



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 05:26 PM EDT

PDB ID : 2ODQ
Title : Complement component C2a, the catalytic fragment of C3- and C5-convertase of human complement
Authors : Narayana, S.V.L.; Krishnan, V.
Deposited on : 2006-12-25
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

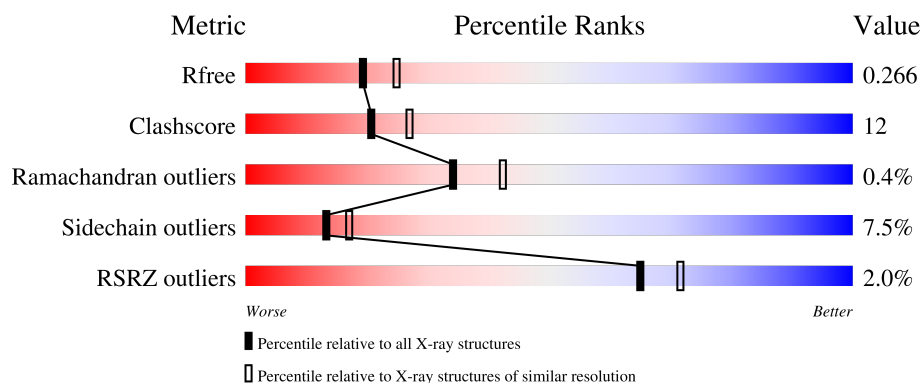
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	509	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>5%</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4129 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.

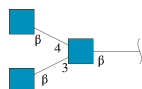
- Molecule 1 is a protein called Complement C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	492	3883	2447	687	723	26	0	0	0

There is a discrepancy between the modelled and reference sequences:

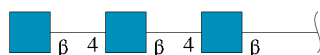
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ALA	CYS	engineered mutation	UNP P06681

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	42	24	3	15	0	0	0

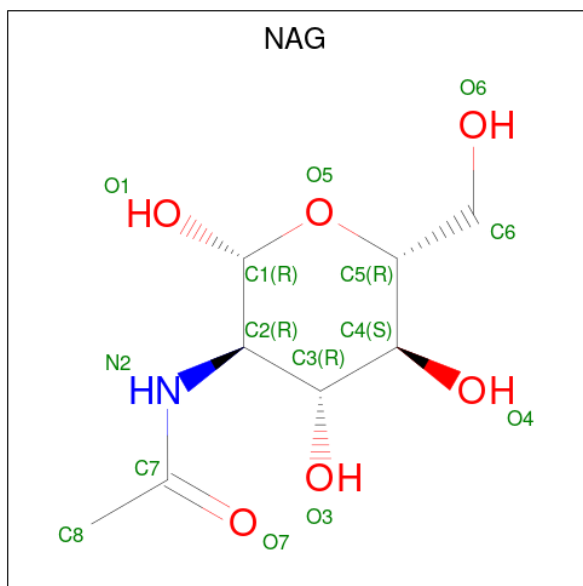
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	42	24	3	15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



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

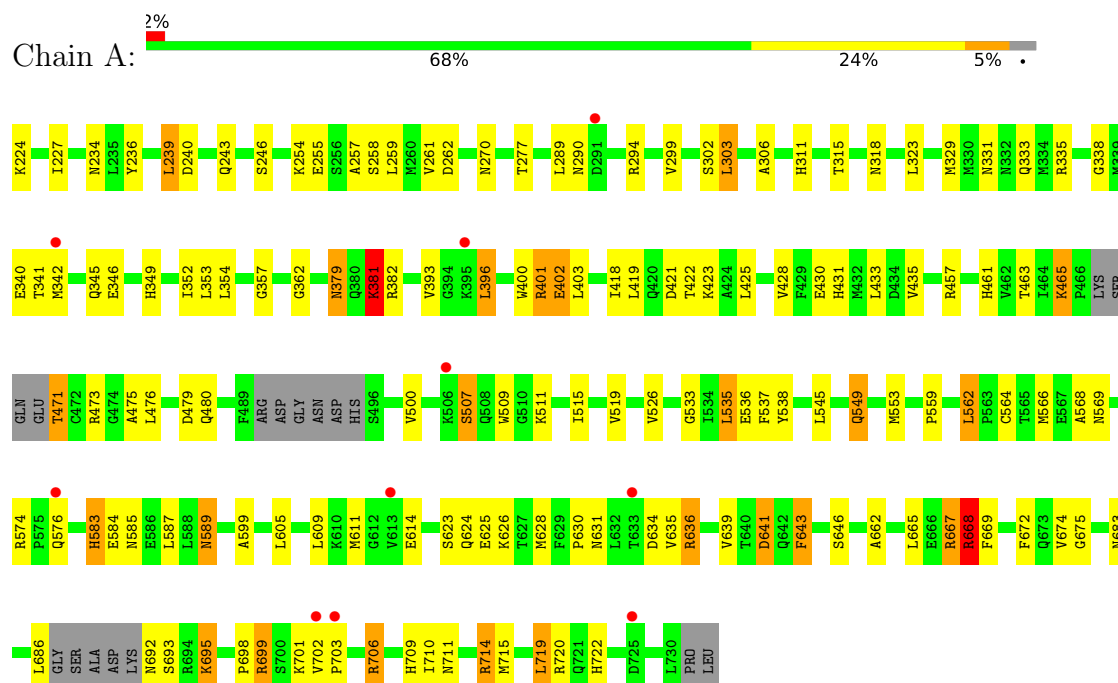
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		

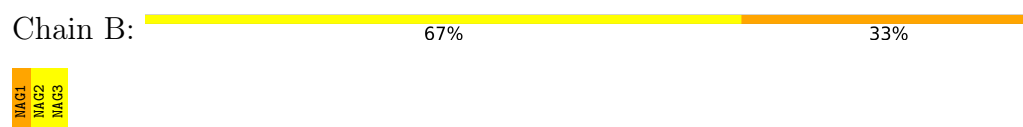
3 Residue-property plots [i](#)

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.

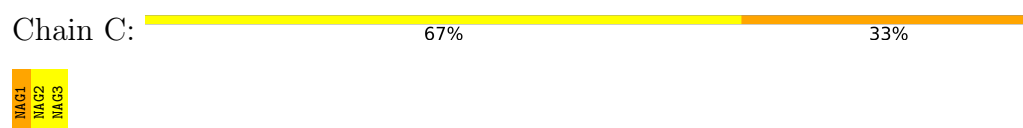
• Molecule 1: Complement C2



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.35Å 84.20Å 74.43Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 19.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.30) 98.8 (19.48-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.39 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.274 0.207 , 0.266	Depositor DCC
R_{free} test set	1397 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4129	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: NAG

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	1.25	12/3959 (0.3%)	1.14	25/5351 (0.5%)

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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLU	CD-OE2	7.57	1.33	1.25
1	A	402	GLU	CB-CG	6.37	1.64	1.52
1	A	435	VAL	CB-CG1	-6.32	1.39	1.52
1	A	674	VAL	CB-CG2	6.14	1.65	1.52
1	A	576	GLN	C-O	6.12	1.34	1.23
1	A	538	TYR	CD2-CE2	5.51	1.47	1.39
1	A	352	ILE	CB-CG2	5.45	1.69	1.52
1	A	549	GLN	CG-CD	5.19	1.62	1.51
1	A	299	VAL	CB-CG2	-5.16	1.42	1.52
1	A	475	ALA	CA-CB	5.12	1.63	1.52
1	A	662	ALA	CA-CB	5.11	1.63	1.52
1	A	720	ARG	CZ-NH1	5.02	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	ARG	NE-CZ-NH2	-10.02	115.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	706	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	720	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	A	706	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	720	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	714	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	479	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	668	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	240	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	715	MET	CG-SD-CE	-6.74	89.42	100.20
1	A	634	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	714	ARG	CG-CD-NE	-6.19	98.80	111.80
1	A	381	LYS	CD-CE-NZ	6.12	125.78	111.70
1	A	641	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	403	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	706	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	719	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	476	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	614	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	A	401	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	699	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	479	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	401	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	303	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	576	GLN	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	643	PHE	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	3883	0	3825	96	1
2	B	42	0	37	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	42	0	37	1	0
4	A	28	0	26	0	0
5	A	134	0	0	8	0
All	All	4129	0	3925	96	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 12.

All (96) 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:631:ASN:HD21	2:B:1:NAG:C1	1.32	1.41
1:A:569:ASN:HD22	1:A:583:HIS:HE1	1.07	0.97
1:A:589:ASN:HD22	1:A:589:ASN:H	0.99	0.95
1:A:564:CYS:H	1:A:583:HIS:HD2	1.09	0.94
1:A:589:ASN:HD22	1:A:589:ASN:N	1.68	0.91
1:A:357:GLY:O	1:A:402:GLU:HG2	1.72	0.89
1:A:589:ASN:H	1:A:589:ASN:ND2	1.72	0.87
1:A:457:ARG:HD2	5:A:57:HOH:O	1.74	0.86
1:A:457:ARG:CD	5:A:57:HOH:O	2.24	0.85
1:A:631:ASN:HD21	2:B:1:NAG:C2	1.89	0.85
1:A:564:CYS:H	1:A:583:HIS:CD2	1.95	0.84
1:A:471:THR:HG23	1:A:473:ARG:HH12	1.42	0.83
1:A:569:ASN:HD22	1:A:583:HIS:CE1	1.95	0.83
1:A:257:ALA:O	1:A:261:VAL:HG23	1.78	0.82
1:A:471:THR:CG2	1:A:473:ARG:HH12	1.94	0.81
1:A:471:THR:HG23	1:A:473:ARG:NH1	1.96	0.80
1:A:243:GLN:HB2	1:A:315:THR:HB	1.64	0.79
1:A:589:ASN:ND2	5:A:82:HOH:O	2.15	0.78
1:A:234:ASN:HD21	1:A:333:GLN:HE22	1.30	0.77
1:A:224:LYS:HE3	1:A:431:HIS:O	1.89	0.72
1:A:686:LEU:O	1:A:695:LYS:HE2	1.92	0.70
1:A:584:GLU:OE2	1:A:714:ARG:NH2	2.22	0.68
1:A:636:ARG:HD2	1:A:639:VAL:O	1.94	0.67
1:A:270:ASN:HD22	1:A:294:ARG:NH2	1.92	0.67
1:A:270:ASN:ND2	1:A:294:ARG:HH22	1.95	0.65
1:A:609:LEU:HB3	1:A:611:MET:HE2	1.79	0.65
1:A:270:ASN:HD22	1:A:294:ARG:HH22	1.45	0.64
1:A:236:TYR:OH	1:A:349:HIS:HD2	1.82	0.62
1:A:277:THR:OG1	1:A:311:HIS:HE1	1.82	0.62
1:A:574:ARG:HD3	5:A:55:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASN:N	5:A:99:HOH:O	2.33	0.61
1:A:535:LEU:HB3	1:A:628:MET:HE3	1.82	0.61
1:A:589:ASN:N	1:A:589:ASN:ND2	2.41	0.61
1:A:587:LEU:HD22	1:A:665:LEU:HD11	1.82	0.60
1:A:254:LYS:HE3	1:A:306:ALA:HB3	1.84	0.58
1:A:533:GLY:O	1:A:630:PRO:HD2	2.04	0.58
1:A:698:PRO:HG2	1:A:701:LYS:HB2	1.86	0.58
1:A:255:GLU:HG2	1:A:422:THR:OG1	2.04	0.57
1:A:533:GLY:HA3	1:A:631:ASN:HB3	1.88	0.56
1:A:553:MET:SD	1:A:559:PRO:HD3	2.45	0.56
1:A:357:GLY:O	1:A:402:GLU:CG	2.50	0.56
1:A:519:VAL:HG11	1:A:722:HIS:CD2	2.40	0.56
1:A:536:GLU:CD	1:A:628:MET:HE1	2.27	0.55
1:A:430:GLU:OE1	3:C:1:NAG:H82	2.07	0.55
1:A:234:ASN:ND2	1:A:333:GLN:HE22	2.04	0.54
1:A:667:ARG:NH2	1:A:668:ARG:NH2	2.55	0.54
1:A:400:TRP:HB2	1:A:418:ILE:HD11	1.89	0.54
1:A:500:VAL:HG23	1:A:515:ILE:HD11	1.90	0.54
1:A:569:ASN:ND2	1:A:583:HIS:HE1	1.90	0.53
1:A:609:LEU:HB3	1:A:611:MET:CE	2.37	0.53
1:A:641:ASP:O	1:A:714:ARG:HG3	2.10	0.52
1:A:646:SER:OG	1:A:709:HIS:HE1	1.91	0.52
1:A:624:GLN:HB3	1:A:702:VAL:HG13	1.93	0.51
1:A:341:THR:O	1:A:345:GLN:HG3	2.12	0.50
1:A:631:ASN:ND2	2:B:1:NAG:C2	2.64	0.50
1:A:631:ASN:CG	2:B:1:NAG:C1	2.78	0.49
1:A:236:TYR:OH	1:A:349:HIS:CD2	2.64	0.49
1:A:262:ASP:HB2	1:A:669:PHE:HE2	1.78	0.48
1:A:461:HIS:HE1	5:A:123:HOH:O	1.96	0.48
1:A:609:LEU:CB	1:A:611:MET:HE2	2.42	0.48
1:A:393:VAL:HA	1:A:419:LEU:O	2.13	0.48
1:A:623:SER:O	1:A:626:LYS:HE2	2.13	0.48
1:A:585:ASN:O	1:A:589:ASN:HB3	2.14	0.47
1:A:471:THR:HG21	1:A:473:ARG:HH12	1.77	0.47
1:A:625:GLU:HB2	1:A:703:PRO:HG3	1.96	0.47
1:A:463:THR:CG2	1:A:465:LYS:HE2	2.45	0.47
1:A:342:MET:O	1:A:346:GLU:HG2	2.14	0.46
1:A:463:THR:HG22	1:A:465:LYS:HE2	1.95	0.46
1:A:683:ASN:OD1	1:A:683:ASN:C	2.54	0.46
1:A:311:HIS:HD2	5:A:60:HOH:O	1.99	0.46
1:A:227:ILE:HD11	1:A:433:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LEU:O	1:A:695:LYS:CE	2.61	0.45
1:A:599:ALA:HB2	1:A:605:LEU:HD11	1.99	0.45
1:A:239:LEU:N	1:A:239:LEU:HD23	2.32	0.45
1:A:675:GLY:HA2	1:A:710:ILE:O	2.17	0.44
1:A:323:LEU:HD21	1:A:353:LEU:HD11	1.99	0.44
1:A:379:ASN:ND2	1:A:381:LYS:HD2	2.32	0.44
1:A:536:GLU:HG3	1:A:628:MET:CE	2.47	0.44
1:A:643:PHE:HA	1:A:709:HIS:O	2.18	0.44
1:A:270:ASN:ND2	5:A:16:HOH:O	2.51	0.44
1:A:562:LEU:O	1:A:568:ALA:HB2	2.17	0.44
1:A:536:GLU:CG	1:A:628:MET:HE1	2.49	0.43
1:A:289:LEU:HD23	1:A:329:MET:HG3	2.00	0.43
1:A:511:LYS:NZ	1:A:549:GLN:HE22	2.17	0.43
1:A:507:SER:C	1:A:509:TRP:H	2.21	0.42
1:A:379:ASN:H	1:A:382:ARG:HB2	1.85	0.41
1:A:331:ASN:HD21	1:A:335:ARG:HH21	1.67	0.41
1:A:609:LEU:CB	1:A:611:MET:CE	2.99	0.41
1:A:239:LEU:HD22	1:A:354:LEU:HD12	2.01	0.41
1:A:536:GLU:CG	1:A:628:MET:CE	2.99	0.41
1:A:526:VAL:HA	1:A:537:PHE:O	2.21	0.41
1:A:672:PHE:CD1	1:A:672:PHE:N	2.89	0.41
1:A:338:GLY:C	1:A:340:GLU:H	2.24	0.41
1:A:507:SER:HB2	1:A:509:TRP:H	1.86	0.41
1:A:419:LEU:HD21	1:A:428:VAL:HG21	2.02	0.40
1:A:318:ASN:OD1	1:A:362:GLY:HA3	2.21	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:402:GLU:OE1	1:A:699:ARG:NH2[2_545]	1.98	0.22

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	484/509 (95%)	463 (96%)	19 (4%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	LEU
1	A	635	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	428/447 (96%)	396 (92%)	32 (8%)	13	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	246	SER
1	A	258	SER
1	A	259	LEU
1	A	290	ASN
1	A	302	SER
1	A	303	LEU
1	A	379	ASN
1	A	381	LYS
1	A	396	LEU
1	A	401	ARG
1	A	421	ASP
1	A	423	LYS
1	A	425	LEU
1	A	465	LYS
1	A	471	THR
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	507	SER
1	A	535	LEU
1	A	545	LEU
1	A	562	LEU
1	A	566	MET
1	A	583	HIS
1	A	589	ASN
1	A	636	ARG
1	A	667	ARG
1	A	668	ARG
1	A	693	SER
1	A	695	LYS
1	A	706	ARG
1	A	711	ASN
1	A	719	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	290	ASN
1	A	311	HIS
1	A	331	ASN
1	A	332	ASN
1	A	333	GLN
1	A	349	HIS
1	A	379	ASN
1	A	426	HIS
1	A	461	HIS
1	A	480	GLN
1	A	532	GLN
1	A	549	GLN
1	A	569	ASN
1	A	583	HIS
1	A	589	ASN
1	A	591	GLN
1	A	608	ASN
1	A	631	ASN
1	A	709	HIS
1	A	711	ASN
1	A	722	HIS

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 ⓘ

6 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	0.86	0	17,19,21	1.52	3 (17%)
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	2.07	2 (11%)
2	NAG	B	3	2	14,14,15	0.76	0	17,19,21	1.39	3 (17%)
3	NAG	C	1	3,1	14,14,15	1.25	2 (14%)	17,19,21	1.83	6 (35%)
3	NAG	C	2	3	14,14,15	1.07	1 (7%)	17,19,21	2.61	7 (41%)
3	NAG	C	3	3	14,14,15	0.79	0	17,19,21	3.28	5 (29%)

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	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	B	3	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3	3	-	5/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	-3.20	1.38	1.43
3	C	1	NAG	C4-C3	2.38	1.58	1.52
3	C	1	NAG	C1-C2	2.18	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NAG	C1-O5-C5	10.21	126.03	112.19
2	B	2	NAG	C1-O5-C5	7.18	121.91	112.19
3	C	2	NAG	O5-C1-C2	-6.35	101.26	111.29
3	C	2	NAG	C1-O5-C5	5.16	119.19	112.19
3	C	3	NAG	C2-N2-C7	5.12	130.20	122.90
3	C	1	NAG	O5-C1-C2	-4.61	104.00	111.29
3	C	3	NAG	C1-C2-N2	-3.99	103.68	110.49
3	C	3	NAG	O5-C5-C6	3.67	112.96	107.20
3	C	3	NAG	O5-C1-C2	3.61	116.99	111.29
2	B	1	NAG	C3-C4-C5	3.53	116.54	110.24
3	C	2	NAG	O4-C4-C5	-3.04	101.75	109.30
2	B	3	NAG	C1-O5-C5	2.93	116.17	112.19
3	C	2	NAG	O7-C7-C8	-2.81	116.84	122.06
3	C	2	NAG	O4-C4-C3	2.79	116.81	110.35
2	B	3	NAG	O5-C1-C2	2.69	115.54	111.29
2	B	2	NAG	O5-C1-C2	2.62	115.43	111.29
3	C	2	NAG	C3-C4-C5	-2.55	105.69	110.24
2	B	1	NAG	O4-C4-C3	-2.51	104.54	110.35
2	B	1	NAG	O3-C3-C4	-2.50	104.57	110.35
3	C	1	NAG	C1-O5-C5	2.49	115.57	112.19
3	C	1	NAG	C6-C5-C4	2.47	118.78	113.00
3	C	1	NAG	O4-C4-C5	2.33	115.08	109.30
3	C	2	NAG	C4-C3-C2	2.14	114.15	111.02
3	C	1	NAG	O5-C5-C6	-2.09	103.93	107.20
3	C	1	NAG	O5-C5-C4	-2.07	105.78	110.83
2	B	3	NAG	O7-C7-C8	-2.07	118.22	122.06

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	3	NAG	C3-C2-N2-C7

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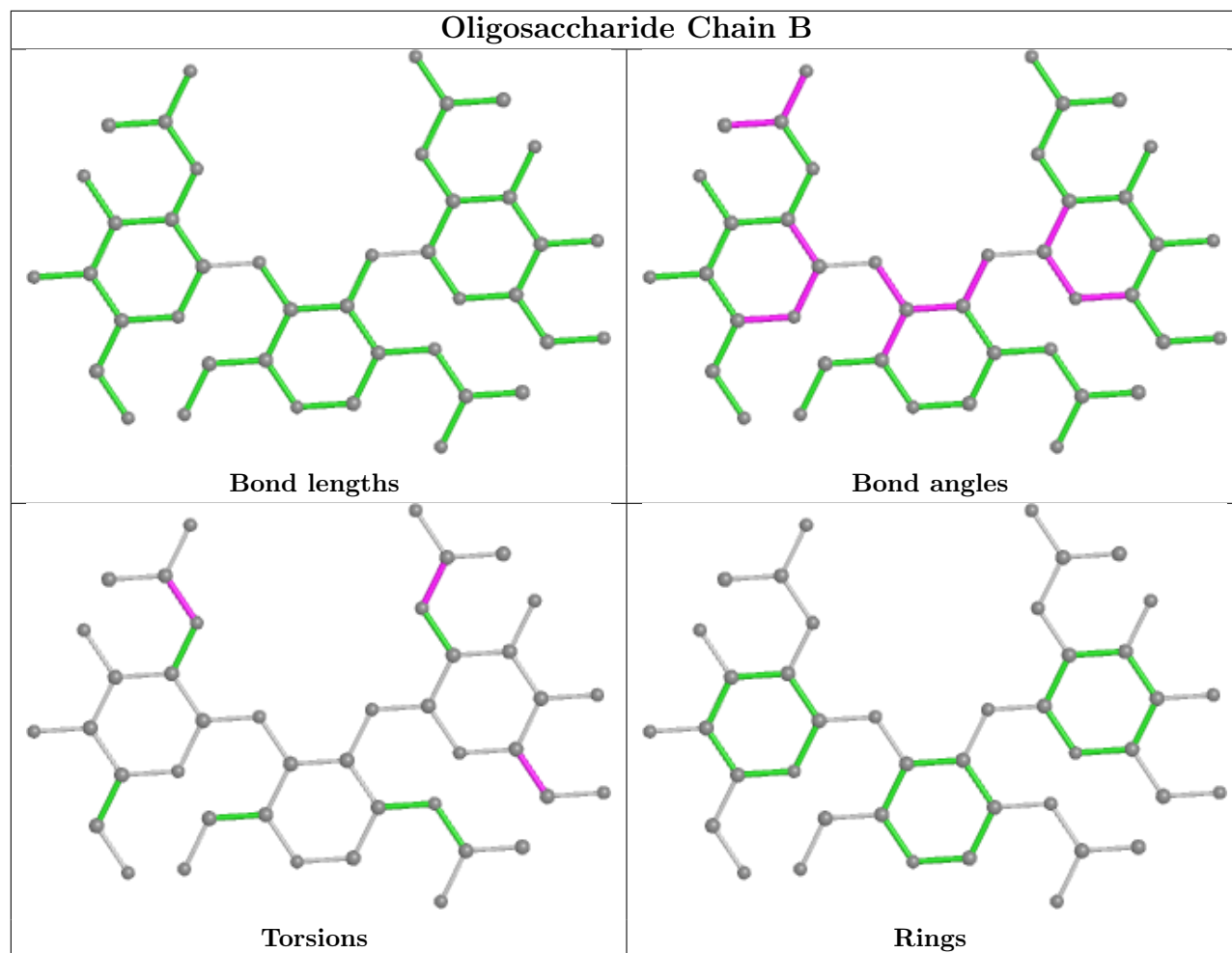
Mol	Chain	Res	Type	Atoms
3	C	3	NAG	C8-C7-N2-C2
3	C	3	NAG	O7-C7-N2-C2
3	C	3	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	3	NAG	C8-C7-N2-C2
2	B	3	NAG	O7-C7-N2-C2
3	C	3	NAG	C4-C5-C6-O6

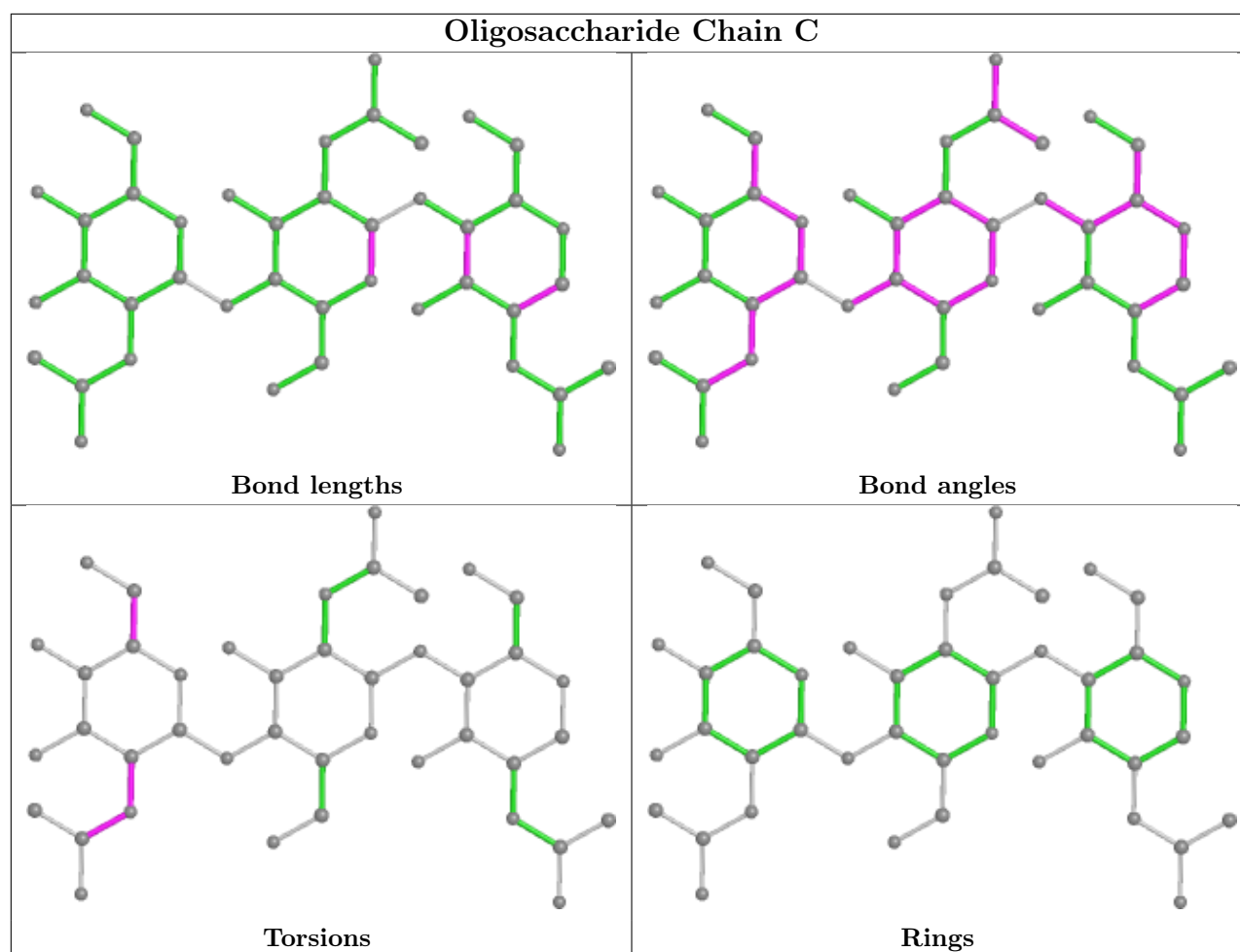
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	4	0
3	C	1	NAG	1	0

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](#)

2 ligands 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
4	NAG	A	807	1	14,14,15	0.97	1 (7%)	17,19,21	2.07	9 (52%)
4	NAG	A	808	1	14,14,15	1.09	1 (7%)	17,19,21	2.09	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
4	NAG	A	807	1	-	2/6/23/26	0/1/1/1
4	NAG	A	808	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	807	NAG	O5-C1	-2.44	1.39	1.43
4	A	808	NAG	C1-C2	2.42	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	808	NAG	C1-O5-C5	6.67	121.23	112.19
4	A	807	NAG	C2-N2-C7	3.53	127.93	122.90
4	A	807	NAG	O4-C4-C3	3.40	118.21	110.35
4	A	807	NAG	C3-C4-C5	-3.01	104.87	110.24
4	A	808	NAG	O3-C3-C4	2.71	116.62	110.35
4	A	807	NAG	C4-C3-C2	-2.68	107.09	111.02
4	A	807	NAG	O5-C1-C2	-2.53	107.29	111.29
4	A	807	NAG	O3-C3-C2	-2.52	104.25	109.47
4	A	807	NAG	O4-C4-C5	2.41	115.28	109.30
4	A	808	NAG	C8-C7-N2	2.41	120.17	116.10
4	A	807	NAG	C1-O5-C5	2.09	115.02	112.19
4	A	807	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	807	NAG	C8-C7-N2-C2
4	A	807	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 [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	492/509 (96%)	-0.09	10 (2%) 65 71	15, 28, 48, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	LYS	3.2
1	A	395	LYS	2.8
1	A	725	ASP	2.6
1	A	576	GLN	2.6
1	A	702	VAL	2.5
1	A	703	PRO	2.3
1	A	633	THR	2.2
1	A	291	ASP	2.1
1	A	613	VAL	2.1
1	A	342	MET	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.

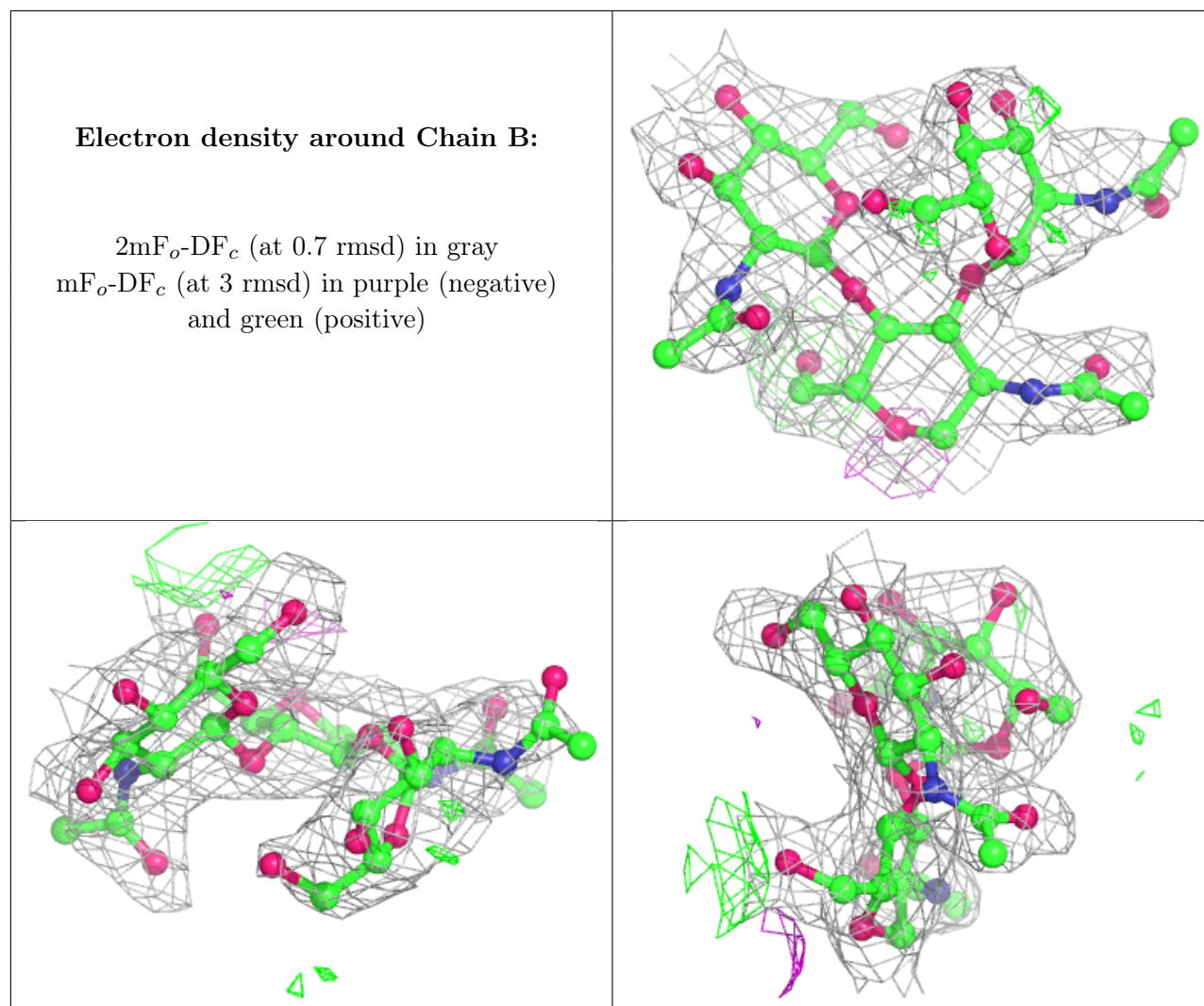
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	3	14/15	0.65	0.32	63,69,76,76	0
2	NAG	B	3	14/15	0.83	0.27	57,61,63,64	0

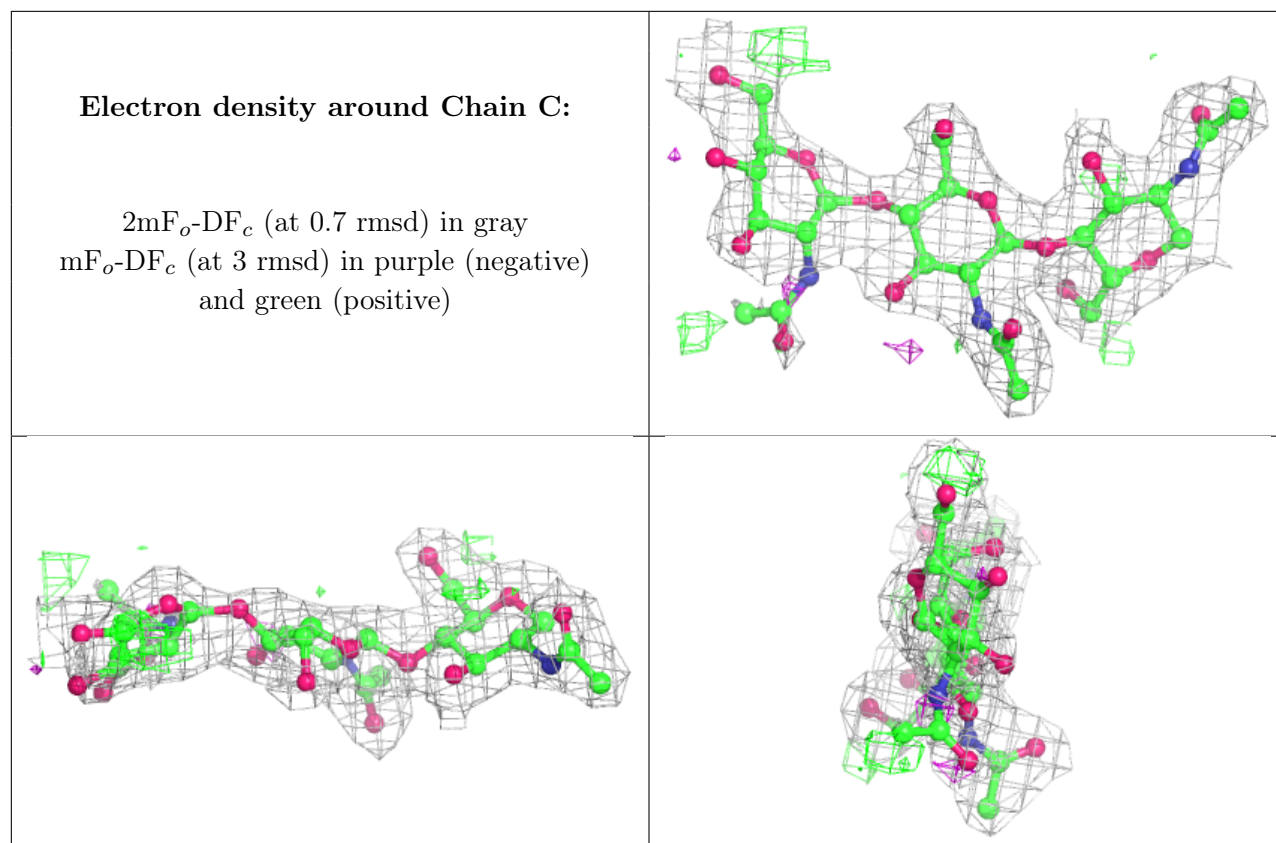
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	1	14/15	0.89	0.15	46,50,55,61	0
2	NAG	B	2	14/15	0.91	0.29	64,69,74,76	0
3	NAG	C	1	14/15	0.93	0.11	23,30,33,34	0
3	NAG	C	2	14/15	0.95	0.14	32,35,44,55	0

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(\AA^2)	Q<0.9
4	NAG	A	808	14/15	0.77	0.23	46,52,57,58	0
4	NAG	A	807	14/15	0.94	0.19	36,45,51,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.