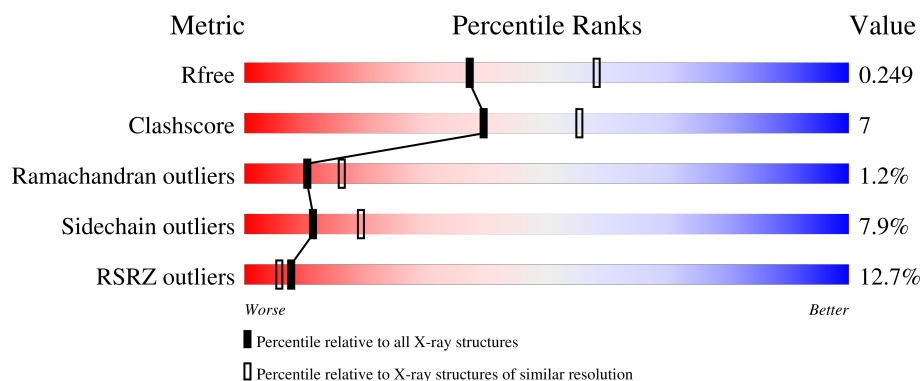
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	12% 80% 13% ...
2	B	2	100%
2	C	2	50% 50%
3	D	3	100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5374 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.

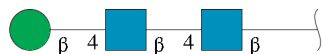
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5155	3313	856	970	16			

- 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 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	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

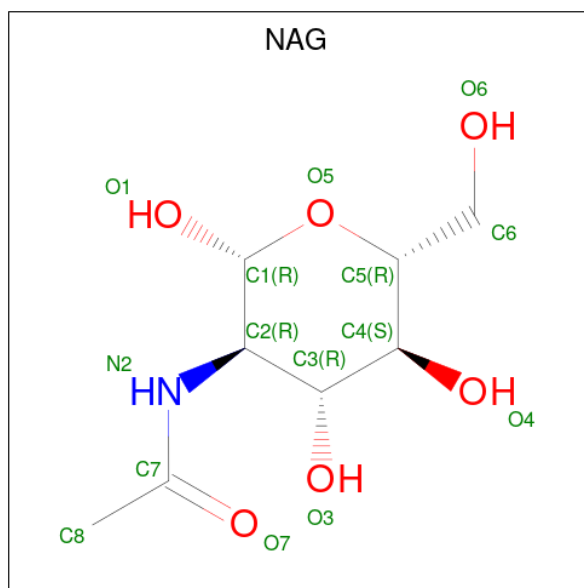
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

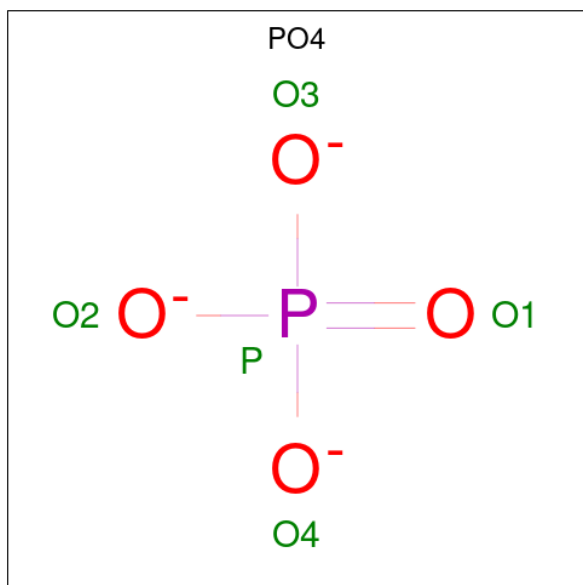
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		

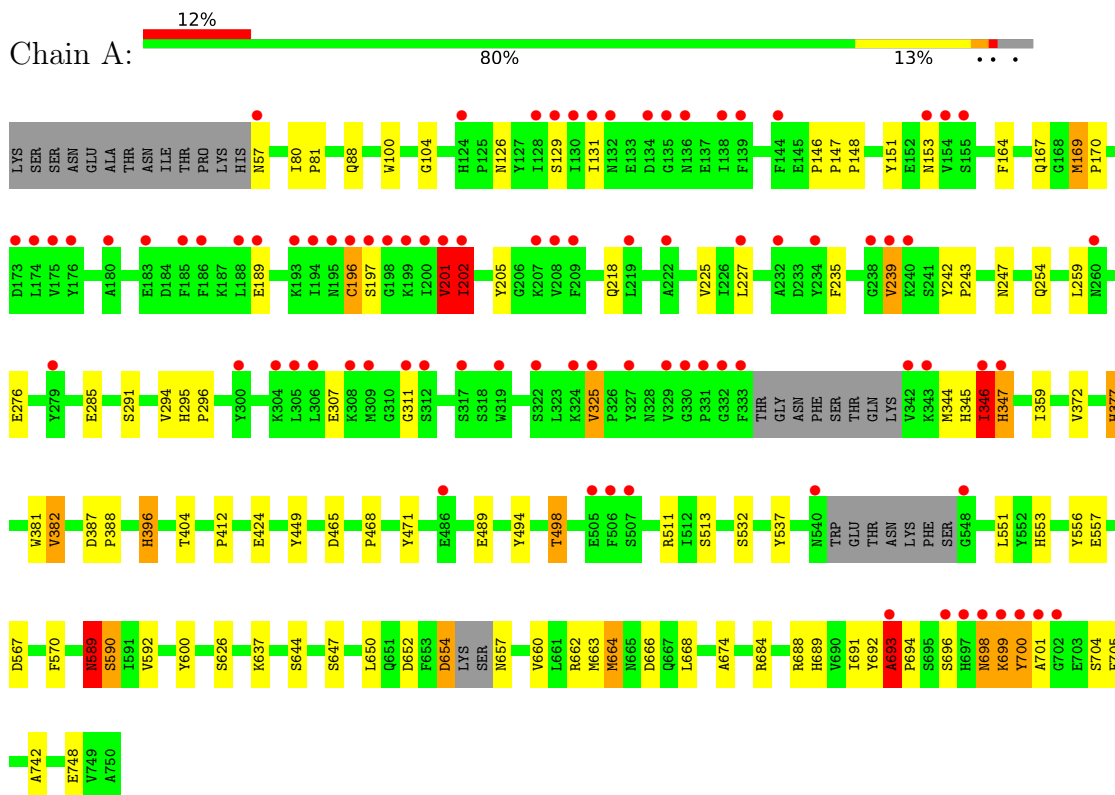
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	87	Total	O	0	0
			87	87		

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

Chain D:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.57Å 130.37Å 159.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.39 47.14 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.14-2.39) 97.3 (47.14-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.251 0.203 , 0.249	Depositor DCC
R_{free} test set	1067 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.0	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	0.94	EDS
Total number of atoms	5374	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: BMA, PO4, NAG, CA, ZN, 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	1.02	7/5299 (0.1%)	1.08	13/7204 (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	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	MET	SD-CE	-7.76	1.60	1.79
1	A	372	VAL	CA-CB	-7.30	1.45	1.54
1	A	705	PHE	C-O	-7.19	1.20	1.23
1	A	693	ALA	CA-C	-6.60	1.44	1.52
1	A	239	VAL	CA-CB	5.29	1.62	1.55
1	A	359	ILE	CA-CB	5.08	1.60	1.53
1	A	589	ASN	CA-C	-5.06	1.46	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	VAL	N-CA-C	-8.59	97.52	109.21
1	A	201	VAL	CA-C-N	7.75	135.66	121.70
1	A	201	VAL	C-N-CA	7.75	135.66	121.70
1	A	202	ILE	N-CA-C	6.61	129.50	111.00
1	A	346	ILE	CA-C-N	6.50	133.95	121.54
1	A	346	ILE	C-N-CA	6.50	133.95	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	ASP	CB-CA-C	-6.31	102.31	111.91
1	A	666	ASP	N-CA-C	-6.11	104.62	111.28
1	A	346	ILE	O-C-N	-5.79	116.37	123.09
1	A	189	GLU	N-CA-C	5.28	116.72	111.07
1	A	652	ASP	N-CA-C	5.22	118.79	110.70
1	A	104	GLY	N-CA-C	5.20	121.87	114.85
1	A	652	ASP	CA-C-O	-5.17	115.52	122.44

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	VAL	Peptide
1	A	346	ILE	Peptide
1	A	699	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5155	0	4747	68	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	D	39	0	34	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	28	0	26	0	0
8	A	5	0	0	0	0
9	A	87	0	0	12	1
All	All	5374	0	4857	68	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 7.

All (68) 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:377:HIS:CE1	1:A:388:PRO:HB3	1.96	0.99
1:A:692:TYR:O	1:A:693:ALA:CB	2.10	0.98
1:A:654:ASP:C	9:A:2059:HOH:O	2.06	0.97
1:A:377:HIS:HD2	1:A:424:GLU:CG	1.85	0.90
1:A:654:ASP:HB2	9:A:2060:HOH:O	1.73	0.88
1:A:377:HIS:CD2	1:A:424:GLU:HB3	2.15	0.81
1:A:377:HIS:HD2	1:A:424:GLU:CD	1.92	0.78
1:A:692:TYR:O	1:A:693:ALA:HB3	1.86	0.76
1:A:692:TYR:O	1:A:693:ALA:HB2	1.90	0.71
1:A:377:HIS:CD2	1:A:424:GLU:CD	2.70	0.69
1:A:657:ASN:CB	9:A:2059:HOH:O	2.39	0.69
1:A:295:HIS:ND1	1:A:296:PRO:HD2	2.08	0.69
1:A:377:HIS:HD2	1:A:424:GLU:CB	2.05	0.69
1:A:377:HIS:HE1	1:A:388:PRO:HB3	1.58	0.69
1:A:377:HIS:CD2	1:A:424:GLU:CB	2.77	0.68
1:A:494:TYR:O	1:A:498:THR:CG2	2.43	0.66
1:A:657:ASN:HB3	9:A:2059:HOH:O	1.94	0.66
1:A:657:ASN:N	9:A:2059:HOH:O	2.32	0.62
1:A:377:HIS:CE1	1:A:388:PRO:CB	2.78	0.61
1:A:494:TYR:O	1:A:498:THR:HG23	2.01	0.61
1:A:377:HIS:CD2	1:A:424:GLU:CG	2.77	0.61
1:A:688:ARG:HD3	9:A:2073:HOH:O	2.00	0.59
1:A:657:ASN:ND2	1:A:660:VAL:HG23	2.16	0.59
1:A:377:HIS:ND1	1:A:388:PRO:HB3	2.15	0.59
1:A:654:ASP:CB	9:A:2060:HOH:O	2.38	0.59
1:A:654:ASP:OD1	1:A:654:ASP:N	2.37	0.58
1:A:377:HIS:ND1	1:A:388:PRO:HG3	2.20	0.57
1:A:100:TRP:HE1	1:A:396:HIS:HD2	1.50	0.56
1:A:126:ASN:OD1	1:A:347:HIS:HB2	2.05	0.56
1:A:494:TYR:O	1:A:498:THR:HG22	2.05	0.55
1:A:345:HIS:CG	9:A:2015:HOH:O	2.60	0.54
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.44	0.52
1:A:377:HIS:CD2	1:A:424:GLU:OE1	2.63	0.52
1:A:567:ASP:OD2	1:A:570:PHE:HA	2.11	0.50
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.92	0.50
1:A:169:MET:HE3	1:A:347:HIS:CE1	2.47	0.50
1:A:227:LEU:O	1:A:296:PRO:HA	2.10	0.50
1:A:381:TRP:HD1	1:A:553:HIS:CD2	2.31	0.48
1:A:699:LYS:HB3	9:A:2042:HOH:O	2.12	0.48
1:A:164:PHE:CE2	1:A:259:LEU:HD11	2.47	0.48
1:A:126:ASN:OD1	1:A:346:ILE:HA	2.13	0.48
1:A:689:HIS:HD2	1:A:691:ILE:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:225:VAL:HA	2.15	0.47
1:A:307:GLU:HA	1:A:325:VAL:HG12	1.97	0.47
1:A:699:LYS:HA	9:A:2075:HOH:O	2.14	0.47
1:A:377:HIS:ND1	1:A:388:PRO:CB	2.79	0.46
1:A:650:LEU:HA	1:A:664:MET:CE	2.45	0.46
1:A:80:ILE:HD12	1:A:88:GLN:HG2	1.97	0.46
1:A:704:SER:HA	9:A:2076:HOH:O	2.16	0.46
1:A:235:PHE:HA	1:A:247:ASN:OD1	2.15	0.45
1:A:196:CYS:O	1:A:197:SER:C	2.58	0.45
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.52	0.45
1:A:225:VAL:HB	1:A:294:VAL:HG22	1.97	0.45
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.18	0.45
1:A:449:TYR:O	1:A:532:SER:HA	2.17	0.44
1:A:225:VAL:O	1:A:294:VAL:HA	2.18	0.44
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.53	0.43
1:A:169:MET:N	1:A:170:PRO:CD	2.82	0.43
1:A:242:TYR:CG	1:A:243:PRO:HA	2.53	0.43
1:A:387:ASP:HA	1:A:388:PRO:HA	1.86	0.43
1:A:81:PRO:HA	1:A:382:VAL:O	2.19	0.43
1:A:590:SER:OG	1:A:592:VAL:O	2.37	0.42
1:A:225:VAL:O	1:A:344:MET:HE1	2.20	0.42
1:A:674:ALA:HB1	1:A:742:ALA:HA	2.01	0.41
1:A:694:PRO:HA	9:A:2075:HOH:O	2.21	0.40
1:A:146:PRO:HA	1:A:147:PRO:HD2	1.95	0.40
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.35	0.40
1:A:684:ARG:NH2	1:A:694:PRO:O	2.49	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)
9:A:2020:HOH:O	9:A:2083:HOH:O[2_565]	2.02	0.18

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	669/707 (95%)	620 (93%)	41 (6%)	8 (1%)	10	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ILE
1	A	693	ALA
1	A	698	ASN
1	A	701	ALA
1	A	311	GLY
1	A	347	HIS
1	A	700	TYR
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	504/603 (84%)	464 (92%)	40 (8%)	11	19

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	129	SER
1	A	131	ILE
1	A	153	ASN
1	A	167	GLN
1	A	169	MET
1	A	196	CYS
1	A	202	ILE
1	A	218	GLN
1	A	239	VAL
1	A	276	GLU

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Mol	Chain	Res	Type
1	A	285	GLU
1	A	291	SER
1	A	325	VAL
1	A	346	ILE
1	A	377	HIS
1	A	396	HIS
1	A	404	THR
1	A	465	ASP
1	A	489	GLU
1	A	498	THR
1	A	511	ARG
1	A	513	SER
1	A	537	TYR
1	A	557	GLU
1	A	589	ASN
1	A	590	SER
1	A	600	TYR
1	A	626	SER
1	A	637	LYS
1	A	644	SER
1	A	647	SER
1	A	654	ASP
1	A	662	ARG
1	A	663	MET
1	A	668	LEU
1	A	696	SER
1	A	698	ASN
1	A	700	TYR
1	A	748	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	112	HIS
1	A	347	HIS
1	A	377	HIS
1	A	396	HIS
1	A	573	HIS
1	A	657	ASN
1	A	689	HIS
1	A	697	HIS

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Mol	Chain	Res	Type
1	A	698	ASN

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 ⓘ

7 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	0.39	0	17,19,21	1.84	5 (29%)
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	2.16	7 (41%)
2	NAG	C	1	2,1	14,14,15	0.80	0	17,19,21	1.23	2 (11%)
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	0.89	0
3	NAG	D	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	1.32	2 (11%)
3	NAG	D	2	3	14,14,15	0.73	0	17,19,21	2.27	8 (47%)
3	BMA	D	3	3	11,11,12	0.91	0	15,15,17	1.32	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/6/23/26	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.43	1.39	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C8-C7-N2	4.33	123.29	116.12
2	B	1	NAG	O5-C5-C6	4.20	115.83	107.66
3	D	2	NAG	C4-C3-C2	-4.14	104.95	111.02
3	D	2	NAG	C1-O5-C5	4.04	117.60	112.19
2	B	2	NAG	C4-C3-C2	3.82	116.62	111.02
2	B	1	NAG	O5-C1-C2	-3.67	105.61	111.29
3	D	3	BMA	C1-C2-C3	3.65	114.95	109.64
3	D	2	NAG	C1-C2-N2	3.19	115.45	110.43
3	D	2	NAG	O3-C3-C4	3.18	117.87	110.38
3	D	1	NAG	O5-C1-C2	-3.13	106.44	111.29
3	D	2	NAG	C8-C7-N2	2.98	121.06	116.12
2	B	2	NAG	C2-N2-C7	2.92	126.81	122.90
2	B	1	NAG	C1-O5-C5	2.91	116.09	112.19
2	B	2	NAG	C3-C4-C5	2.68	115.09	110.23
2	C	1	NAG	O4-C4-C3	-2.60	104.26	110.38
2	B	2	NAG	C1-O5-C5	2.51	115.55	112.19
3	D	1	NAG	C1-O5-C5	2.49	115.53	112.19
2	B	1	NAG	O4-C4-C3	-2.46	104.57	110.38
3	D	2	NAG	O4-C4-C3	2.31	115.83	110.38
3	D	2	NAG	O5-C1-C2	-2.29	107.75	111.29
2	B	1	NAG	O6-C6-C5	2.27	119.06	111.33
2	C	1	NAG	O5-C1-C2	-2.26	107.80	111.29
3	D	3	BMA	O2-C2-C3	-2.25	105.49	110.15
2	B	2	NAG	O7-C7-C8	-2.20	118.14	122.05
2	B	2	NAG	O5-C1-C2	-2.11	108.03	111.29
3	D	2	NAG	O7-C7-C8	-2.06	118.39	122.05

There are no chirality outliers.

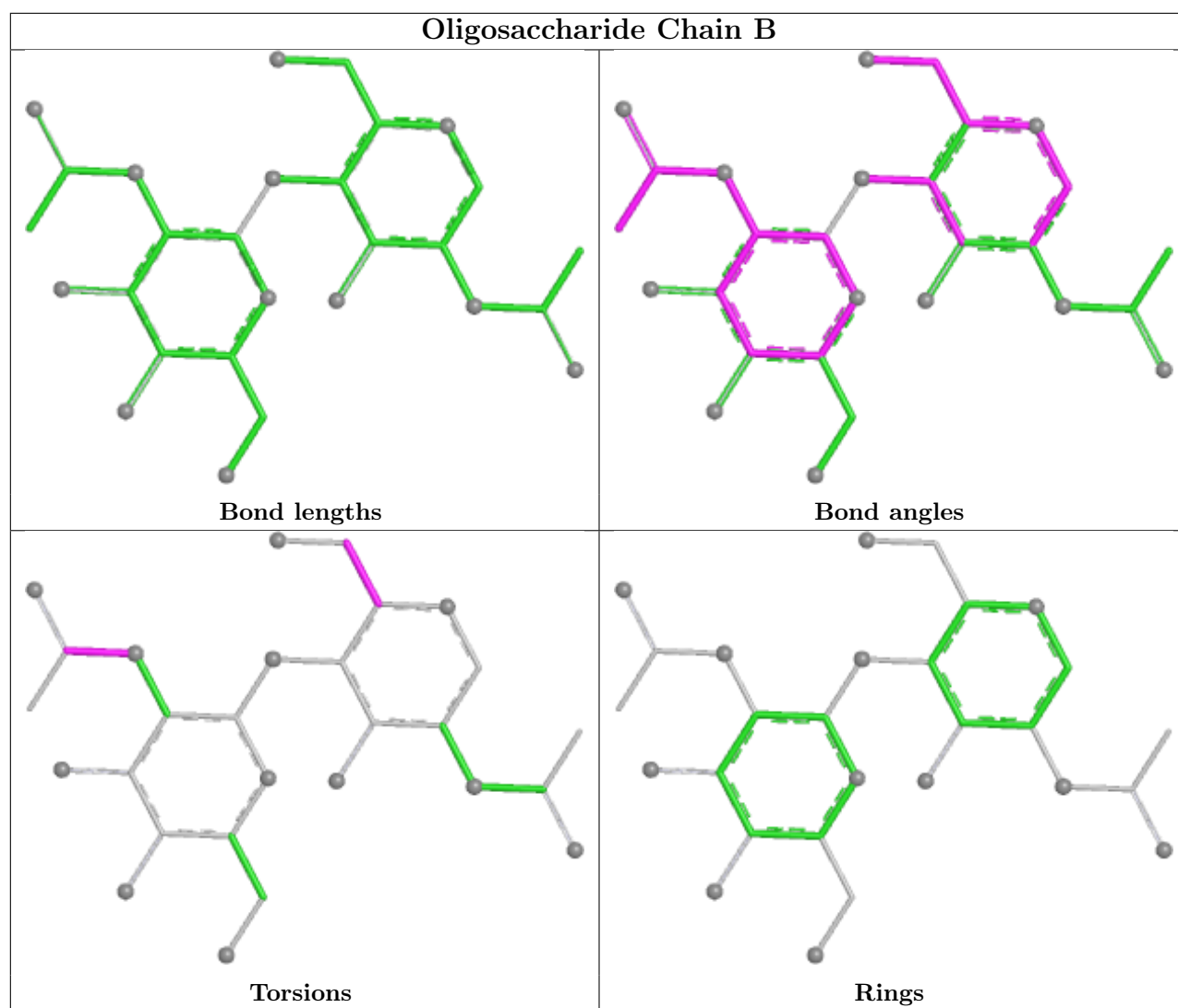
All (8) torsion outliers are listed below:

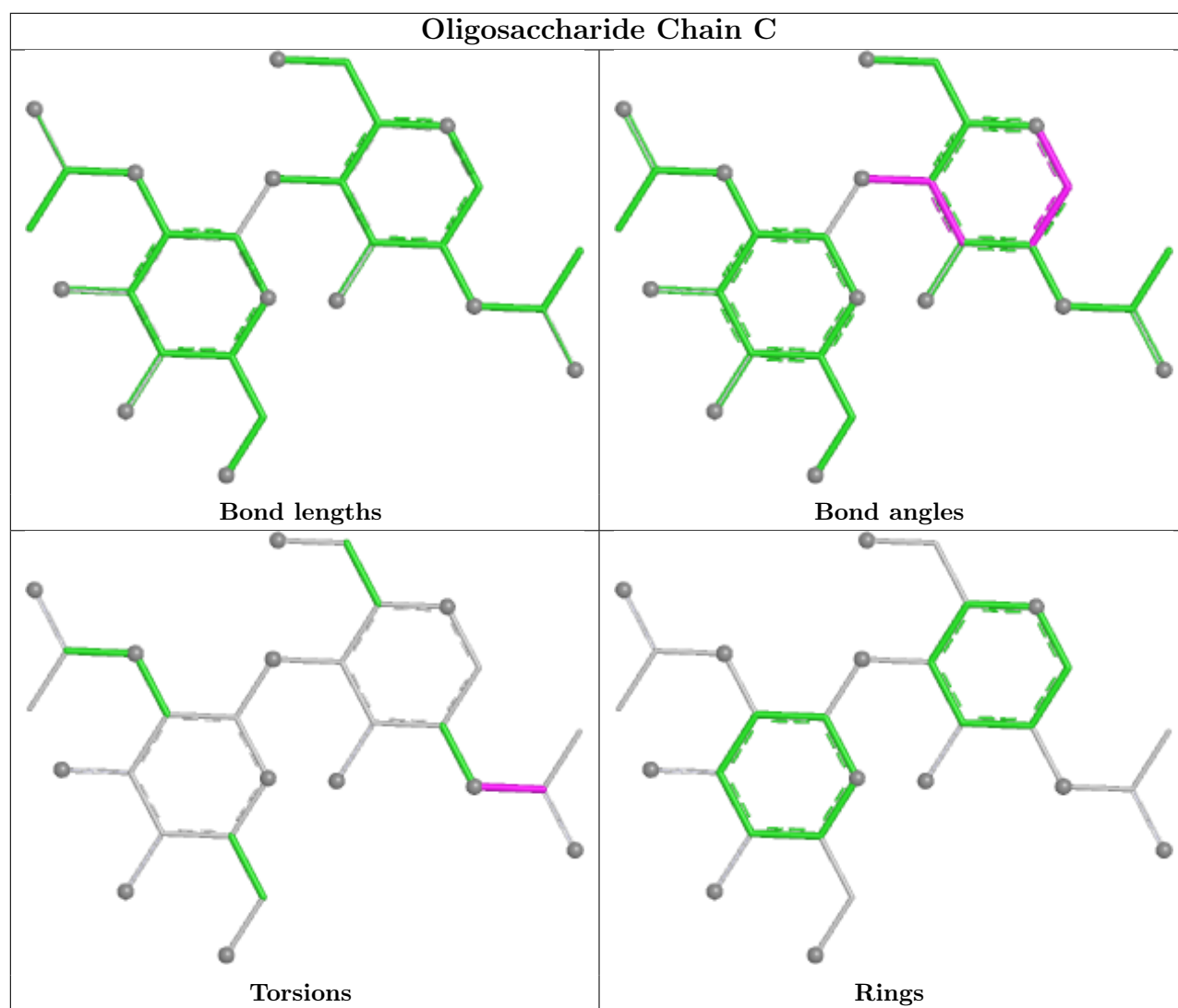
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2

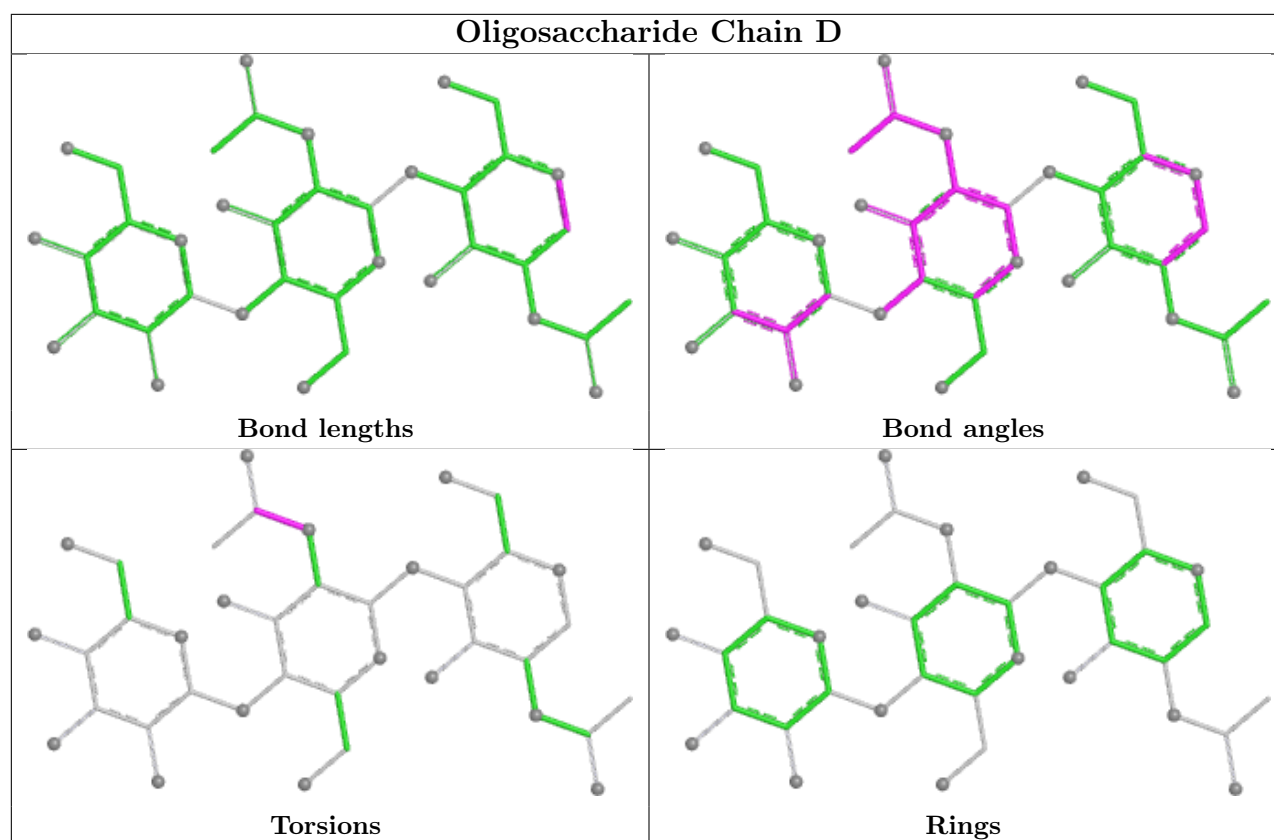
There are no ring outliers.

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	PO4	A	1764	4	4,4,4	1.23	1 (25%)	6,6,6	0.94	0
7	NAG	A	1758	1	14,14,15	0.67	0	17,19,21	2.08	1 (5%)
7	NAG	A	1757	1	14,14,15	0.92	0	17,19,21	1.89	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1758	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1757	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)
8	A	1764	PO4	P-O4	-2.26	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1758	NAG	C1-O5-C5	7.01	121.58	112.19
7	A	1757	NAG	C1-O5-C5	4.58	118.32	112.19
7	A	1757	NAG	C1-C2-N2	3.46	115.89	110.43
7	A	1757	NAG	O5-C1-C2	-2.43	107.53	111.29
7	A	1757	NAG	O3-C3-C4	2.04	115.19	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1758	NAG	C4-C5-C6-O6
7	A	1758	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	677/707 (95%)	0.53	86 (12%) 8 6	23, 44, 86, 100	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	TYR	7.8
1	A	139	PHE	6.2
1	A	131	ILE	5.1
1	A	194	ILE	4.9
1	A	701	ALA	4.5
1	A	188	LEU	4.5
1	A	136	ASN	4.4
1	A	195	ASN	4.0
1	A	129	SER	3.9
1	A	124	HIS	3.9
1	A	138	ILE	3.9
1	A	219	LEU	3.8
1	A	185	PHE	3.8
1	A	209	PHE	3.7
1	A	319	TRP	3.7
1	A	200	ILE	3.7
1	A	130	ILE	3.5
1	A	308	LYS	3.5
1	A	699	LYS	3.4
1	A	342	VAL	3.4
1	A	197	SER	3.4
1	A	128	ILE	3.3
1	A	186	PHE	3.3
1	A	506	PHE	3.3
1	A	279	TYR	3.3
1	A	325	VAL	3.3
1	A	208	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	329	VAL	3.2
1	A	183	GLU	3.1
1	A	332	GLY	3.1
1	A	201	VAL	3.1
1	A	189	GLU	3.0
1	A	331	PRO	2.9
1	A	193	LYS	2.9
1	A	196	CYS	2.9
1	A	698	ASN	2.9
1	A	312	SER	2.8
1	A	507	SER	2.8
1	A	347	HIS	2.8
1	A	322	SER	2.8
1	A	134	ASP	2.8
1	A	222	ALA	2.8
1	A	173	ASP	2.7
1	A	199	LYS	2.7
1	A	300	TYR	2.7
1	A	144	PHE	2.7
1	A	153	ASN	2.7
1	A	309	MET	2.7
1	A	333	PHE	2.7
1	A	696	SER	2.7
1	A	324	LYS	2.6
1	A	343	LYS	2.6
1	A	505	GLU	2.6
1	A	239	VAL	2.6
1	A	180	ALA	2.5
1	A	176	TYR	2.5
1	A	486	GLU	2.5
1	A	697	HIS	2.5
1	A	702	GLY	2.5
1	A	57	ASN	2.5
1	A	154	VAL	2.4
1	A	304	LYS	2.4
1	A	132	ASN	2.3
1	A	238	GLY	2.3
1	A	346	ILE	2.3
1	A	232	ALA	2.3
1	A	305	LEU	2.2
1	A	202	ILE	2.2
1	A	227	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	540	ASN	2.2
1	A	330	GLY	2.2
1	A	260	ASN	2.2
1	A	198	GLY	2.2
1	A	155	SER	2.2
1	A	317	SER	2.2
1	A	311	GLY	2.1
1	A	174	LEU	2.1
1	A	548	GLY	2.1
1	A	240	LYS	2.1
1	A	693	ALA	2.1
1	A	234	TYR	2.1
1	A	175	VAL	2.1
1	A	135	GLY	2.1
1	A	207	LYS	2.0
1	A	306	LEU	2.0
1	A	327	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

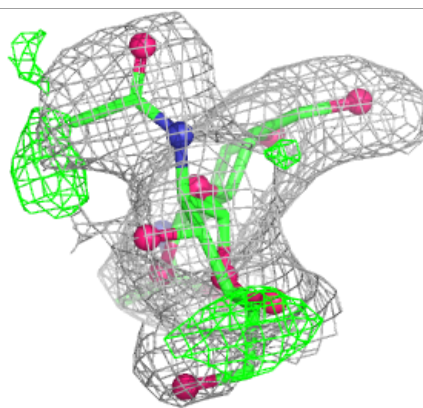
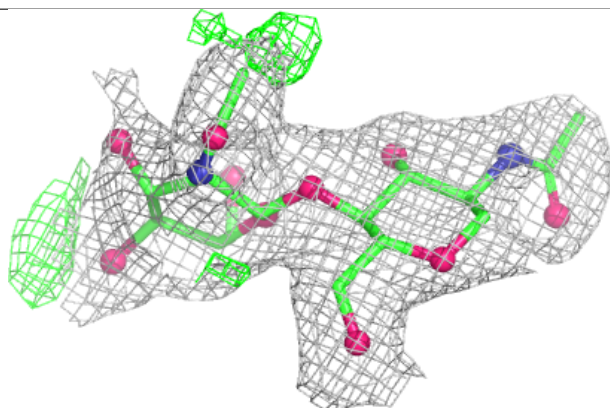
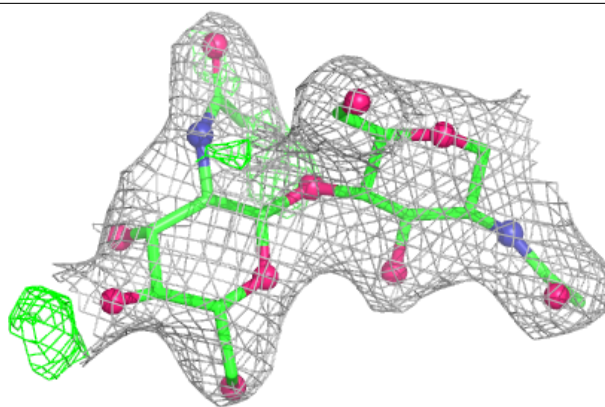
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.67	0.17	71,78,80,81	0
3	BMA	D	3	11/12	0.76	0.14	75,77,79,79	0
3	NAG	D	2	14/15	0.85	0.13	63,69,71,73	0
2	NAG	C	2	14/15	0.85	0.12	63,67,69,70	0
2	NAG	C	1	14/15	0.88	0.12	52,55,59,61	0
2	NAG	B	1	14/15	0.93	0.09	53,57,61,67	0
3	NAG	D	1	14/15	0.97	0.05	34,40,52,57	0

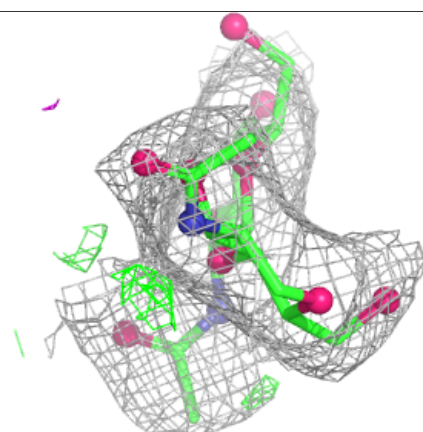
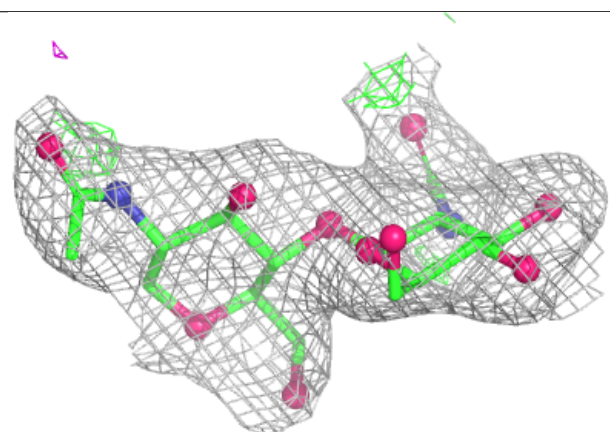
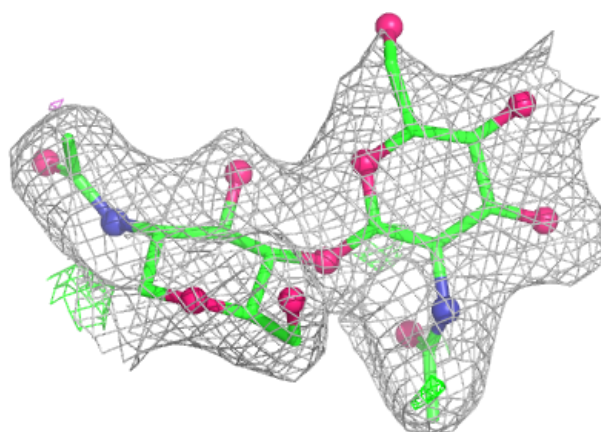
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

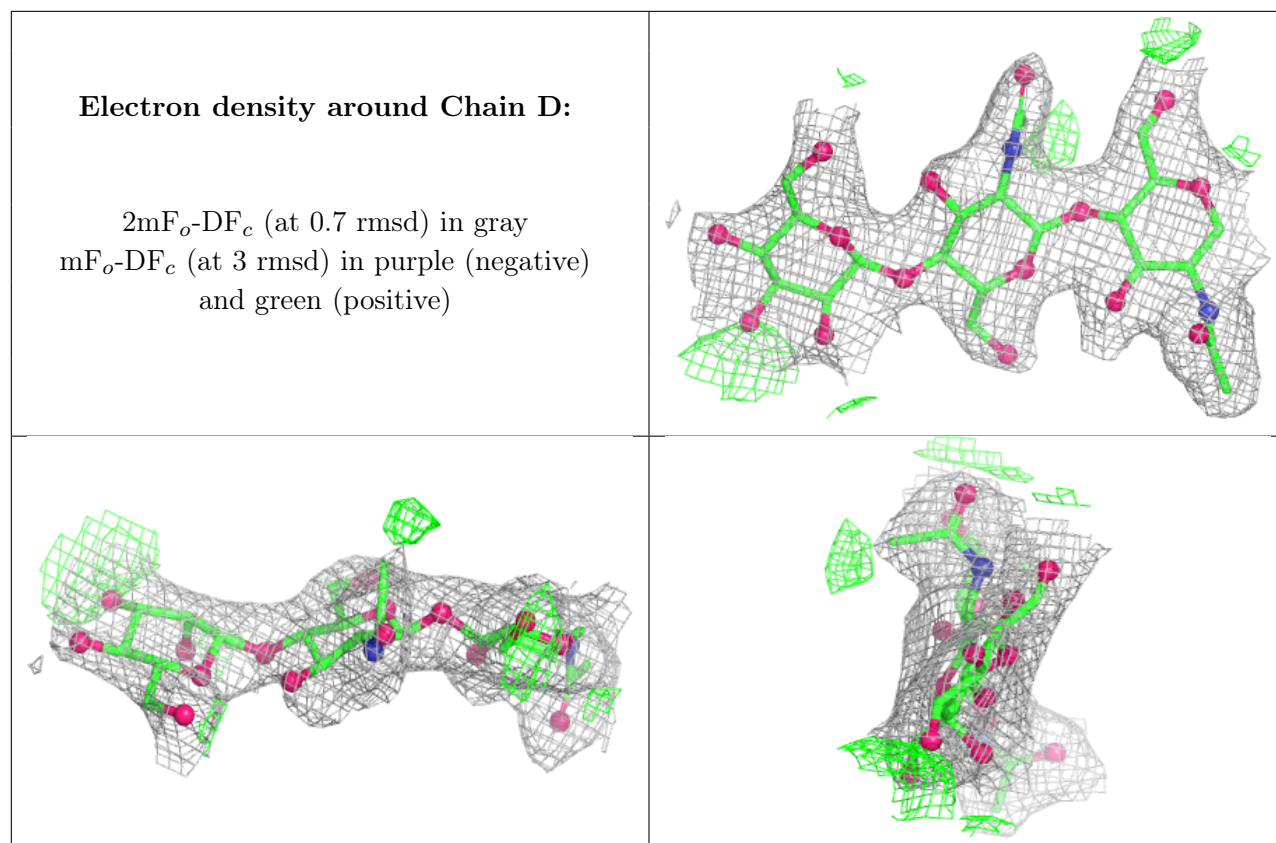
Electron density around Chain B:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	NAG	A	1757	14/15	0.71	0.16	74,77,79,80	0
7	NAG	A	1758	14/15	0.81	0.15	53,69,73,73	0
6	CL	A	1754	1/1	0.99	0.03	35,35,35,35	0
8	PO4	A	1764	5/5	0.99	0.05	35,38,41,41	0
4	ZN	A	1752	1/1	1.00	0.02	30,30,30,30	0
5	CA	A	1753	1/1	1.00	0.01	25,25,25,25	0
4	ZN	A	1751	1/1	1.00	0.01	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.