Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2026 – 04:10 PM EST

PDB ID	:	11CW / pdb_000011cw
Title	:	Crystal structure of mouse IgG2a Fc in complex with mouse Fc gamma receptor IV
Authors	:	Mo, G.; Yan, Z.
Deposited on	:	2026-02-17
Resolution	:	3.16 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:

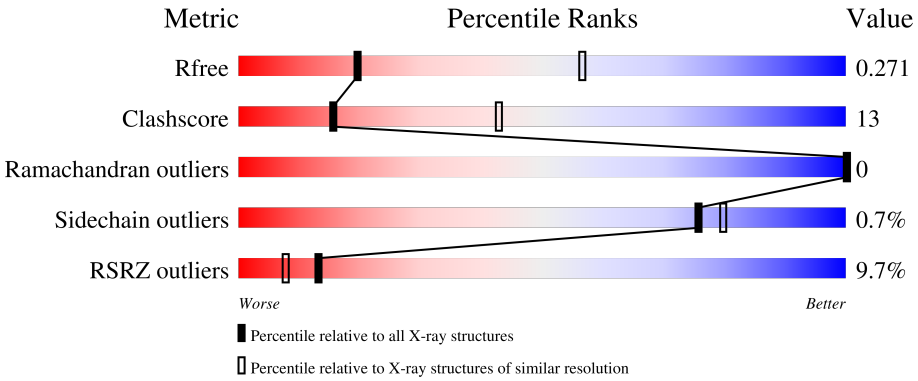
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 <=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	233	5% 56% 30% · 12%
1	B	233	7% 63% 27% 10%
2	C	249	11% 46% 19% · 35%
3	D	8	25% 38% 38%
3	E	8	75% 25%

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Mol	Chain	Length	Quality of chain
4	F	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4897 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.

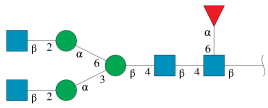
- Molecule 1 is a protein called Ig gamma-2A chain C region, A allele.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1050	277	319	10			
1	B	209	Total	C	N	O	S	0	0	0
			1676	1064	280	322	10			

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	0	0
			1325	835	242	242	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



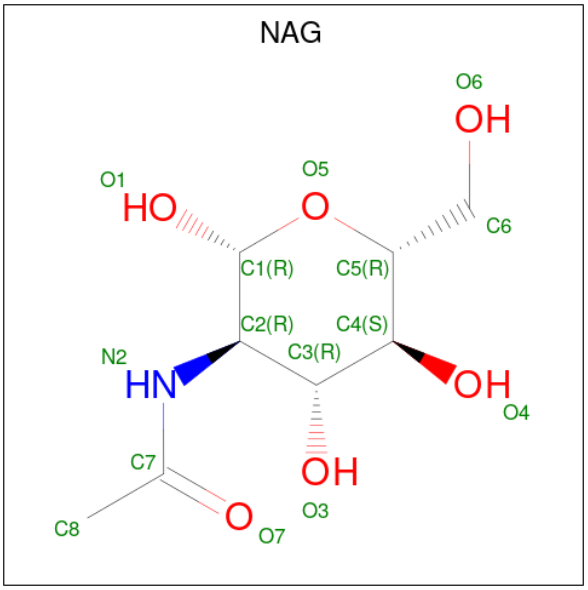
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	E	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



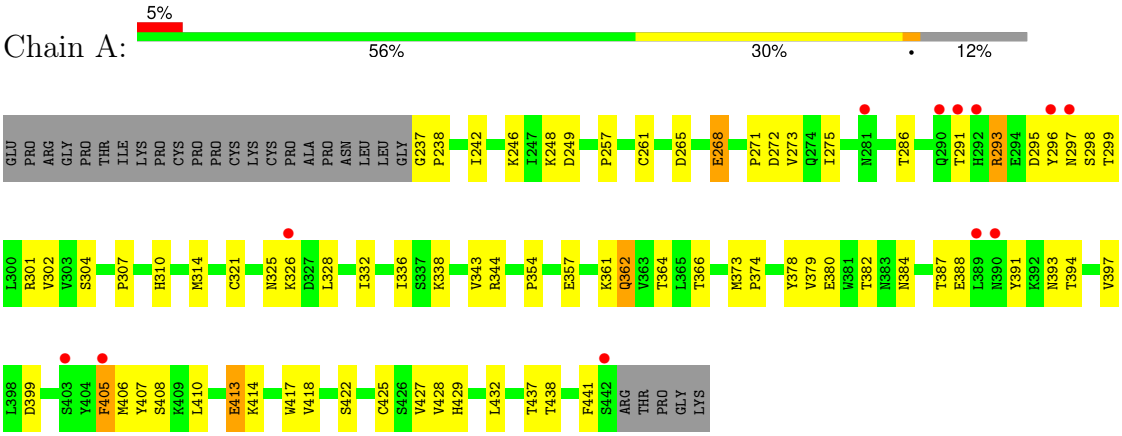
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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.

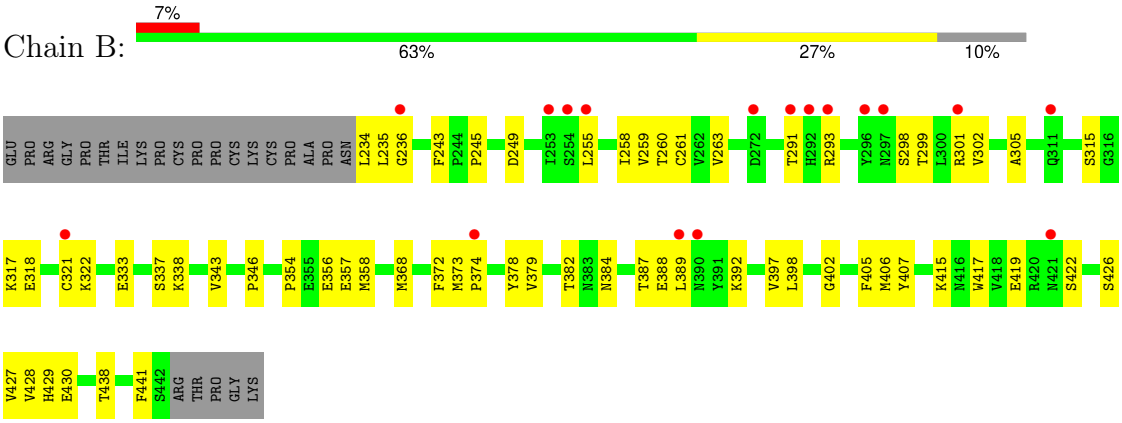
• Molecule 1: Ig gamma-2A chain C region, A allele

Chain A:



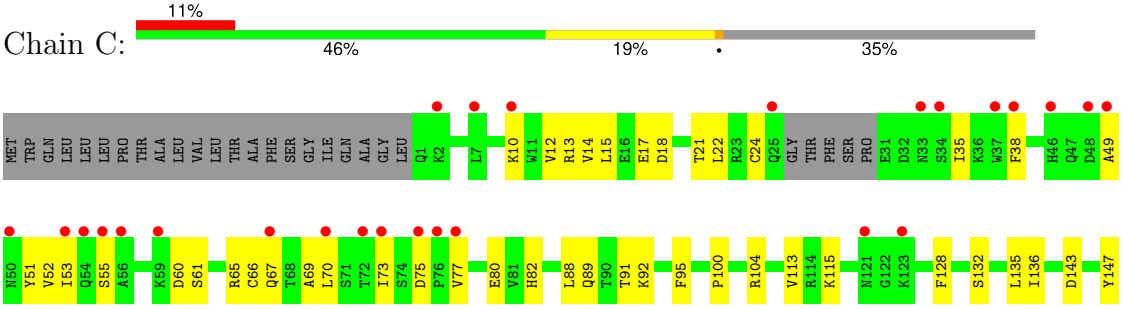
• Molecule 1: Ig gamma-2A chain C region, A allele

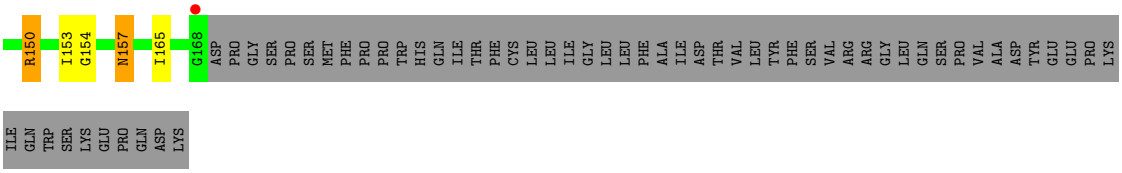
Chain B:



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

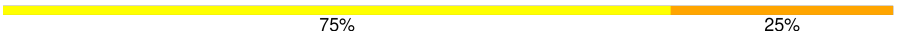
Chain D:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

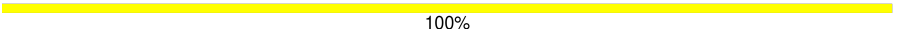
Chain E:





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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	113.75Å 185.06Å 93.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.23 – 3.16 54.23 – 3.16	Depositor EDS
% Data completeness (in resolution range)	90.4 (54.23-3.16) 90.5 (54.23-3.16)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.226 , 0.272 0.226 , 0.271	Depositor DCC
R_{free} test set	1554 reflections (8.93%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4897	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, BMA, MAN, 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	0.66	1/1699 (0.1%)	1.19	7/2314 (0.3%)
1	B	0.66	0/1719	1.08	4/2341 (0.2%)
2	C	0.71	0/1357	1.03	2/1835 (0.1%)
All	All	0.67	1/4775 (0.0%)	1.10	13/6490 (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	1
2	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	GLU	CD-OE1	10.53	1.45	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	362	GLN	OE1-CD-NE2	28.97	151.57	122.60
1	A	362	GLN	CG-CD-OE1	-17.77	85.25	120.80
1	B	261	CYS	CA-CB-SG	10.20	137.86	114.40
2	C	136	ILE	N-CA-C	-8.94	98.70	107.55
1	A	265	ASP	N-CA-C	-8.81	99.18	111.52
1	B	298	SER	N-CA-C	-8.06	100.40	111.28
1	A	405	PHE	CA-CB-CG	6.18	119.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	CYS	N-CA-C	5.99	118.44	108.20
2	C	157	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	413	GLU	OE1-CD-OE2	-5.54	109.59	122.90
1	B	298	SER	CB-CA-C	-5.37	104.26	112.11
1	A	293	ARG	CB-CA-C	5.36	119.52	109.71
1	A	268	GLU	N-CA-C	-5.17	105.72	112.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	GLN	Sidechain
2	C	104	ARG	Sidechain
2	C	150	ARG	Sidechain

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	1656	0	1618	60	0
1	B	1676	0	1643	44	0
2	C	1325	0	1297	33	0
3	D	99	0	85	3	0
3	E	99	0	85	2	0
4	F	28	0	25	1	0
5	C	14	0	13	0	0
All	All	4897	0	4766	129	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 13.

All (129) 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:405:PHE:HZ	1:B:392:LYS:HB3	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PHE:HZ	1:B:392:LYS:CB	1.86	0.88
2:C:35:ILE:HG13	2:C:49:ALA:HA	1.57	0.85
2:C:21:THR:HG23	2:C:52:VAL:HG22	1.62	0.79
1:A:405:PHE:CZ	1:B:392:LYS:CB	2.69	0.76
1:A:382:THR:HG22	1:A:387:THR:HA	1.69	0.73
1:B:243:PHE:HB2	1:B:260:THR:HG23	1.72	0.72
2:C:10:LYS:O	2:C:10:LYS:HG3	1.88	0.72
1:B:374:PRO:HD2	1:B:429:HIS:CE1	2.26	0.70
1:A:388:GLU:HG2	1:A:410:LEU:HD11	1.74	0.69
1:A:405:PHE:CZ	1:B:392:LYS:HB3	2.23	0.68
2:C:13:ARG:NH1	2:C:88:LEU:O	2.27	0.67
1:A:405:PHE:CZ	1:B:392:LYS:HB2	2.31	0.66
1:A:237:GLY:O	2:C:115:LYS:NZ	2.24	0.65
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.80	0.63
2:C:17:GLU:HA	2:C:55:SER:HB2	1.79	0.63
2:C:80:GLU:OE1	2:C:82:HIS:NE2	2.31	0.63
1:B:293:ARG:HB2	1:B:301:ARG:HB3	1.79	0.63
1:B:384:ASN:H	1:B:422:SER:HB3	1.64	0.63
1:A:344:ARG:N	1:A:373:MET:HB2	2.16	0.61
3:E:4:MAN:O2	3:E:5:NAG:O7	2.18	0.61
1:B:379:VAL:HG22	1:B:427:VAL:HG12	1.83	0.60
1:A:374:PRO:HD2	1:A:429:HIS:CE1	2.36	0.60
1:B:291:THR:HA	1:B:302:VAL:HG13	1.83	0.60
1:A:406:MET:HE1	1:A:408:SER:HB2	1.84	0.59
2:C:10:LYS:O	2:C:10:LYS:CG	2.48	0.59
1:B:235:LEU:HD21	1:B:299:THR:HG22	1.84	0.59
2:C:91:THR:OG1	2:C:92:LYS:NZ	2.32	0.58
1:A:314:MET:HA	1:A:338:LYS:HD2	1.83	0.58
1:A:399:ASP:HB2	1:A:405:PHE:HD2	1.68	0.58
1:A:275:ILE:HD12	1:A:304:SER:HB2	1.85	0.58
1:B:397:VAL:HG13	1:B:405:PHE:CE1	2.40	0.56
1:B:374:PRO:HD2	1:B:429:HIS:HE1	1.68	0.56
1:A:328:LEU:HD13	1:A:332:ILE:HG13	1.88	0.56
2:C:61:SER:O	4:F:1:NAG:H3	2.06	0.56
2:C:10:LYS:O	2:C:91:THR:HG22	2.06	0.55
1:B:382:THR:HG22	1:B:387:THR:HA	1.88	0.55
1:B:260:THR:HG21	3:E:7:NAG:H61	1.89	0.55
2:C:53:ILE:CG2	2:C:55:SER:O	2.54	0.55
1:A:393:ASN:HB3	1:A:406:MET:HE3	1.89	0.54
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.40	0.54
2:C:15:LEU:O	2:C:18:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:THR:HA	1:A:302:VAL:HG13	1.91	0.53
2:C:53:ILE:HG22	2:C:55:SER:O	2.09	0.53
2:C:143:ASP:O	2:C:147:TYR:OH	2.26	0.52
2:C:67:GLN:HB2	2:C:73:ILE:HA	1.91	0.52
1:A:297:ASN:HB3	1:A:299:THR:HG23	1.92	0.51
1:A:380:GLU:HB2	1:A:391:TYR:OH	2.09	0.51
1:B:343:VAL:HA	1:B:374:PRO:HD3	1.93	0.51
1:A:296:TYR:CE1	3:D:8:FUC:H5	2.45	0.51
1:B:354:PRO:HG2	1:B:357:GLU:HB2	1.93	0.50
2:C:113:VAL:HG22	2:C:153:ILE:HG13	1.93	0.49
2:C:24:CYS:SG	2:C:66:CYS:HB2	2.53	0.49
1:A:344:ARG:HB2	1:A:373:MET:CG	2.43	0.49
1:A:246:LYS:HD2	1:A:249:ASP:OD2	2.12	0.48
1:A:397:VAL:HG13	1:A:405:PHE:CD1	2.48	0.48
1:A:361:LYS:HE2	1:A:413:GLU:OE1	2.14	0.48
1:A:394:THR:HG23	1:A:407:TYR:O	2.13	0.48
1:B:415:LYS:O	1:B:419:GLU:HG2	2.14	0.48
2:C:69:ALA:O	2:C:70:LEU:HB2	2.14	0.47
2:C:100:PRO:HB2	2:C:135:LEU:HD11	1.96	0.47
1:A:297:ASN:OD1	2:C:150:ARG:NH2	2.47	0.47
1:B:354:PRO:HD2	1:B:357:GLU:OE1	2.15	0.47
2:C:12:VAL:HG23	2:C:13:ARG:HG3	1.98	0.46
1:A:242:ILE:HG12	1:A:336:ILE:HB	1.97	0.46
1:A:344:ARG:H	1:A:373:MET:HB2	1.80	0.46
2:C:53:ILE:HD13	2:C:60:ASP:CG	2.41	0.45
1:A:378:TYR:HB3	1:A:428:VAL:HB	1.97	0.45
1:B:263:VAL:CG1	1:B:302:VAL:HB	2.45	0.45
1:B:378:TYR:HB3	1:B:428:VAL:HB	1.97	0.45
1:A:379:VAL:HG11	1:A:406:MET:CE	2.46	0.45
1:B:315:SER:OG	1:B:317:LYS:HG2	2.15	0.45
1:A:295:ASP:OD2	3:D:1:NAG:H62	2.16	0.45
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.81	0.45
1:B:322:LYS:HG3	1:B:333:GLU:HG2	1.98	0.45
1:A:384:ASN:H	1:A:422:SER:HB3	1.81	0.45
1:A:427:VAL:HG13	1:A:432:LEU:HD11	1.99	0.45
1:B:236:GLY:HA3	2:C:154:GLY:HA3	1.99	0.45
3:D:2:NAG:H83	3:D:6:MAN:O4	2.16	0.45
1:B:417:TRP:HH2	1:B:441:PHE:CG	2.35	0.45
2:C:66:CYS:O	2:C:66:CYS:SG	2.74	0.45
1:B:249:ASP:HA	1:B:255:LEU:HB2	1.99	0.44
2:C:38:PHE:HB2	2:C:65:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:PHE:CG	2:C:132:SER:HB3	2.53	0.44
1:A:397:VAL:HG13	1:A:405:PHE:CE1	2.53	0.44
2:C:15:LEU:HD23	2:C:15:LEU:HA	1.80	0.44
1:B:249:ASP:OD1	1:B:249:ASP:N	2.50	0.44
1:A:238:PRO:HD2	1:A:328:LEU:CD2	2.47	0.44
1:A:366:THR:HG23	1:B:407:TYR:OH	2.17	0.44
2:C:75:ASP:N	2:C:75:ASP:OD1	2.49	0.43
1:A:257:PRO:HD3	1:A:310:HIS:CE1	2.53	0.43
1:A:343:VAL:HA	1:A:374:PRO:HD3	1.99	0.43
1:A:248:LYS:HD2	1:A:378:TYR:CD2	2.54	0.43
1:B:318:GLU:HG2	1:B:337:SER:HB2	1.99	0.43
1:A:414:LYS:O	1:A:418:VAL:HG12	2.19	0.43
1:A:293:ARG:HB2	1:A:301:ARG:O	2.19	0.42
1:A:399:ASP:HA	1:A:405:PHE:HE2	1.84	0.42
1:B:379:VAL:HG11	1:B:406:MET:HE1	2.01	0.42
1:B:398:LEU:HD11	1:B:402:GLY:HA2	2.01	0.42
2:C:95:PHE:CD2	2:C:165:ILE:HG23	2.54	0.42
1:A:273:VAL:HG22	1:A:325:ASN:HB2	2.00	0.42
1:B:358:MET:HE3	1:B:358:MET:HB3	1.83	0.42
1:A:388:GLU:HG2	1:A:410:LEU:CD1	2.47	0.42
1:A:272:ASP:O	1:A:325:ASN:ND2	2.52	0.42
1:A:432:LEU:HD13	1:A:437:THR:HG22	2.00	0.42
1:A:364:THR:HG21	1:B:368:MET:SD	2.59	0.42
1:A:379:VAL:HG11	1:A:406:MET:HE1	2.01	0.42
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.79	0.42
1:B:426:SER:OG	1:B:438:THR:HG22	2.20	0.42
1:A:406:MET:HE2	1:A:407:TYR:O	2.19	0.42
1:B:258:ILE:HG21	1:B:305:ALA:HB1	2.02	0.42
2:C:22:LEU:HD13	2:C:51:TYR:CD2	2.55	0.42
1:A:417:TRP:HH2	1:A:441:PHE:CG	2.38	0.42
1:A:425:CYS:O	1:A:438:THR:HA	2.19	0.41
1:A:399:ASP:CG	1:A:405:PHE:CD2	2.99	0.41
1:A:374:PRO:HD2	1:A:429:HIS:HE1	1.84	0.41
1:A:354:PRO:HG2	1:A:357:GLU:HB2	2.02	0.41
2:C:67:GLN:HE21	2:C:73:ILE:HB	1.86	0.41
1:A:325:ASN:ND2	1:A:326:LYS:H	2.19	0.41
1:B:384:ASN:H	1:B:422:SER:CB	2.32	0.41
1:A:268:GLU:O	1:A:271:PRO:HD3	2.21	0.41
1:B:245:PRO:HD3	1:B:259:VAL:HG12	2.03	0.41
1:B:356:GLU:H	1:B:356:GLU:CD	2.29	0.41
1:B:373:MET:HB3	1:B:374:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:VAL:HA	2:C:89:GLN:HE21	1.86	0.41
1:A:406:MET:HE2	1:A:407:TYR:C	2.46	0.40
1:B:388:GLU:OE2	1:B:389:LEU:N	2.49	0.40
1:A:286:THR:HG23	1:A:307:PRO:HD2	2.04	0.40
1:A:297:ASN:O	1:A:298:SER:HB3	2.22	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	204/233 (88%)	201 (98%)	3 (2%)	0	100	100
1	B	207/233 (89%)	203 (98%)	4 (2%)	0	100	100
2	C	159/249 (64%)	156 (98%)	3 (2%)	0	100	100
All	All	570/715 (80%)	560 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/219 (90%)	194 (99%)	2 (1%)	68	76
1	B	198/219 (90%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	148/223 (66%)	146 (99%)	2 (1%)	59 73
All	All	542/661 (82%)	538 (99%)	4 (1%)	76 80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	CYS
1	A	321	CYS
2	C	77	VAL
2	C	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	325	ASN
1	A	436	HIS
1	B	310	HIS
2	C	1	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	$\#\|Z\|>2$
3	NAG	D	1	3,1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.67	0
3	BMA	D	3	3	11,11,12	0.65	0	15,15,17	1.04	1 (6%)
3	MAN	D	4	3	11,11,12	1.23	2 (18%)	15,15,17	1.22	2 (13%)
3	NAG	D	5	3	14,14,15	0.34	0	17,19,21	0.47	0
3	MAN	D	6	3	11,11,12	1.48	3 (27%)	15,15,17	1.44	3 (20%)
3	NAG	D	7	3	14,14,15	0.44	0	17,19,21	0.74	0
3	FUC	D	8	3	10,10,11	1.37	1 (10%)	14,14,16	1.08	1 (7%)
3	NAG	E	1	3,1	14,14,15	0.28	0	17,19,21	1.02	2 (11%)
3	NAG	E	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.60	0
3	BMA	E	3	3	11,11,12	1.13	1 (9%)	15,15,17	1.16	1 (6%)
3	MAN	E	4	3	11,11,12	1.20	2 (18%)	15,15,17	1.19	1 (6%)
3	NAG	E	5	3	14,14,15	0.43	0	17,19,21	0.93	1 (5%)
3	MAN	E	6	3	11,11,12	1.14	1 (9%)	15,15,17	1.00	2 (13%)
3	NAG	E	7	3	14,14,15	0.51	0	17,19,21	0.54	0
3	FUC	E	8	3	10,10,11	1.86	4 (40%)	14,14,16	1.88	4 (28%)
4	NAG	F	1	4,2	14,14,15	0.50	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.45	0	17,19,21	0.78	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
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	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
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	NAG	D	7	3	-	0/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	6	3	-	2/2/19/22	0/1/1/1
3	NAG	E	7	3	-	0/6/23/26	0/1/1/1
3	FUC	E	8	3	-	-	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	MAN	O5-C1	-3.26	1.38	1.43
3	E	6	MAN	O5-C1	-3.15	1.38	1.43
3	E	8	FUC	C1-C2	3.04	1.59	1.52
3	E	3	BMA	O5-C1	-2.80	1.39	1.43
3	E	8	FUC	C2-C3	2.69	1.56	1.52
3	E	2	NAG	O5-C1	-2.64	1.39	1.43
3	D	4	MAN	C4-C3	2.50	1.58	1.52
3	D	6	MAN	C2-C3	2.47	1.56	1.52
3	E	8	FUC	C6-C5	2.44	1.57	1.51
3	E	8	FUC	O5-C5	-2.44	1.38	1.43
3	D	8	FUC	C2-C3	-2.40	1.48	1.52
3	E	4	MAN	C4-C5	2.33	1.58	1.53
3	D	6	MAN	O3-C3	2.23	1.48	1.43
3	D	4	MAN	C4-C5	2.04	1.57	1.53
3	E	4	MAN	C4-C3	2.02	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	8	FUC	C1-C2-C3	4.01	115.48	109.64
3	E	4	MAN	C1-O5-C5	3.40	116.74	112.19
3	D	6	MAN	C1-O5-C5	3.12	116.36	112.19
3	E	8	FUC	C6-C5-C4	2.99	118.54	113.08
3	E	1	NAG	C1-O5-C5	2.95	116.14	112.19
3	E	8	FUC	O5-C1-C2	2.71	117.26	110.79
3	E	5	NAG	C2-N2-C7	2.70	126.52	122.90
3	D	6	MAN	O3-C3-C2	2.66	115.49	110.05
3	E	3	BMA	O2-C2-C3	-2.61	104.74	110.15
3	D	1	NAG	C1-O5-C5	2.59	115.66	112.19
3	D	6	MAN	O2-C2-C3	-2.46	105.05	110.15
3	D	4	MAN	O2-C2-C3	-2.45	105.08	110.15
3	D	8	FUC	O2-C2-C1	2.45	114.83	109.22
3	E	1	NAG	O4-C4-C5	-2.38	103.46	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	NAG	C1-O5-C5	2.31	115.28	112.19
3	D	4	MAN	C1-O5-C5	2.27	115.22	112.19
3	E	8	FUC	C1-O5-C5	2.26	118.28	112.97
3	E	6	MAN	C1-O5-C5	2.18	115.11	112.19
3	D	3	BMA	O4-C4-C3	-2.01	105.64	110.38
3	E	6	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	5	NAG	C1-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6

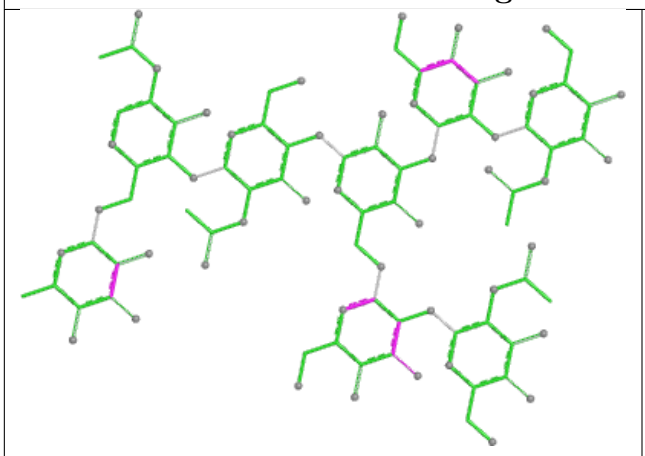
There are no ring outliers.

8 monomers are involved in 6 short contacts:

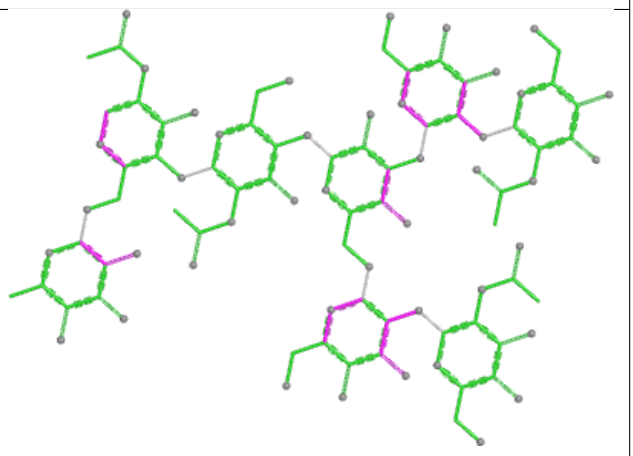
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	NAG	1	0
3	E	4	MAN	1	0
3	E	7	NAG	1	0
4	F	1	NAG	1	0
3	D	6	MAN	1	0
3	D	8	FUC	1	0
3	D	1	NAG	1	0
3	D	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

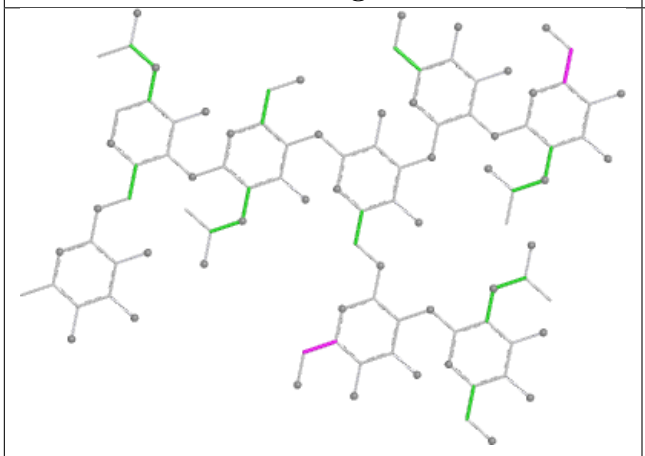
Oligosaccharide Chain D



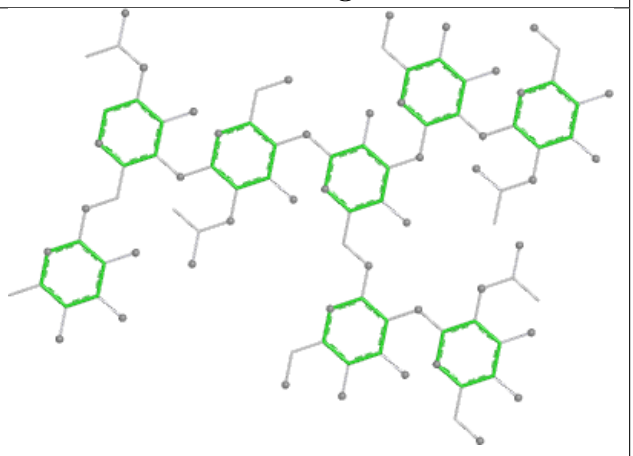
Bond lengths



Bond angles

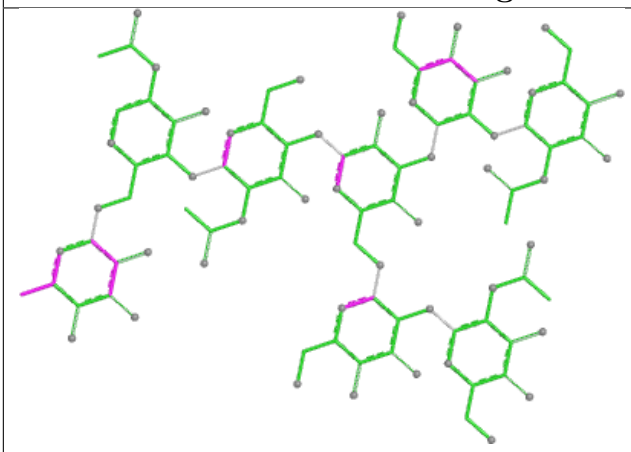


Torsions

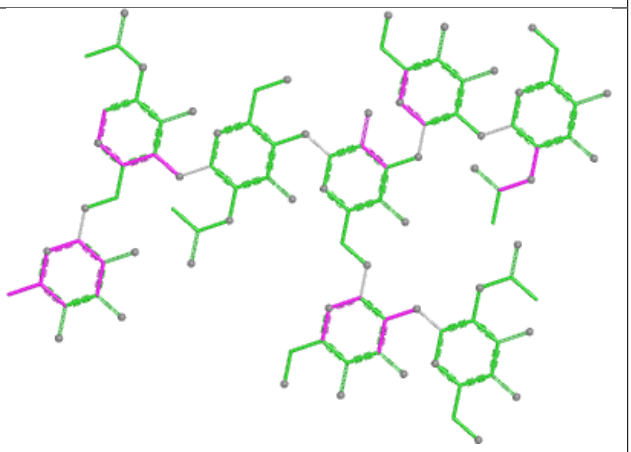


Rings

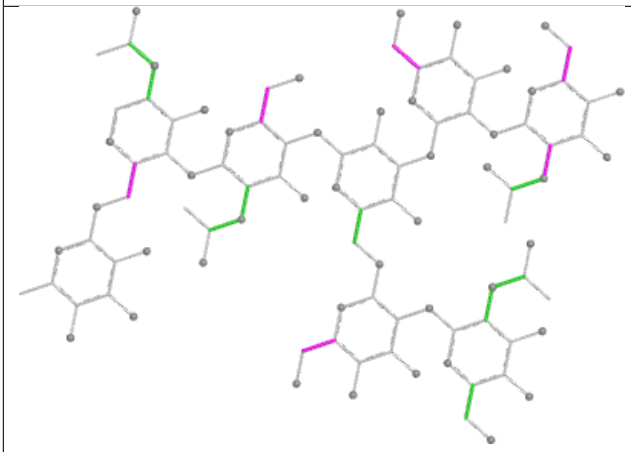
Oligosaccharide Chain E



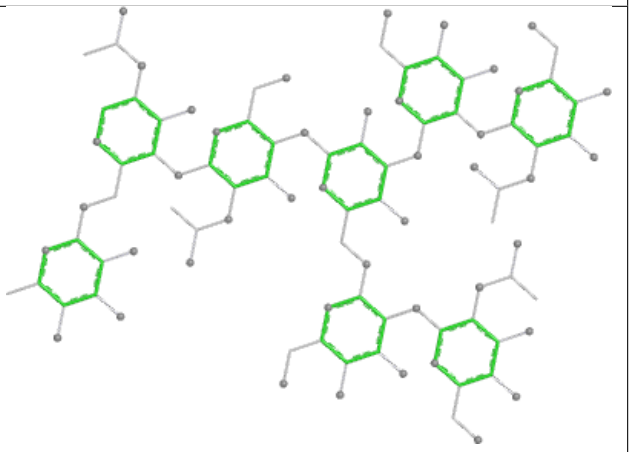
Bond lengths



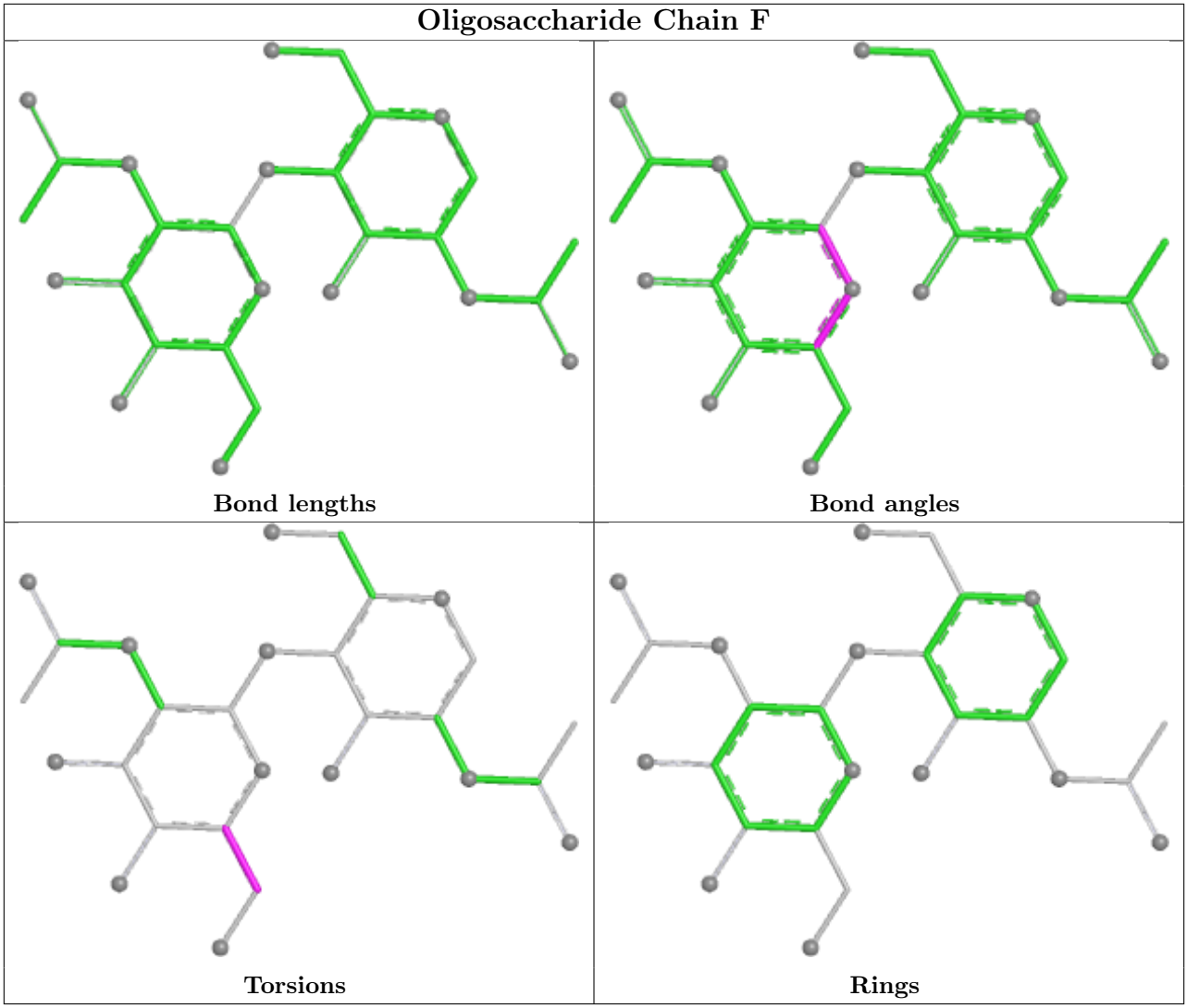
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	NAG	C	301	2	14,14,15	0.87	1 (7%)	17,19,21	0.82	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
5	NAG	C	301	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	NAG	O5-C1	2.54	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	301	NAG	C1-O5-C5	2.67	115.76	112.19

There are no chirality outliers.

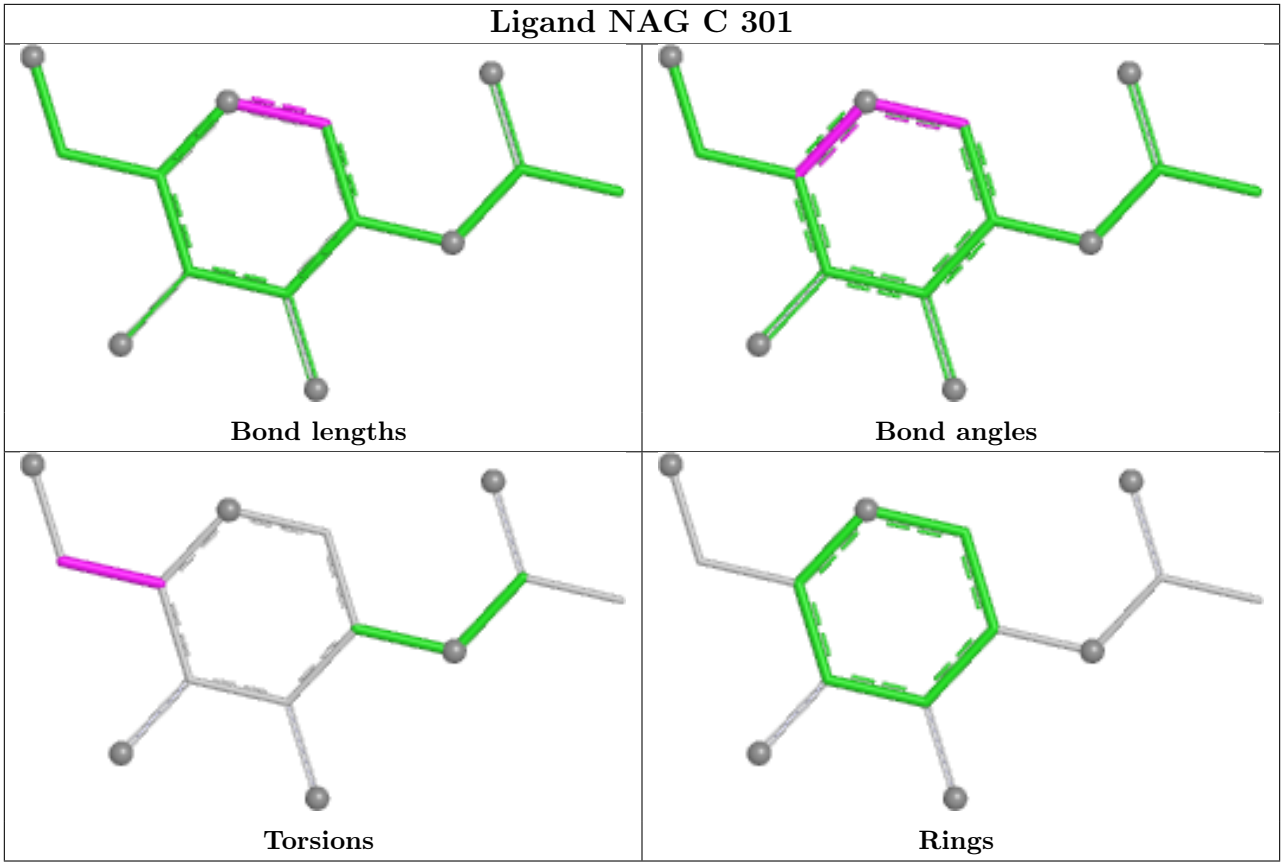
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	NAG	O5-C5-C6-O6
5	C	301	NAG	C4-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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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, 95^{th} 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	206/233 (88%)	0.28	12 (5%) 29 16	28, 44, 64, 75	0
1	B	209/233 (89%)	0.41	17 (8%) 18 10	28, 46, 73, 84	0
2	C	163/249 (65%)	0.84	27 (16%) 4 2	30, 51, 104, 118	0
All	All	578/715 (80%)	0.48	56 (9%) 13 8	28, 46, 92, 118	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	HIS	4.7
1	B	291	THR	4.2
1	A	292	HIS	3.9
2	C	34	SER	3.8
1	A	297	ASN	3.8
2	C	33	ASN	3.7
1	B	253	ILE	3.6
1	B	293	ARG	3.6
2	C	38	PHE	3.4
1	A	291	THR	3.3
1	A	405	PHE	3.3
2	C	56	ALA	3.3
2	C	53	ILE	3.2
2	C	123	LYS	3.1
1	B	321	CYS	3.1
2	C	168	GLY	3.0
2	C	7	LEU	3.0
1	B	389	LEU	3.0
2	C	46	HIS	3.0
2	C	48	ASP	3.0
2	C	49	ALA	2.9
1	B	296	TYR	2.9
2	C	10	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	442	SER	2.9
2	C	75	ASP	2.8
1	B	297	ASN	2.7
1	A	389	LEU	2.7
1	B	301	ARG	2.7
2	C	2	LYS	2.7
2	C	76	PRO	2.7
1	B	255	LEU	2.6
2	C	73	ILE	2.6
1	A	296	TYR	2.6
1	B	254	SER	2.6
2	C	59	LYS	2.6
1	B	390	ASN	2.5
1	B	311	GLN	2.5
2	C	55	SER	2.4
1	B	374	PRO	2.4
1	A	390	ASN	2.4
1	A	281	ASN	2.3
2	C	121	ASN	2.3
2	C	50	ASN	2.3
2	C	54	GLN	2.3
2	C	70	LEU	2.2
2	C	72	THR	2.2
1	A	290	GLN	2.2
2	C	37	TRP	2.2
2	C	67	GLN	2.2
2	C	25	GLN	2.1
2	C	77	VAL	2.1
1	B	236	GLY	2.1
1	B	421	ASN	2.1
1	A	326	LYS	2.0
1	A	403	SER	2.0
1	B	272	ASP	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)

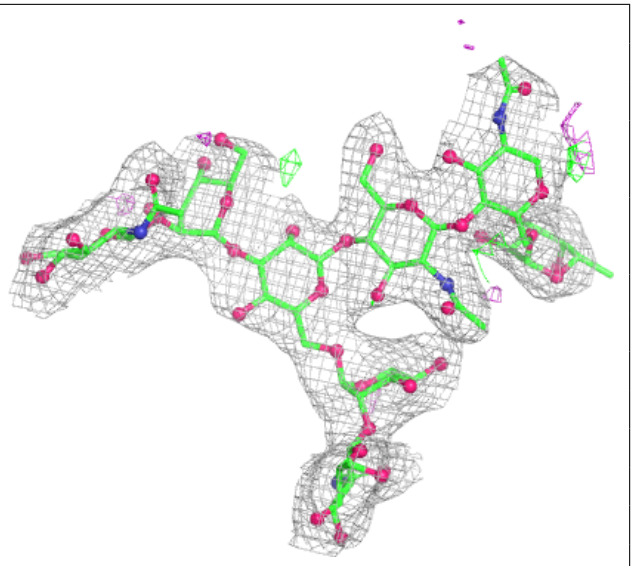
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

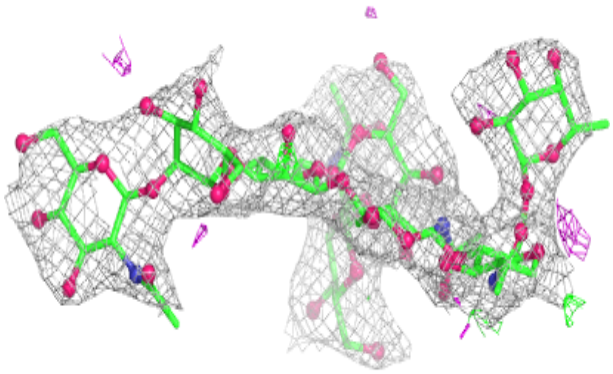
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	F	1	14/15	0.66	0.16	62,71,78,80	0
3	FUC	E	8	10/11	0.67	0.19	54,66,72,74	0
3	NAG	E	5	14/15	0.69	0.17	80,91,100,107	0
3	MAN	D	4	11/12	0.74	0.13	65,67,72,73	0
4	NAG	F	2	14/15	0.75	0.19	58,77,92,96	0
3	FUC	D	8	10/11	0.79	0.15	55,61,66,67	0
3	NAG	D	5	14/15	0.80	0.13	63,79,86,87	0
3	MAN	E	4	11/12	0.88	0.10	64,74,81,82	0
3	MAN	E	6	11/12	0.89	0.10	48,50,54,67	0
3	NAG	D	7	14/15	0.90	0.10	43,51,56,60	0
3	MAN	D	6	11/12	0.91	0.09	44,50,55,59	0
3	NAG	D	1	14/15	0.91	0.12	45,53,58,60	0
3	NAG	E	7	14/15	0.91	0.10	41,50,57,61	0
3	BMA	E	3	11/12	0.93	0.08	49,57,66,68	0
3	BMA	D	3	11/12	0.93	0.09	44,50,54,61	0
3	NAG	E	2	14/15	0.95	0.08	46,52,56,59	0
3	NAG	D	2	14/15	0.95	0.09	37,44,46,47	0
3	NAG	E	1	14/15	0.95	0.10	52,62,66,69	0

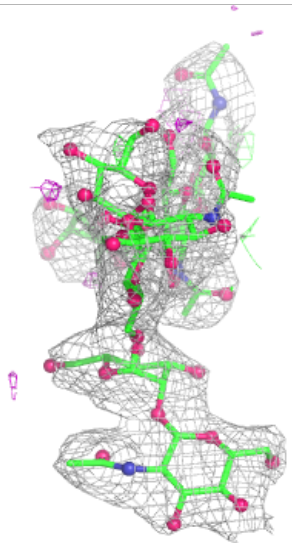
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

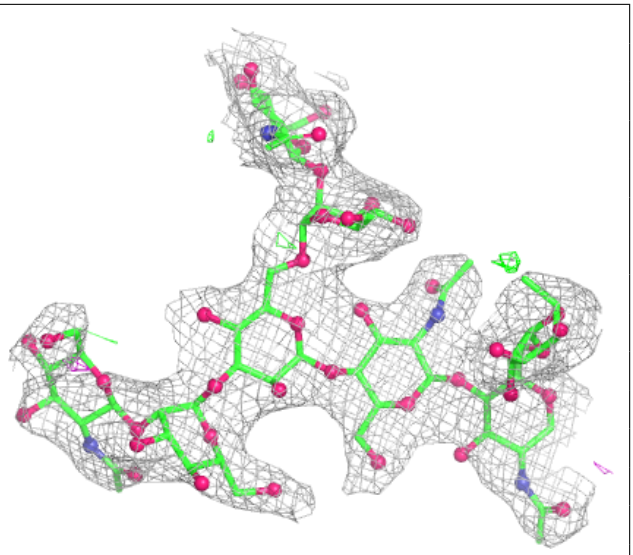


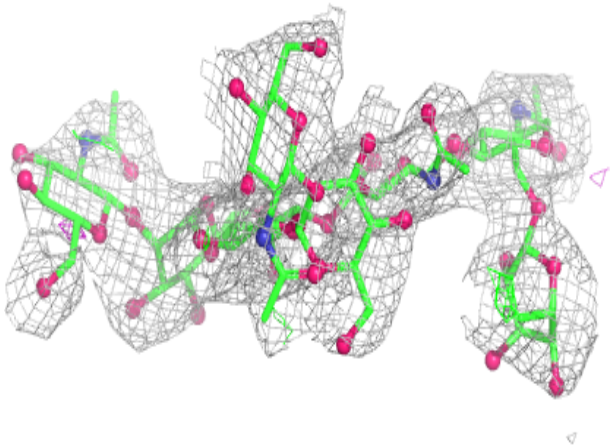


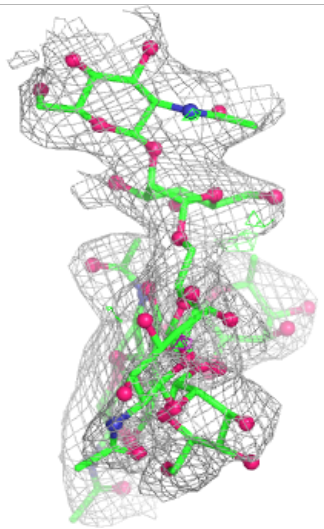


Electron density around Chain E:

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

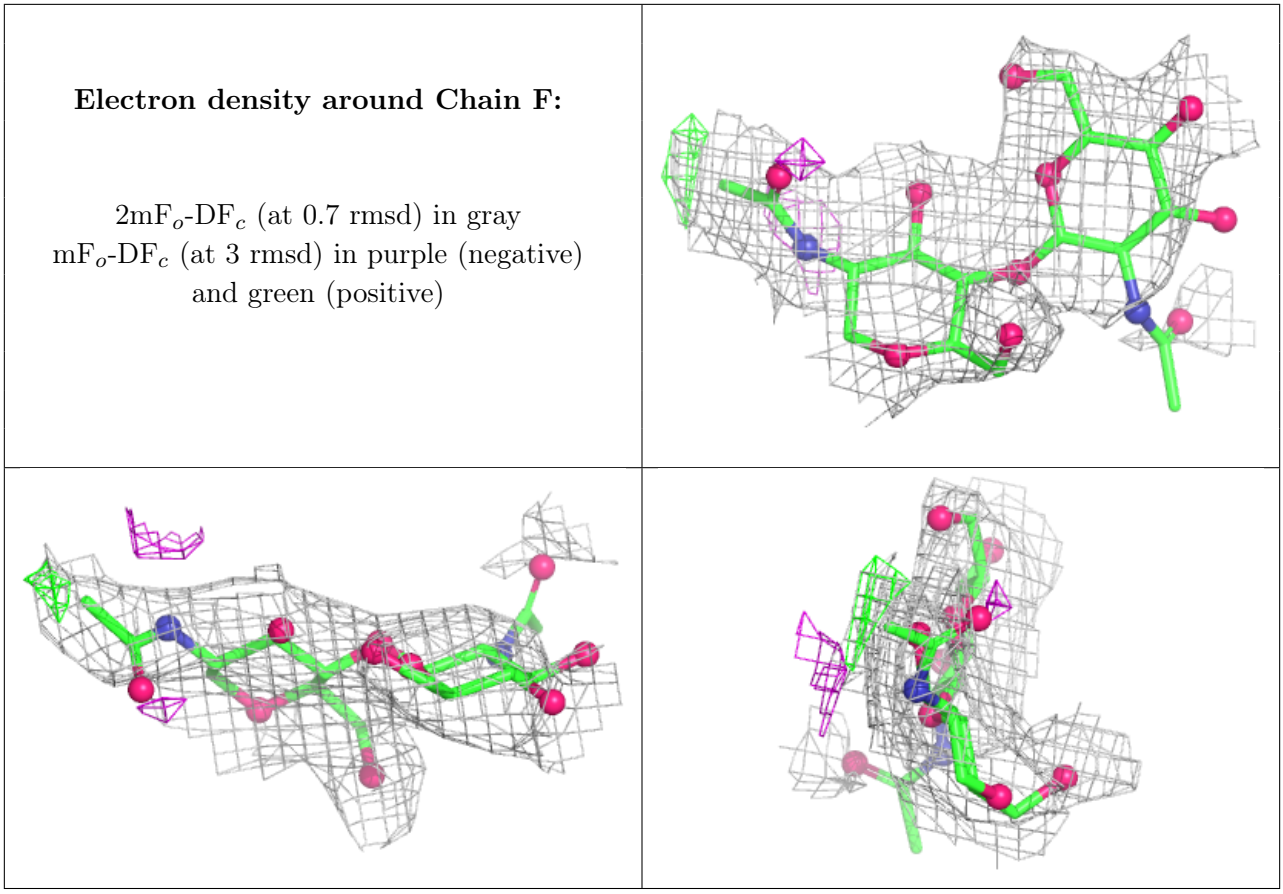






Electron density around Chain F:

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



6.4 Ligands

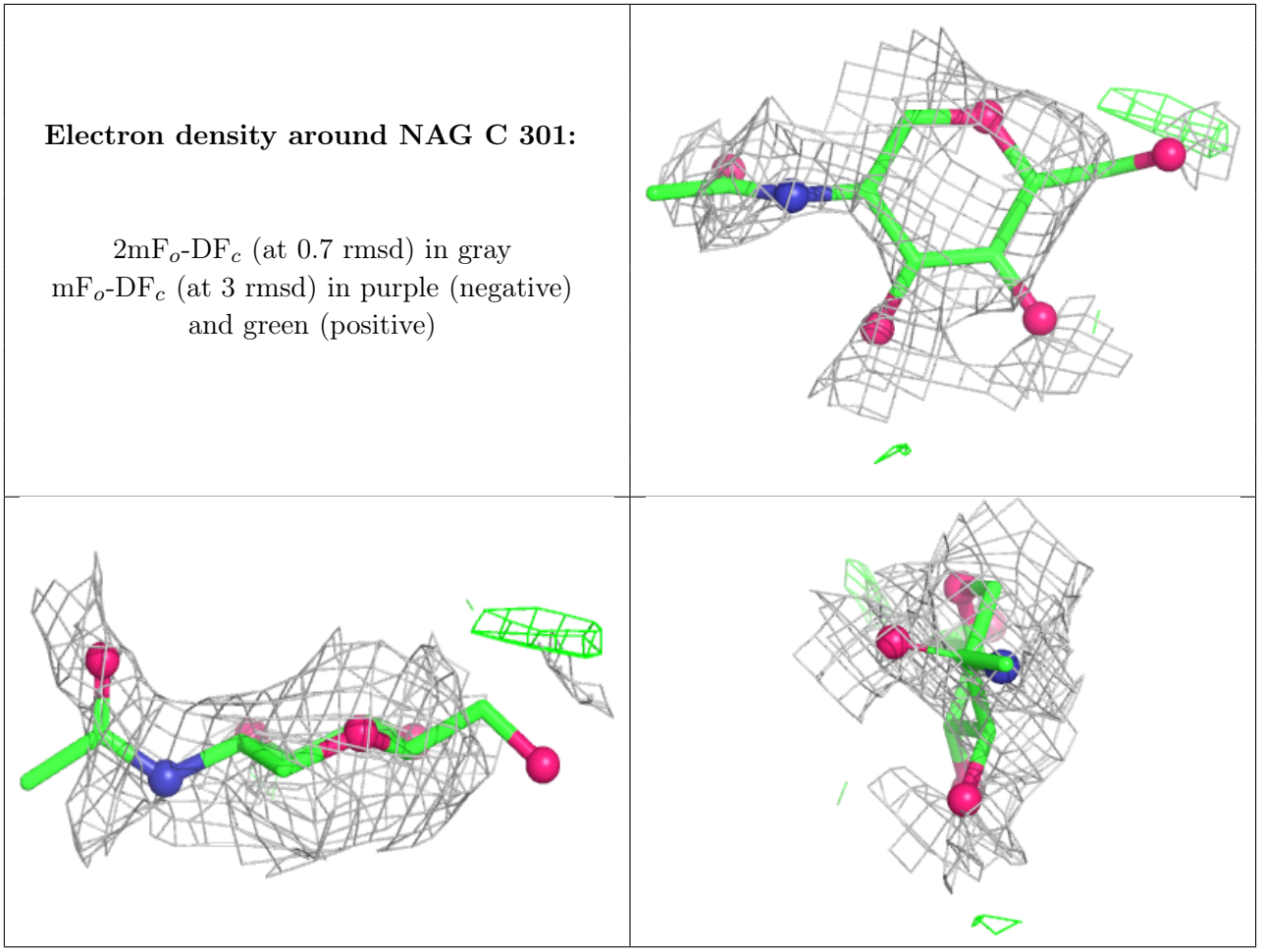
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NAG	C	301	14/15	0.64	0.17	71,84,89,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG C 301:

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



6.5 Other polymers

There are no such residues in this entry.