



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 6IDV / pdb_00006idv
Title : Peptide Asparaginyl Ligases from *Viola yedoensis*
Authors : El Sahili, A.; Hu, S.; Lescar, J.
Deposited on : 2018-09-11
Resolution : 2.40 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

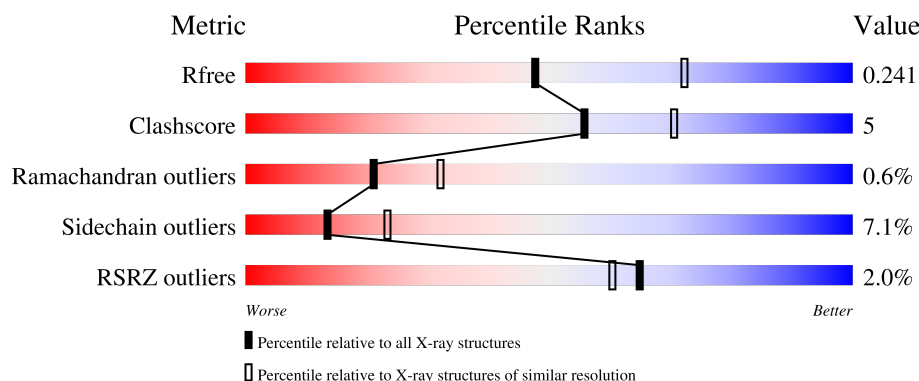
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	483	2% 71% 15% • 12%
1	B	483	2% 72% 14% • 12%
2	C	3	33% 67%
2	E	3	33% 67%
3	D	2	50% 50%

2 Entry composition [i](#)

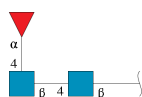
There are 7 unique types of molecules in this entry. The entry contains 7199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptide Asparaginyl Ligases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	1	0
			3305	2104	550	629	22			
1	B	426	Total	C	N	O	S	0	1	0
			3306	2101	550	633	22			

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



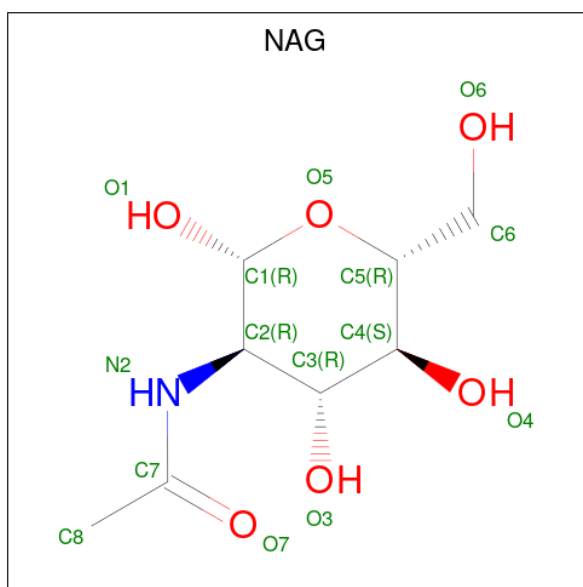
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



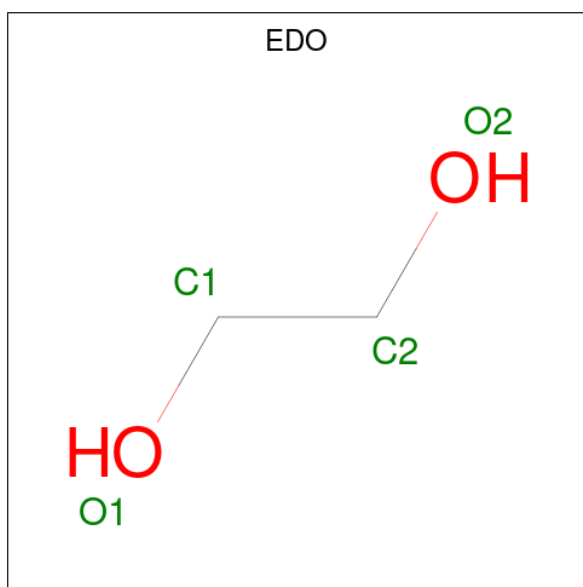
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



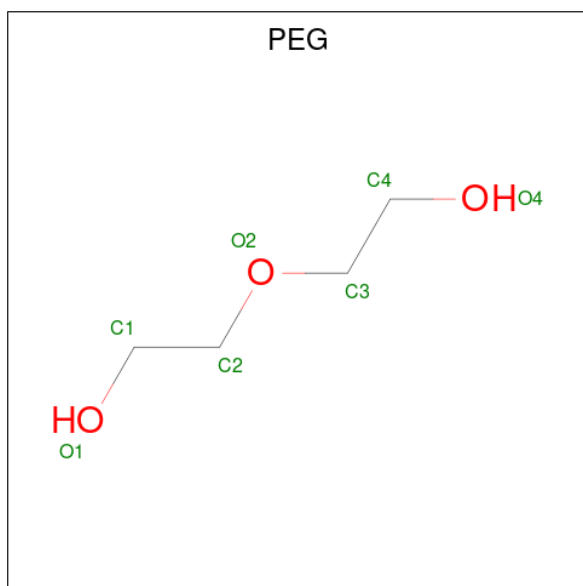
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

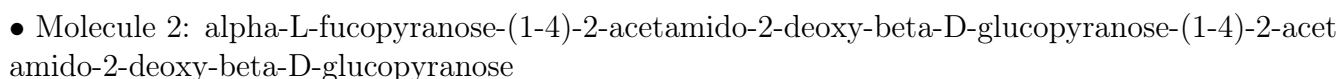


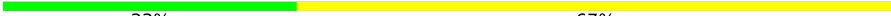
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total	O	0	0
			212	212		
7	B	215	Total	O	0	0
			215	215		

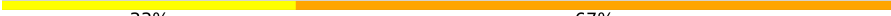
- Molecule 1: Peptide Asparaginyl Ligases



Chain C:  33% 67%

MAG1
MAG2
FUC3

- Molecule 2: α -L-fucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1
MAG2
FUC3

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

Chain D:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.80Å 69.80Å 104.48Å 90.00° 110.22° 90.00°	Depositor
Resolution (Å)	48.00 – 2.40 48.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.00-2.40) 99.6 (48.00-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	128.47 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.195 , 0.236 0.200 , 0.241	Depositor DCC
R_{free} test set	2077 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7199	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 5.30% 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: SNN, PEG, FUC, EDO, 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	0.82	1/3377 (0.0%)	1.38	16/4579 (0.3%)
1	B	0.82	1/3378 (0.0%)	1.41	16/4580 (0.3%)
All	All	0.82	2/6755 (0.0%)	1.40	32/9159 (0.3%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	-7.74	1.60	1.79
1	B	180	MET	SD-CE	-7.39	1.61	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	SER	CA-C-N	6.73	129.28	120.60
1	B	266	SER	C-N-CA	6.73	129.28	120.60
1	A	305	ASP	CA-C-N	6.57	124.38	120.24
1	A	305	ASP	C-N-CA	6.57	124.38	120.24
1	B	305	ASP	CA-C-N	6.35	124.24	120.24
1	B	305	ASP	C-N-CA	6.35	124.24	120.24
1	B	67	ASN	CA-C-N	5.86	129.62	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ASN	C-N-CA	5.86	129.62	120.82
1	A	73	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	73	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	67	ASN	CA-C-N	5.66	129.30	120.82
1	A	67	ASN	C-N-CA	5.66	129.30	120.82
1	B	237	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	366	ILE	CA-C-N	5.61	127.73	120.44
1	B	366	ILE	C-N-CA	5.61	127.73	120.44
1	B	94	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	237	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	366	ILE	CA-C-N	5.51	127.60	120.44
1	A	366	ILE	C-N-CA	5.51	127.60	120.44
1	A	252	ASP	CA-C-N	5.48	128.01	120.39
1	A	252	ASP	C-N-CA	5.48	128.01	120.39
1	A	209	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	274	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	269	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	253	PHE	N-CA-C	5.12	116.28	109.93
1	B	320	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	68	TYR	CA-C-N	5.09	127.41	120.54
1	A	68	TYR	C-N-CA	5.09	127.41	120.54
1	A	399	ALA	N-CA-C	5.08	117.20	111.11
1	B	209	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	269	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	277	ASN	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ALA	Mainchain
1	B	170	ALA	Mainchain

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	3305	0	3206	34	0
1	B	3306	0	3194	27	0
2	C	38	0	34	0	0
2	E	38	0	34	3	0
3	D	28	0	25	1	0
4	A	14	0	13	1	0
4	B	28	0	26	1	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	B	7	0	10	2	0
7	A	212	0	0	1	0
7	B	215	0	0	2	0
All	All	7199	0	6554	63	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 5.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:PRO:HD2	1:B:253:PHE:HB2	1.63	0.80
1:A:323:ASN:HD22	1:A:326:ARG:HE	1.33	0.76
1:A:145:ASN:HD21	4:A:501:NAG:C1	1.98	0.75
1:B:145:ASN:HD21	4:B:702:NAG:C1	2.00	0.75
1:A:131:GLU:H	6:B:703:PEG:H12	1.51	0.74
1:B:137:ASN:HD21	1:B:150:ILE:H	1.36	0.72
1:A:137:ASN:HD21	1:A:150:ILE:H	1.36	0.72
1:B:282:THR:HA	1:B:312:SER:HA	1.81	0.63
1:A:282:THR:HA	1:A:312:SER:HA	1.80	0.63
1:B:351:ILE:HD12	1:B:375:LEU:HD13	1.83	0.61
1:A:250:THR:HG23	1:A:251:PRO:HD3	1.83	0.60
1:A:280:THR:HG21	1:A:327:THR:HG22	1.85	0.59
1:B:243:TRP:HB3	1:B:340:VAL:HG22	1.85	0.58
1:B:280:THR:HG21	1:B:327:THR:HG22	1.87	0.56
1:B:243:TRP:HB3	1:B:340:VAL:CG2	2.36	0.55
1:B:243:TRP:CD1	1:B:297:ALA:HB1	2.42	0.55
1:B:398:LYS:HA	1:B:401:LYS:HD2	1.90	0.53
1:B:268:THR:OG1	1:B:294:ILE:HD11	2.10	0.51
1:A:243:TRP:HB3	1:A:340:VAL:HG22	1.93	0.51
1:A:244:ILE:HD11	1:A:343:GLN:HA	1.94	0.50
1:A:75:CYS:SG	1:A:95:MET:HE1	2.52	0.49
1:B:198:LYS:O	1:B:201:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ALA:O	1:A:426:THR:HG23	2.12	0.49
1:A:57:VAL:HG22	1:A:92:ILE:HD12	1.95	0.48
1:A:287:PHE:CE1	1:A:302:GLN:HG3	2.48	0.48
1:B:287:PHE:CE1	1:B:302:GLN:HG3	2.49	0.48
1:B:64:GLY:HA2	2:E:1:NAG:H61	1.96	0.47
1:A:251:PRO:HD2	1:A:253:PHE:HB2	1.96	0.47
1:B:114:LYS:HG2	1:B:115:PRO:HD2	1.97	0.47
6:B:703:PEG:H21	7:B:923:HOH:O	2.14	0.47
1:A:243:TRP:HB3	1:A:340:VAL:CG2	2.45	0.47
2:E:2:NAG:H4	2:E:3:FUC:O2	2.15	0.46
1:B:141:ALA:HA	1:B:156:VAL:HG12	1.98	0.46
1:A:141:ALA:HA	1:A:156:VAL:HG12	1.98	0.46
1:B:178:ILE:HD11	1:B:186:LEU:HD23	1.98	0.46
1:A:244:ILE:CD1	1:A:343:GLN:HA	2.46	0.46
1:B:57:VAL:HG22	1:B:92:ILE:HD12	1.96	0.46
1:A:58:LEU:HB3	1:A:74:VAL:HG13	1.97	0.46
1:A:425:ARG:O	1:A:429:THR:HG23	2.16	0.46
1:A:470:PRO:HG2	1:A:475:SER:HB3	1.97	0.46
1:B:142:ILE:HA	1:B:157:LEU:HD12	1.97	0.45
1:B:244:ILE:CD1	1:B:343:GLN:HA	2.47	0.45
1:B:425:ARG:O	1:B:429:THR:HG23	2.16	0.45
1:B:244:ILE:HG13	1:B:343:GLN:HG2	1.99	0.45
1:A:426:THR:HG21	1:A:455:LYS:HB2	1.99	0.45
1:A:236:SER:HB2	1:A:240:GLU:HG2	1.98	0.45
1:B:102:ASN:HA	2:E:1:NAG:O7	2.17	0.45
1:B:418:GLN:HG2	7:B:959:HOH:O	2.16	0.45
1:A:64:GLY:HA2	3:D:1:NAG:H61	1.99	0.44
1:A:142:ILE:HA	1:A:157:LEU:HD12	1.99	0.44
1:A:262:GLY:HA3	1:A:267[A]:ILE:HD11	1.99	0.44
1:A:178:ILE:HD11	1:A:186:LEU:HD23	1.99	0.44
1:A:323:ASN:HD22	1:A:326:ARG:NE	2.09	0.44
1:A:188:ALA:HB3	1:A:417:TRP:CH2	2.52	0.43
1:B:58:LEU:HB3	1:B:74:VAL:HG13	1.99	0.43
1:B:178:ILE:HG12	1:B:219:MET:HE2	2.00	0.43
1:A:423:MET:CE	1:A:455:LYS:HA	2.49	0.43
1:B:250:THR:HG22	1:B:251:PRO:HD3	2.01	0.43
1:A:165:ILE:HB	1:A:207:MET:HG3	2.01	0.42
1:A:178:ILE:HG12	1:A:219:MET:HE2	2.02	0.42
1:A:181:PRO:HB2	7:A:616:HOH:O	2.20	0.41
1:A:134:ASN:CA	1:A:180:MET:HE2	2.51	0.41
1:A:170:ALA:HA	1:A:212:GLU:HB3	2.03	0.41

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	421/483 (87%)	411 (98%)	8 (2%)	2 (0%)	24	37
1	B	421/483 (87%)	410 (97%)	8 (2%)	3 (1%)	18	28
All	All	842/966 (87%)	821 (98%)	16 (2%)	5 (1%)	21	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	PRO
1	B	250	THR
1	B	251	PRO
1	A	250	THR
1	B	97	ASP

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	355/402 (88%)	329 (93%)	26 (7%)	13	22
1	B	355/402 (88%)	330 (93%)	25 (7%)	14	24
All	All	710/804 (88%)	659 (93%)	51 (7%)	13	23

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	196	LYS
1	A	250	THR
1	A	256	GLU
1	A	264	LEU
1	A	267[A]	ILE
1	A	267[B]	ILE
1	A	269	PHE
1	A	277	ASN
1	A	341	ILE
1	A	342	HIS
1	A	343	GLN
1	A	344	HIS
1	A	365	LYS
1	A	386	ILE
1	A	388	LEU
1	A	392	LEU
1	A	393	LEU
1	A	401	LYS
1	A	423	MET
1	A	426	THR
1	A	429	THR
1	A	434	LEU
1	A	455	LYS
1	A	458	LEU
1	A	468	THR
1	B	196	LYS
1	B	201	THR
1	B	211	VAL
1	B	256	GLU
1	B	264	LEU
1	B	267	ILE
1	B	269	PHE
1	B	276	HIS
1	B	277	ASN
1	B	324	ASP
1	B	341	ILE
1	B	342	HIS
1	B	343	GLN
1	B	344	HIS
1	B	365	LYS
1	B	388	LEU
1	B	392	LEU

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Mol	Chain	Res	Type
1	B	393	LEU
1	B	423	MET
1	B	429	THR
1	B	434	LEU
1	B	435	SER
1	B	455	LYS
1	B	457	GLN
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	137	ASN
1	A	145	ASN
1	A	162	ASN
1	A	215	ASN
1	A	277	ASN
1	A	302	GLN
1	A	323	ASN
1	A	325	ASN
1	A	369	GLN
1	A	371	GLN
1	A	418	GLN
1	A	430	HIS
1	B	135	ASN
1	B	137	ASN
1	B	145	ASN
1	B	215	ASN
1	B	277	ASN
1	B	325	ASN
1	B	369	GLN
1	B	371	GLN
1	B	418	GLN
1	B	430	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SNN	B	171	1	7,8,8	3.23	2 (28%)	10,11,11	3.09	5 (50%)
1	SNN	A	171	1	7,8,8	3.14	2 (28%)	10,11,11	2.98	5 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SNN	B	171	1	-	-	0/1/1/1
1	SNN	A	171	1	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	SNN	C4-C5	-8.21	1.39	1.51
1	A	171	SNN	C4-C5	-7.77	1.39	1.51
1	A	171	SNN	C-N1	-2.43	1.34	1.37
1	B	171	SNN	C-N1	-2.07	1.35	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	SNN	C5-N1-C	-5.28	108.65	113.96
1	B	171	SNN	CA-C-N1	5.03	111.25	107.30
1	A	171	SNN	C5-N1-C	-5.03	108.91	113.96
1	A	171	SNN	CA-C-N1	5.02	111.24	107.30
1	A	171	SNN	O-C-CA	-4.48	122.97	126.19
1	B	171	SNN	O-C-CA	-4.32	123.08	126.19
1	B	171	SNN	O5-C5-C4	-3.45	122.08	126.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	SNN	C4-C5-N1	3.31	111.96	108.02
1	A	171	SNN	C4-C5-N1	3.19	111.81	108.02
1	A	171	SNN	O5-C5-C4	-2.59	123.18	126.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	1.26	2 (14%)	17,19,21	1.46	2 (11%)
2	NAG	C	2	2	14,14,15	1.04	1 (7%)	17,19,21	0.74	0
2	FUC	C	3	2	10,10,11	0.42	0	14,14,16	0.84	0
3	NAG	D	1	3,1	14,14,15	1.33	3 (21%)	17,19,21	0.97	1 (5%)
3	NAG	D	2	3	14,14,15	1.00	0	17,19,21	1.26	1 (5%)
2	NAG	E	1	2,1	14,14,15	1.91	4 (28%)	17,19,21	2.99	6 (35%)
2	NAG	E	2	2	14,14,15	1.53	3 (21%)	17,19,21	1.17	1 (5%)
2	FUC	E	3	2	10,10,11	0.46	0	14,14,16	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	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	C	2	2	-	0/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	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
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C5	4.68	1.52	1.43
2	E	1	NAG	C2-N2	3.21	1.51	1.46
2	C	1	NAG	O5-C1	-3.06	1.38	1.43
3	D	1	NAG	O5-C5	2.99	1.49	1.43
2	E	2	NAG	C3-C2	2.66	1.58	1.52
2	E	1	NAG	C4-C5	2.58	1.58	1.53
3	D	1	NAG	C4-C5	2.46	1.58	1.53
2	E	2	NAG	C1-C2	2.41	1.55	1.52
2	E	2	NAG	O4-C4	2.39	1.48	1.43
2	C	1	NAG	C1-C2	2.37	1.55	1.52
2	C	2	NAG	C4-C3	2.17	1.58	1.52
2	E	1	NAG	O5-C1	-2.14	1.40	1.43
3	D	1	NAG	C4-C3	2.13	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C2-N2-C7	7.61	133.10	122.90
2	E	1	NAG	C1-C2-N2	6.25	120.28	110.43
2	E	1	NAG	C4-C3-C2	-4.14	104.95	111.02
2	E	1	NAG	O5-C1-C2	-3.38	106.06	111.29
2	C	1	NAG	C1-O5-C5	-3.29	107.78	112.19
3	D	2	NAG	C1-O5-C5	3.23	116.51	112.19
2	E	1	NAG	C6-C5-C4	-2.86	106.00	113.02
2	E	2	NAG	C4-C3-C2	2.61	114.84	111.02
2	C	1	NAG	C4-C3-C2	2.61	114.84	111.02
2	E	1	NAG	O7-C7-N2	2.50	126.40	121.98
3	D	1	NAG	C3-C4-C5	2.13	114.09	110.23

There are no chirality outliers.

All (9) torsion outliers are listed below:

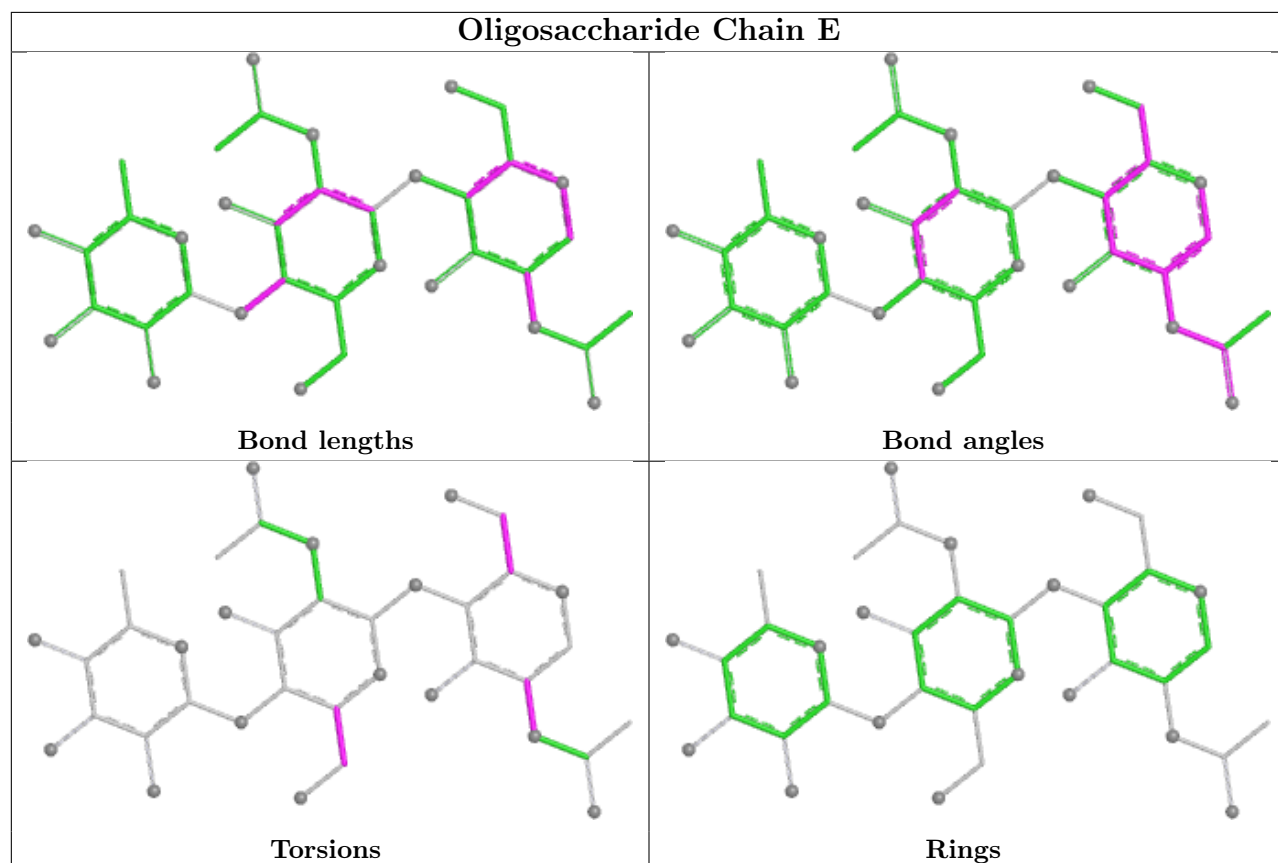
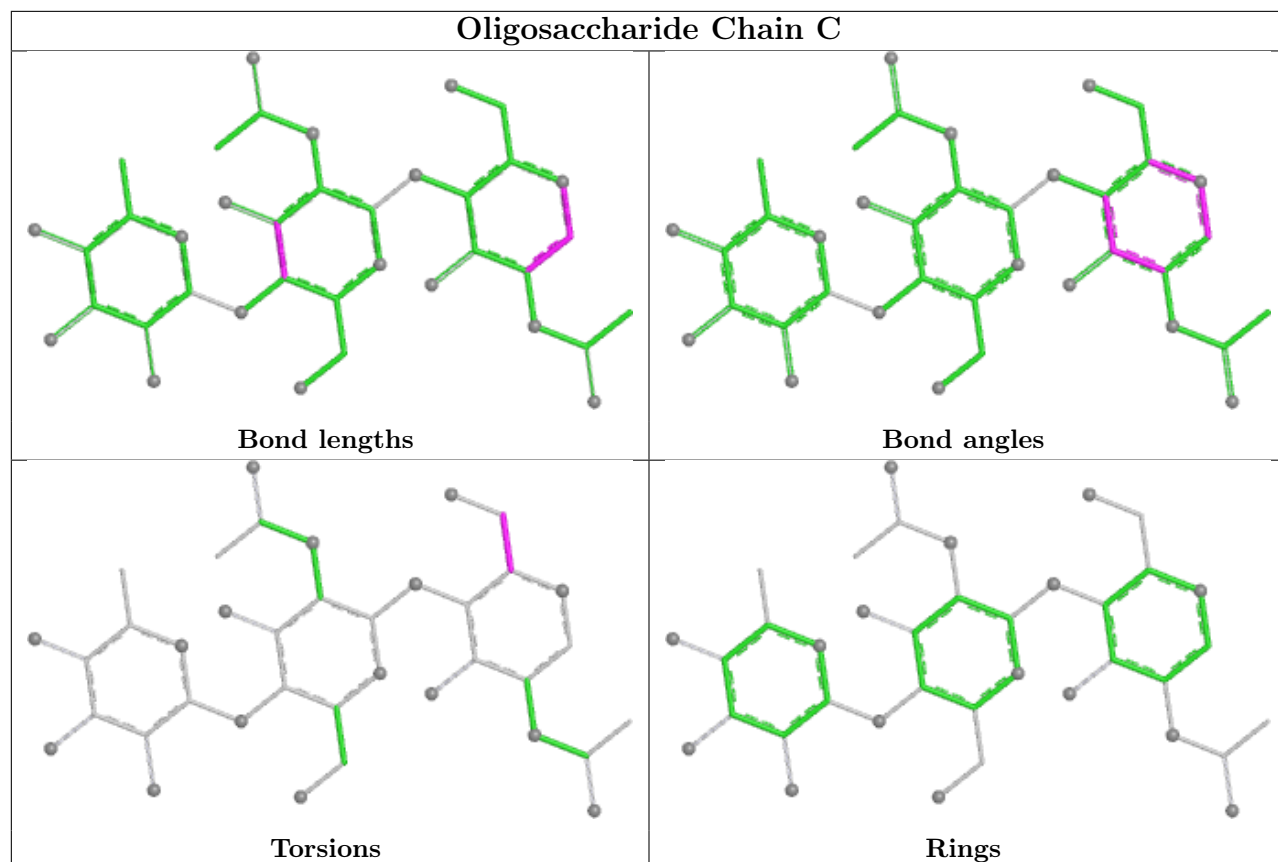
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

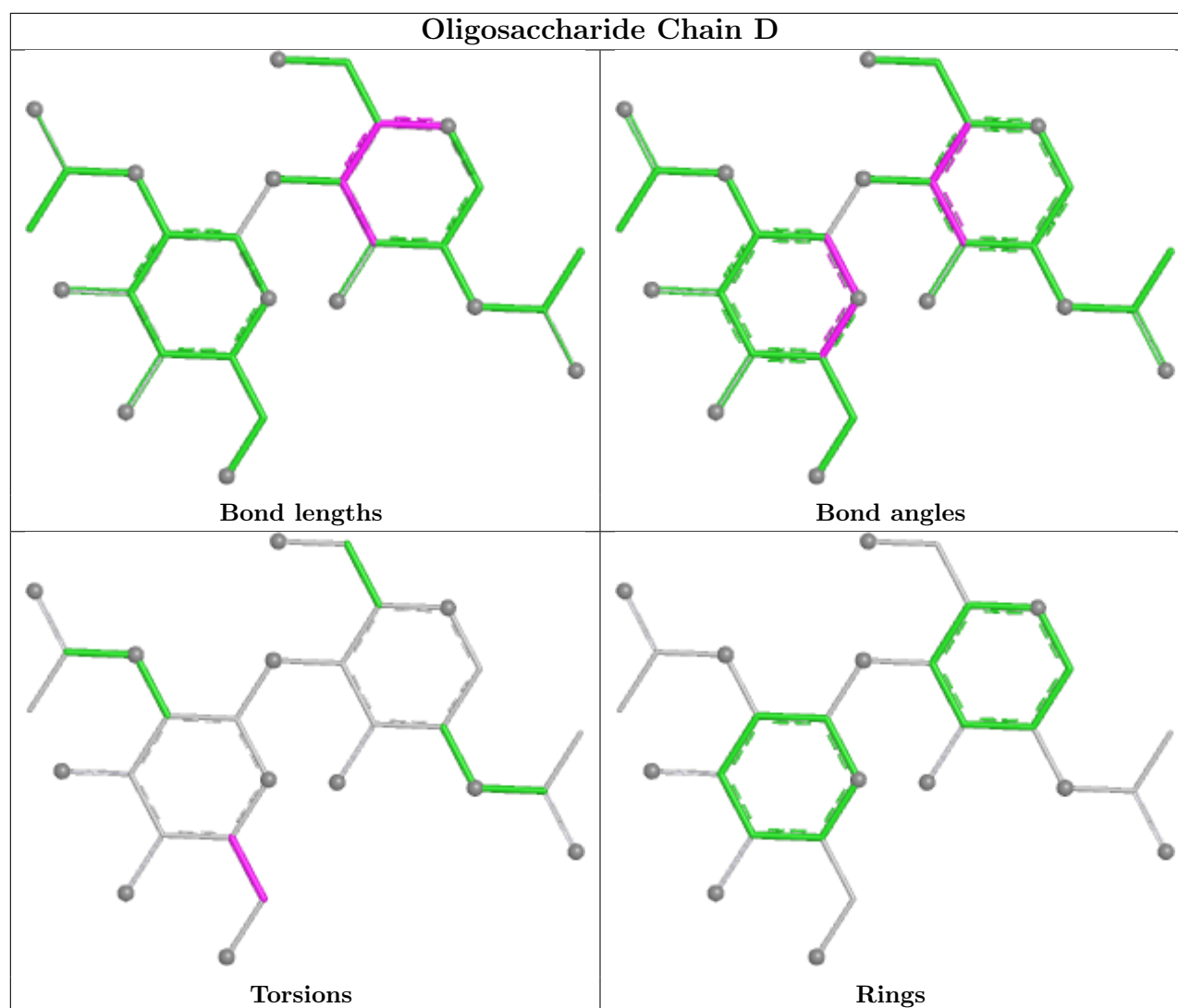
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	FUC	1	0
2	E	1	NAG	2	0
3	D	1	NAG	1	0
2	E	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.





5.6 Ligand geometry [i](#)

6 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	501	-	14,14,15	1.16	1 (7%)	17,19,21	0.90	0
6	PEG	B	703	-	6,6,6	0.16	0	5,5,5	0.09	0
5	EDO	B	704	-	3,3,3	0.56	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	702	-	14,14,15	1.10	1 (7%)	17,19,21	0.90	0
4	NAG	B	701	1	14,14,15	1.79	4 (28%)	17,19,21	1.18	1 (5%)
5	EDO	A	502	-	3,3,3	0.56	0	2,2,2	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	501	-	-	0/6/23/26	0/1/1/1
6	PEG	B	703	-	-	3/4/4/4	-
5	EDO	B	704	-	-	0/1/1/1	-
4	NAG	B	702	-	-	0/6/23/26	0/1/1/1
4	NAG	B	701	1	-	2/6/23/26	0/1/1/1
5	EDO	A	502	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	NAG	C1-C2	3.81	1.57	1.52
4	B	701	NAG	O5-C5	2.65	1.48	1.43
4	B	701	NAG	C3-C2	2.53	1.57	1.52
4	B	702	NAG	C4-C5	2.27	1.57	1.53
4	B	701	NAG	O5-C1	-2.21	1.40	1.43
4	A	501	NAG	C4-C5	2.09	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAG	C4-C3-C2	2.50	114.68	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	NAG	C4-C5-C6-O6
6	B	703	PEG	O2-C3-C4-O4
4	B	701	NAG	O5-C5-C6-O6
6	B	703	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	B	703	PEG	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0
6	B	703	PEG	2	0
4	B	702	NAG	1	0

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 [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	425/483 (87%)	0.20	8 (1%) 66 62	19, 42, 64, 88	1 (0%)
1	B	425/483 (87%)	0.24	9 (2%) 63 59	22, 45, 65, 88	1 (0%)
All	All	850/966 (87%)	0.22	17 (2%) 65 60	19, 44, 65, 88	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	GLY	4.7
1	B	250	THR	4.2
1	A	250	THR	4.0
1	B	396	VAL	4.0
1	A	329	VAL	3.7
1	A	251	PRO	3.2
1	B	251	PRO	3.0
1	B	467	VAL	2.6
1	A	360	GLU	2.3
1	A	436	GLU	2.3
1	A	252	ASP	2.1
1	B	344	HIS	2.1
1	A	51	ILE	2.1
1	B	199	ALA	2.0
1	B	436[A]	GLU	2.0
1	A	337	PRO	2.0
1	B	347	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SNN	B	171	8/8	0.93	0.08	32,35,39,40	0
1	SNN	A	171	8/8	0.95	0.08	32,36,37,38	0

6.3 Carbohydrates

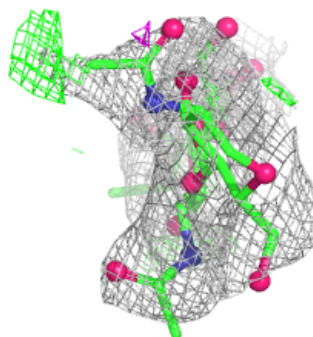
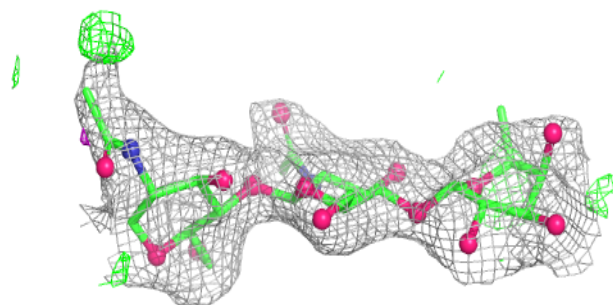
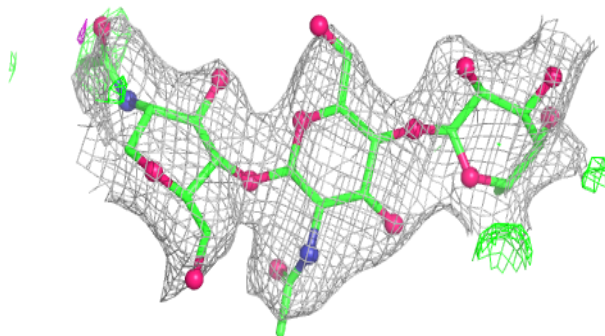
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	E	3	10/11	0.10	0.21	93,97,99,99	0
2	FUC	C	3	10/11	0.54	0.17	97,98,99,100	0
2	NAG	C	1	14/15	0.75	0.17	75,80,82,83	0
2	NAG	E	2	14/15	0.79	0.13	71,75,82,88	0
2	NAG	C	2	14/15	0.80	0.13	85,86,90,94	0
2	NAG	E	1	14/15	0.86	0.15	55,57,62,65	0
3	NAG	D	2	14/15	0.86	0.10	53,57,60,60	0
3	NAG	D	1	14/15	0.94	0.08	36,39,48,48	0

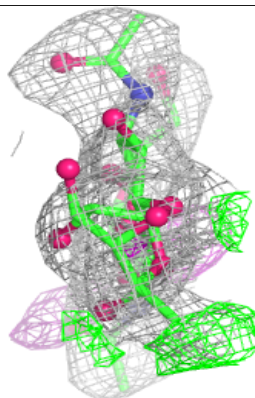
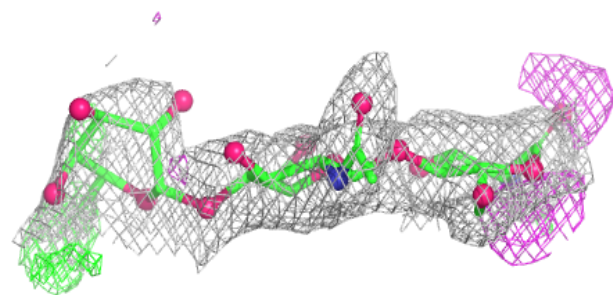
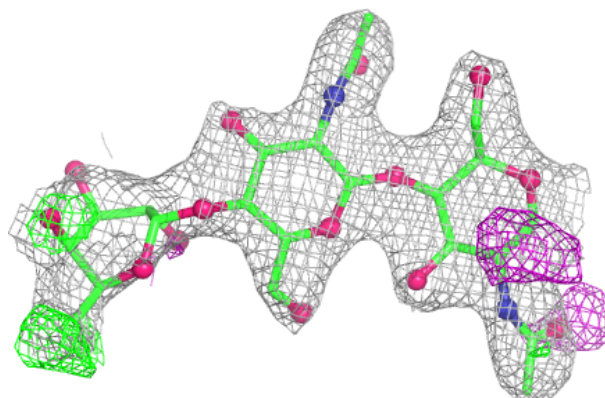
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

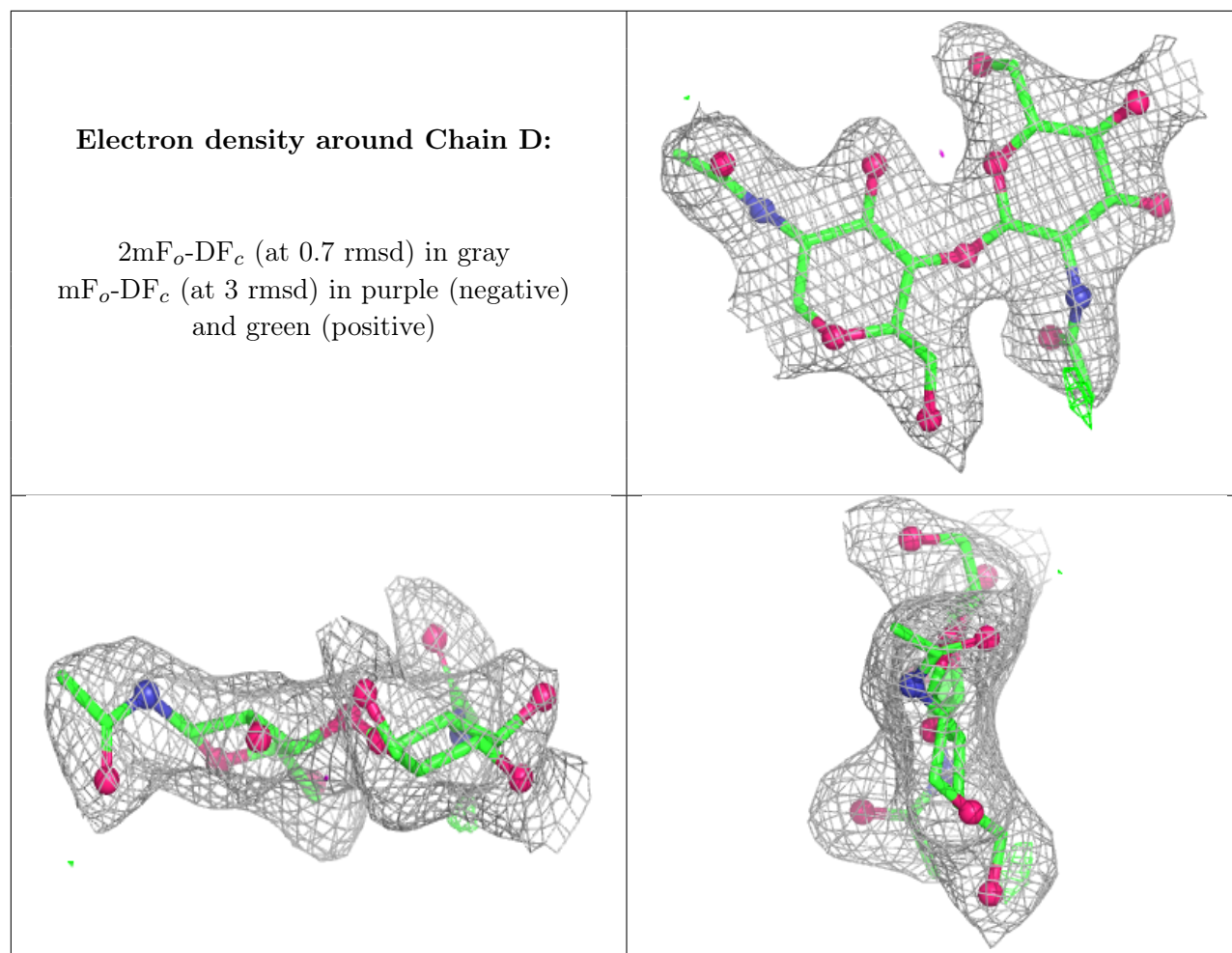
Electron density around Chain C:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	702	14/15	0.70	0.19	106,109,111,111	0
4	NAG	A	501	14/15	0.71	0.20	104,106,109,109	0
4	NAG	B	701	14/15	0.77	0.15	76,80,81,82	0
5	EDO	B	704	4/4	0.79	0.16	70,71,71,71	0
5	EDO	A	502	4/4	0.82	0.15	53,54,54,55	0
6	PEG	B	703	7/7	0.84	0.13	56,59,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.