



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 07:27 AM EDT

PDB ID : 7RDW / pdb_00007rdw
Title : Crystal Structure of FH1 Fab bound to HXb2 HIV-1 gp120 core
Authors : Weidle, C.; Pancera, M.
Deposited on : 2021-07-12
Resolution : 3.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

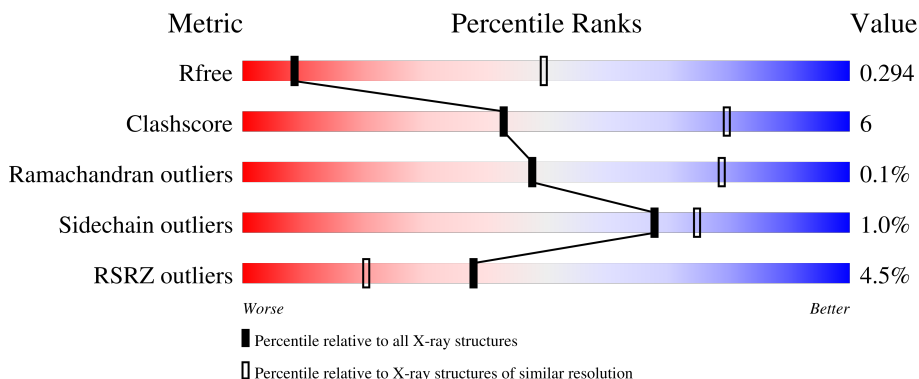
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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.



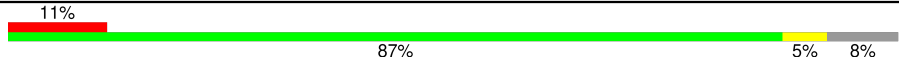

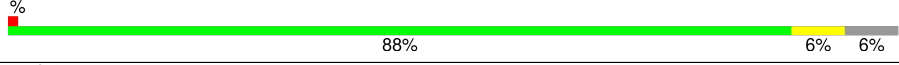

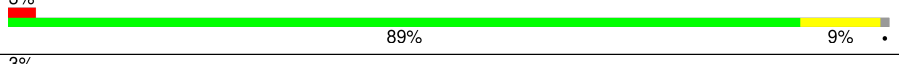
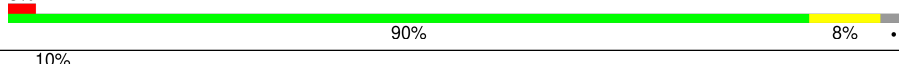


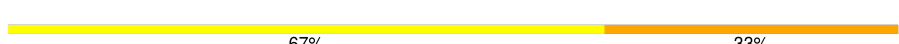
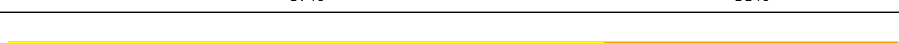
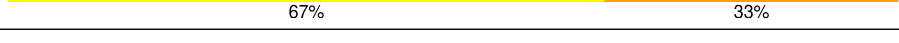
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	C	373	 2% 75% 12% 13%
1	D	373	 2% 71% 17% 12%
1	M	373	 % 72% 16% 12%
1	N	373	 2% 75% 12% 12%
2	G	225	 7% 81% 12% 7%

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Mol	Chain	Length	Quality of chain
2	U	225	
3	H	225	
3	Q	225	
4	I	211	
4	L	211	
4	R	211	
4	V	211	
5	O	3	
5	c	3	
5	m	3	
5	y	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	O	2	X	-	-	-
5	NAG	c	2	X	-	-	-
5	BMA	c	3	X	-	-	-
5	NAG	m	2	X	-	-	-
5	NAG	y	2	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21960 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 Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	326	Total 2390	C 1500	N 416	O 451	S 23	0	0	0
1	D	329	Total 2440	C 1524	N 428	O 466	S 22	0	0	0
1	M	328	Total 2405	C 1509	N 417	O 456	S 23	0	0	0
1	N	329	Total 2413	C 1513	N 423	O 454	S 23	0	0	0

- Molecule 2 is a protein called FH1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	210	Total 1483	C 932	N 260	O 283	S 8	0	0	0
2	U	208	Total 1454	C 915	N 258	O 273	S 8	0	0	0

- Molecule 3 is a protein called FH1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	209	Total 1502	C 953	N 262	O 279	S 8	0	0	0
3	Q	212	Total 1595	C 1010	N 271	O 306	S 8	0	0	0

- Molecule 4 is a protein called FH1 Fab Light Chain.

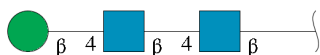
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	209	Total 1391	C 861	N 255	O 270	S 5	0	0	0
4	L	208	Total 1424	C 901	N 246	O 272	S 5	0	0	0

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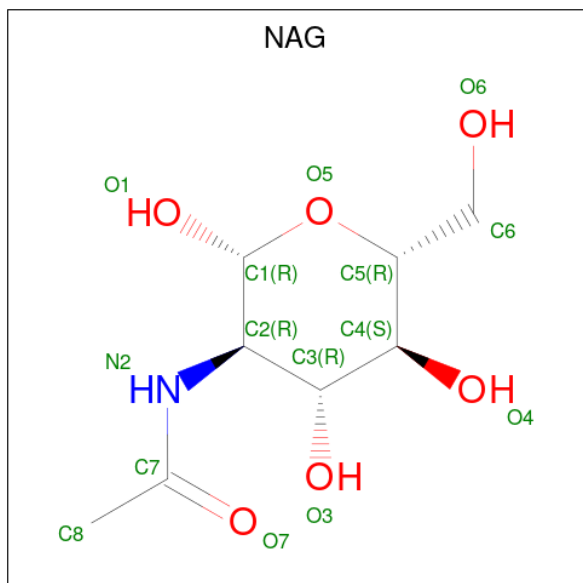
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	R	205	Total 1439	C 901	N 244	O 289	S 5	0	0	0
4	V	200	Total 1344	C 838	N 240	O 261	S 5	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	O	3	Total 39	C 22	N 2	O 15	0	0	0
5	c	3	Total 39	C 22	N 2	O 15	0	0	0
5	m	3	Total 39	C 22	N 2	O 15	0	0	0
5	y	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



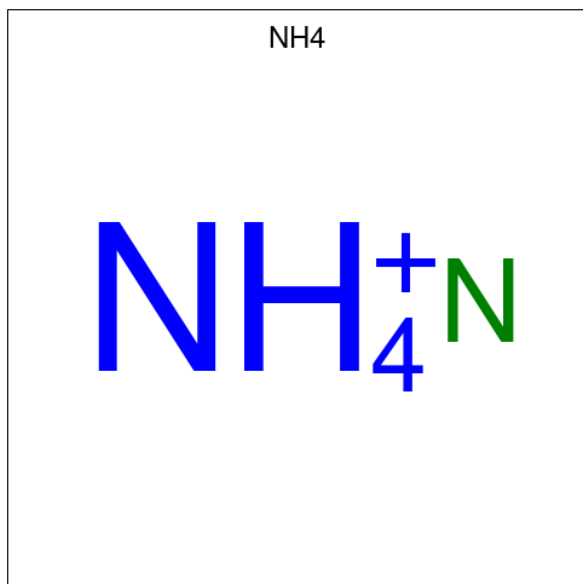
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1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

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

- Molecule 7 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



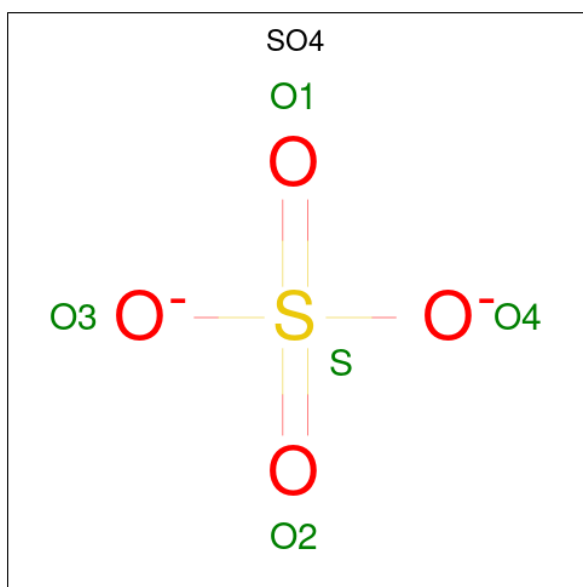
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	N	0	0
			1	1		
7	C	1	Total	N	0	0
			1	1		
7	D	1	Total	N	0	0
			1	1		
7	I	1	Total	N	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	N	1	Total C O 4 2 2	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	M	1	Total O S 5 4 1	0	0

- Molecule 10 is water.

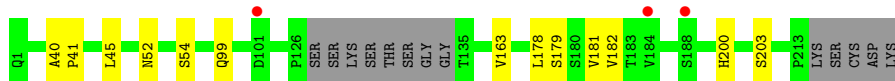
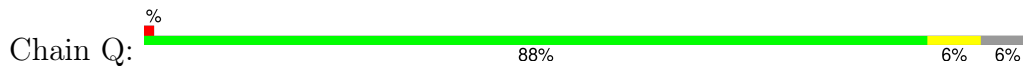
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	11	Total O 11 11	0	0
10	D	15	Total O 15 15	0	0
10	G	8	Total O 8 8	0	0
10	H	4	Total O 4 4	0	0
10	I	1	Total O 1 1	0	0
10	L	5	Total O 5 5	0	0
10	M	12	Total O 12 12	0	0
10	N	16	Total O 16 16	0	0
10	Q	2	Total O 2 2	0	0

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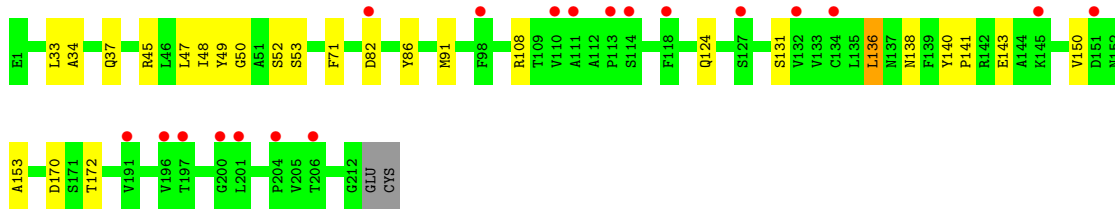
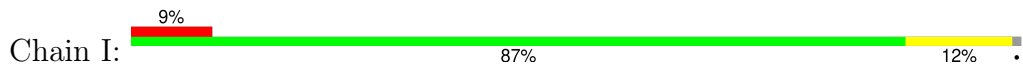
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	R	4	Total O 4 4	0	0
10	U	7	Total O 7 7	0	0
10	V	4	Total O 4 4	0	0

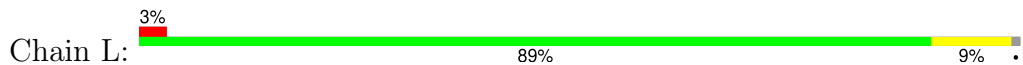
- Molecule 3: FH1 Fab Heavy Chain



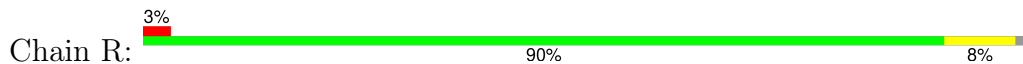
- Molecule 4: FH1 Fab Light Chain



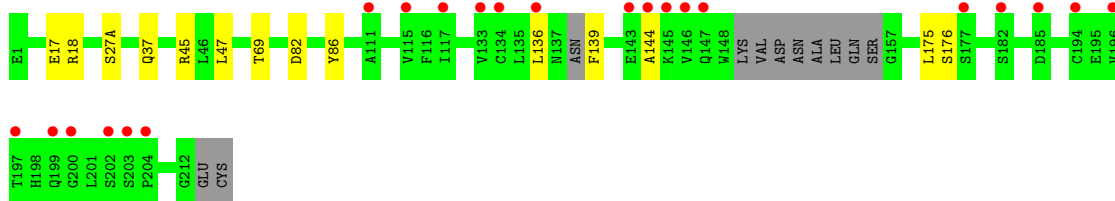
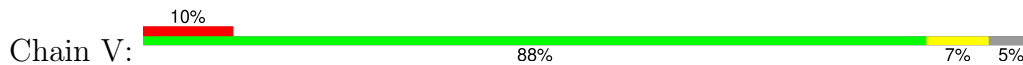
- Molecule 4: FH1 Fab Light Chain



- Molecule 4: FH1 Fab Light Chain



- Molecule 4: FH1 Fab Light Chain



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  67% 33%

MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  67% 33%

MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.36Å 106.27Å 113.22Å 67.57° 76.67° 60.99°	Depositor
Resolution (Å)	50.18 – 3.55 50.18 – 3.55	Depositor EDS
% Data completeness (in resolution range)	76.8 (50.18-3.55) 77.0 (50.18-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.260 , 0.295 0.262 , 0.294	Depositor DCC
R_{free} test set	1842 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	21960	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: EDO, BMA, SO4, PCA, NH4, 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	C	0.09	0/2440	0.23	0/3333
1	D	0.12	0/2489	0.26	0/3393
1	M	0.09	0/2455	0.24	0/3358
1	N	0.16	0/2462	0.37	3/3361 (0.1%)
2	G	0.14	0/1518	0.27	0/2084
2	U	0.12	0/1486	0.27	0/2039
3	H	0.08	0/1547	0.22	0/2120
3	Q	0.08	0/1641	0.21	0/2245
4	I	0.10	0/1416	0.24	0/1939
4	L	0.08	0/1456	0.23	0/1996
4	R	0.08	0/1473	0.22	0/2019
4	V	0.08	0/1371	0.23	0/1878
All	All	0.11	0/21754	0.26	3/29765 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	74	CYS	CA-CB-SG	-9.96	91.49	114.40
1	N	73	ALA	CA-C-N	-5.39	113.48	122.21
1	N	73	ALA	C-N-CA	-5.39	113.48	122.21

There are no chirality outliers.

There are no planarity outliers.

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	C	2390	0	2159	35	0
1	D	2440	0	2222	51	0
1	M	2405	0	2180	38	0
1	N	2413	0	2183	40	0
2	G	1483	0	1225	17	0
2	U	1454	0	1203	15	0
3	H	1502	0	1276	12	0
3	Q	1595	0	1475	10	0
4	I	1391	0	1145	17	0
4	L	1424	0	1194	11	0
4	R	1439	0	1202	11	1
4	V	1344	0	1107	7	1
5	O	39	0	34	3	0
5	c	39	0	34	2	0
5	m	39	0	34	1	0
5	y	39	0	34	5	0
6	C	98	0	91	6	0
6	D	70	0	65	1	0
6	M	84	0	78	2	0
6	N	140	0	130	3	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
8	C	8	0	12	0	0
8	D	4	0	6	0	0
8	H	8	0	12	0	0
8	N	4	0	6	0	0
9	C	5	0	0	0	0
9	D	5	0	0	1	0
9	M	5	0	0	0	0
10	C	11	0	0	1	0
10	D	15	0	0	0	0
10	G	8	0	0	0	0
10	H	4	0	0	1	0
10	I	1	0	0	0	0
10	L	5	0	0	0	0
10	M	12	0	0	0	0
10	N	16	0	0	1	0
10	Q	2	0	0	0	0
10	R	4	0	0	0	0
10	U	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	V	4	0	0	0	0
All	All	21960	0	19107	255	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 6.

The worst 5 of 255 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:D:57:ASP:OD1	1:D:77:THR:OG1	1.83	0.96
1:N:249:HIS:HD1	1:N:486:TYR:HH	1.19	0.90
1:M:444:ARG:O	5:m:2:NAG:O3	1.90	0.89
1:M:358:THR:HG1	1:M:466:GLU:N	1.71	0.89
3:H:200:HIS:HD1	3:H:203:SER:HG	1.16	0.88

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)
4:R:57:GLY:O	4:V:45:ARG:NH1[1_565]	2.14	0.06

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	C	318/373 (85%)	302 (95%)	16 (5%)	0	100	100
1	D	319/373 (86%)	299 (94%)	20 (6%)	0	100	100
1	M	320/373 (86%)	302 (94%)	17 (5%)	1 (0%)	36	65
1	N	319/373 (86%)	305 (96%)	14 (4%)	0	100	100
2	G	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U	204/225 (91%)	191 (94%)	13 (6%)	0	100	100
3	H	205/225 (91%)	195 (95%)	10 (5%)	0	100	100
3	Q	208/225 (92%)	202 (97%)	6 (3%)	0	100	100
4	I	207/211 (98%)	193 (93%)	14 (7%)	0	100	100
4	L	204/211 (97%)	189 (93%)	14 (7%)	1 (0%)	24	57
4	R	201/211 (95%)	182 (90%)	19 (10%)	0	100	100
4	V	194/211 (92%)	183 (94%)	11 (6%)	0	100	100
All	All	2905/3236 (90%)	2740 (94%)	162 (6%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	2	VAL
4	L	91	MET
1	M	269	GLU

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	C	244/328 (74%)	240 (98%)	4 (2%)	55	69
1	D	254/328 (77%)	250 (98%)	4 (2%)	55	69
1	M	247/328 (75%)	244 (99%)	3 (1%)	63	73
1	N	247/328 (75%)	244 (99%)	3 (1%)	63	73
2	G	124/190 (65%)	122 (98%)	2 (2%)	55	69
2	U	119/190 (63%)	118 (99%)	1 (1%)	73	77
3	H	130/191 (68%)	129 (99%)	1 (1%)	73	77
3	Q	166/191 (87%)	166 (100%)	0	100	100
4	I	108/184 (59%)	107 (99%)	1 (1%)	70	76
4	L	118/184 (64%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	129/184 (70%)	129 (100%)	0	100	100
4	V	109/184 (59%)	109 (100%)	0	100	100
All	All	1995/2810 (71%)	1976 (99%)	19 (1%)	68	75

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	491	ILE
1	N	353	PHE
2	U	99	GLN
1	N	74	CYS
2	G	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	U	52	ASN
2	U	164	HIS
4	V	38	GLN
4	L	38	GLN
3	Q	39	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](#)

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
2	PCA	U	1	2	7,8,9	1.86	1 (14%)	9,10,12	1.60	4 (44%)
2	PCA	G	1	2	7,8,9	1.81	1 (14%)	9,10,12	1.75	4 (44%)

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	PCA	U	1	2	-	0/0/11/13	0/1/1/1
2	PCA	G	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	1	PCA	CD-N	4.80	1.46	1.34
2	G	1	PCA	CD-N	4.64	1.46	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	PCA	CB-CA-C	-2.80	108.82	112.66
2	U	1	PCA	CB-CA-N	2.36	109.74	103.24
2	U	1	PCA	OE-CD-CG	-2.27	122.67	126.72
2	G	1	PCA	OE-CD-CG	-2.25	122.70	126.72
2	U	1	PCA	O-C-CA	-2.17	119.20	124.77

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

12 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
5	NAG	O	1	1,5	14,14,15	2.07	6 (42%)	17,19,21	3.96	6 (35%)
5	NAG	O	2	5	14,14,15	2.00	5 (35%)	17,19,21	4.69	10 (58%)
5	BMA	O	3	5	11,11,12	0.93	1 (9%)	15,15,17	2.24	4 (26%)
5	NAG	c	1	1,5	14,14,15	2.06	5 (35%)	17,19,21	3.68	5 (29%)
5	NAG	c	2	5	14,14,15	2.18	5 (35%)	17,19,21	4.21	7 (41%)
5	BMA	c	3	5	11,11,12	1.54	2 (18%)	15,15,17	3.99	7 (46%)
5	NAG	m	1	1,5	14,14,15	2.08	5 (35%)	17,19,21	3.94	5 (29%)
5	NAG	m	2	5	14,14,15	1.76	4 (28%)	17,19,21	4.49	7 (41%)
5	BMA	m	3	5	11,11,12	0.83	0	15,15,17	2.14	6 (40%)
5	NAG	y	1	1,5	14,14,15	1.99	5 (35%)	17,19,21	4.22	6 (35%)
5	NAG	y	2	5	14,14,15	1.91	5 (35%)	17,19,21	4.84	11 (64%)
5	BMA	y	3	5	11,11,12	1.62	2 (18%)	15,15,17	1.18	1 (6%)

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	O	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	c	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	c	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	m	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	m	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	m	3	5	-	2/2/19/22	0/1/1/1
5	NAG	y	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	y	2	5	1/1/5/7	3/6/23/26	0/1/1/1
5	BMA	y	3	5	-	1/2/19/22	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2	NAG	O5-C5	4.25	1.51	1.43
5	c	2	NAG	C7-N2	4.22	1.48	1.34
5	y	2	NAG	C7-N2	4.10	1.47	1.34
5	O	2	NAG	C7-N2	4.00	1.47	1.34
5	m	1	NAG	C7-N2	3.98	1.47	1.34

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	y	1	NAG	O5-C1-C2	14.99	134.48	111.29
5	y	2	NAG	O5-C1-C2	14.94	134.40	111.29
5	O	2	NAG	O5-C1-C2	14.77	134.14	111.29
5	O	1	NAG	O5-C1-C2	14.27	133.37	111.29
5	m	1	NAG	O5-C1-C2	14.17	133.22	111.29

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	2	NAG	C1
5	c	2	NAG	C1
5	c	3	BMA	C1
5	m	2	NAG	C1
5	y	2	NAG	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	2	NAG	C3-C2-N2-C7
5	c	3	BMA	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
5	m	3	BMA	C4-C5-C6-O6
5	c	3	BMA	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

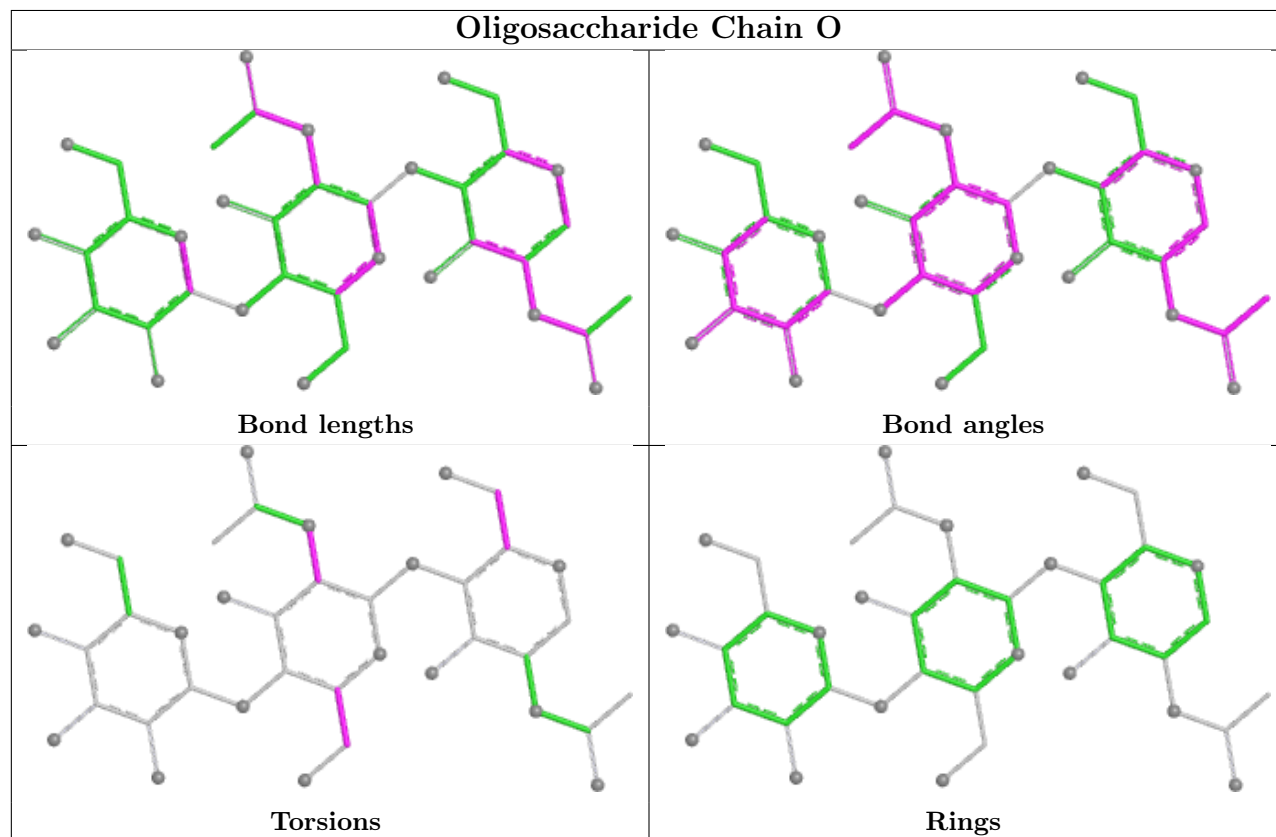
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	c	1	NAG	2	0
5	y	1	NAG	4	0
5	m	2	NAG	1	0
5	y	2	NAG	1	0
5	O	2	NAG	1	0

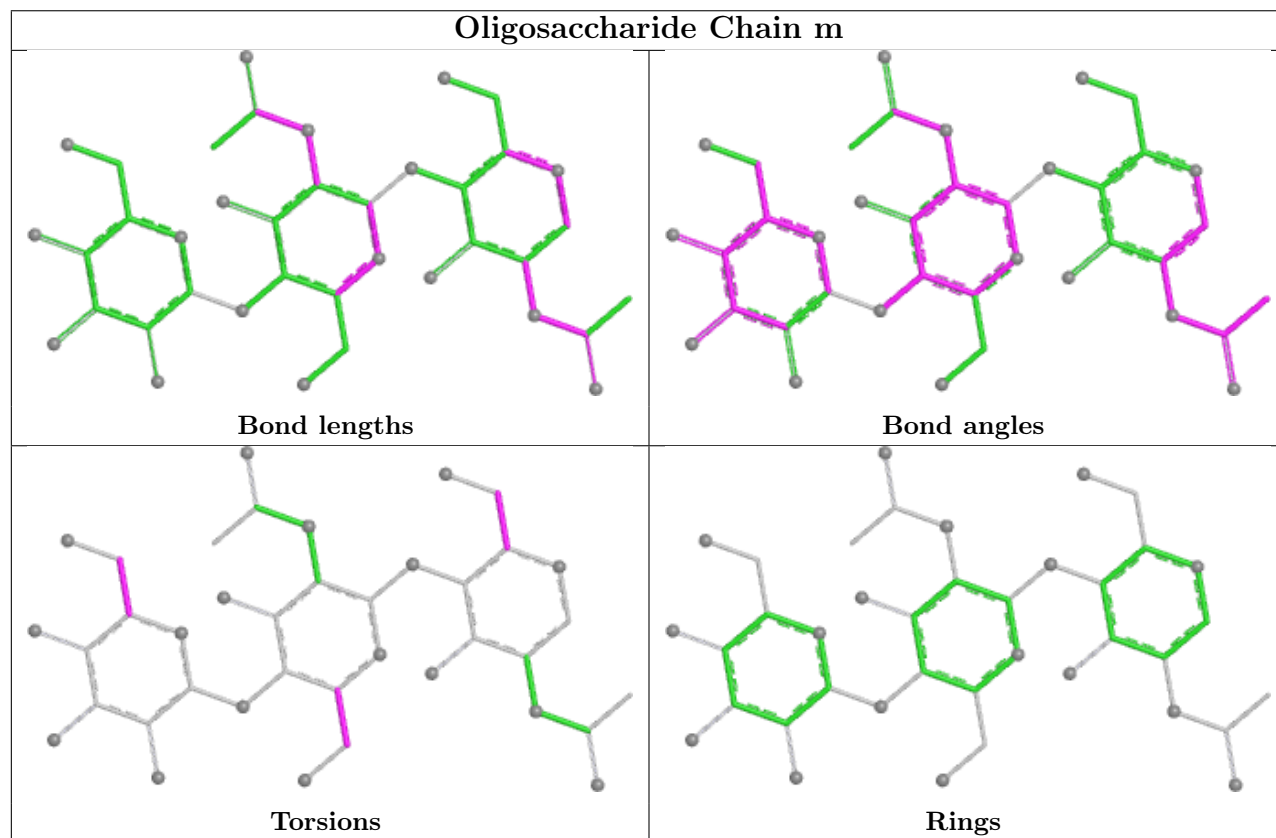
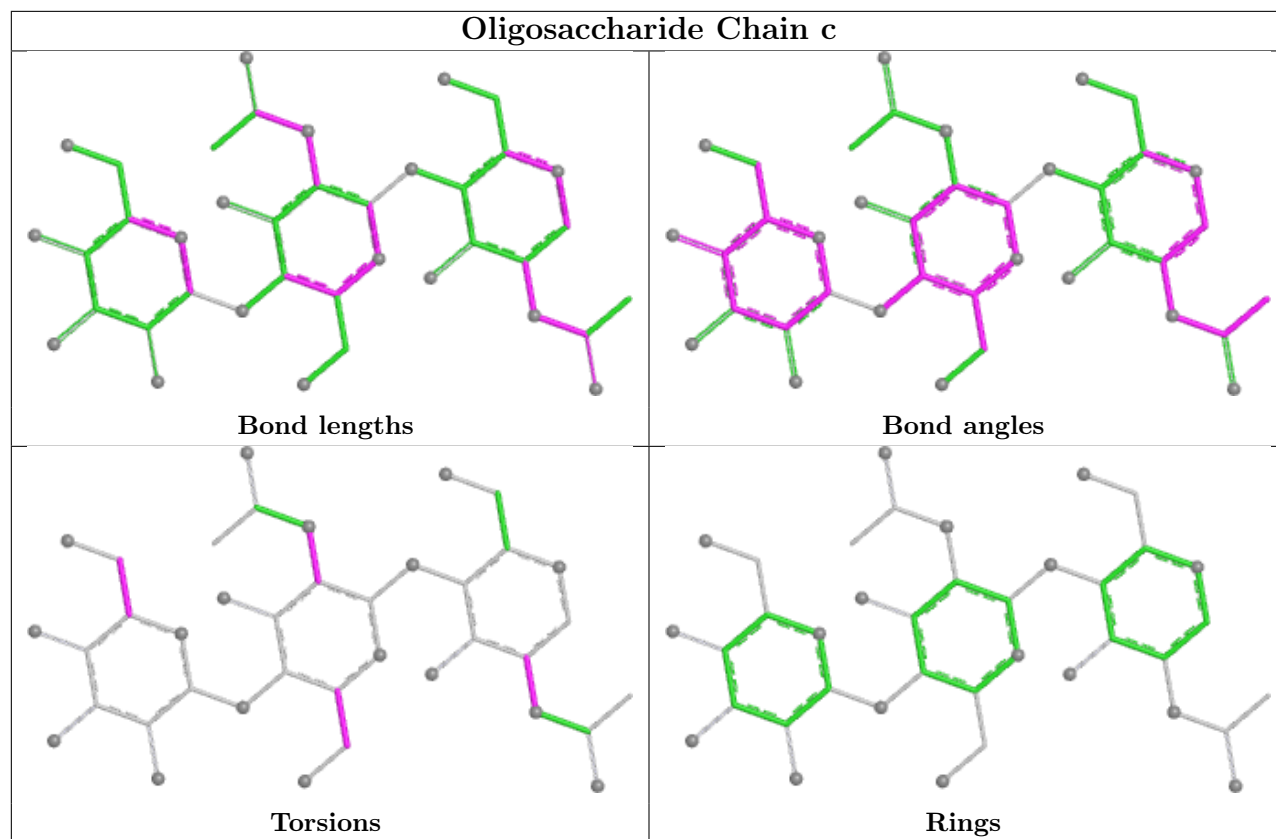
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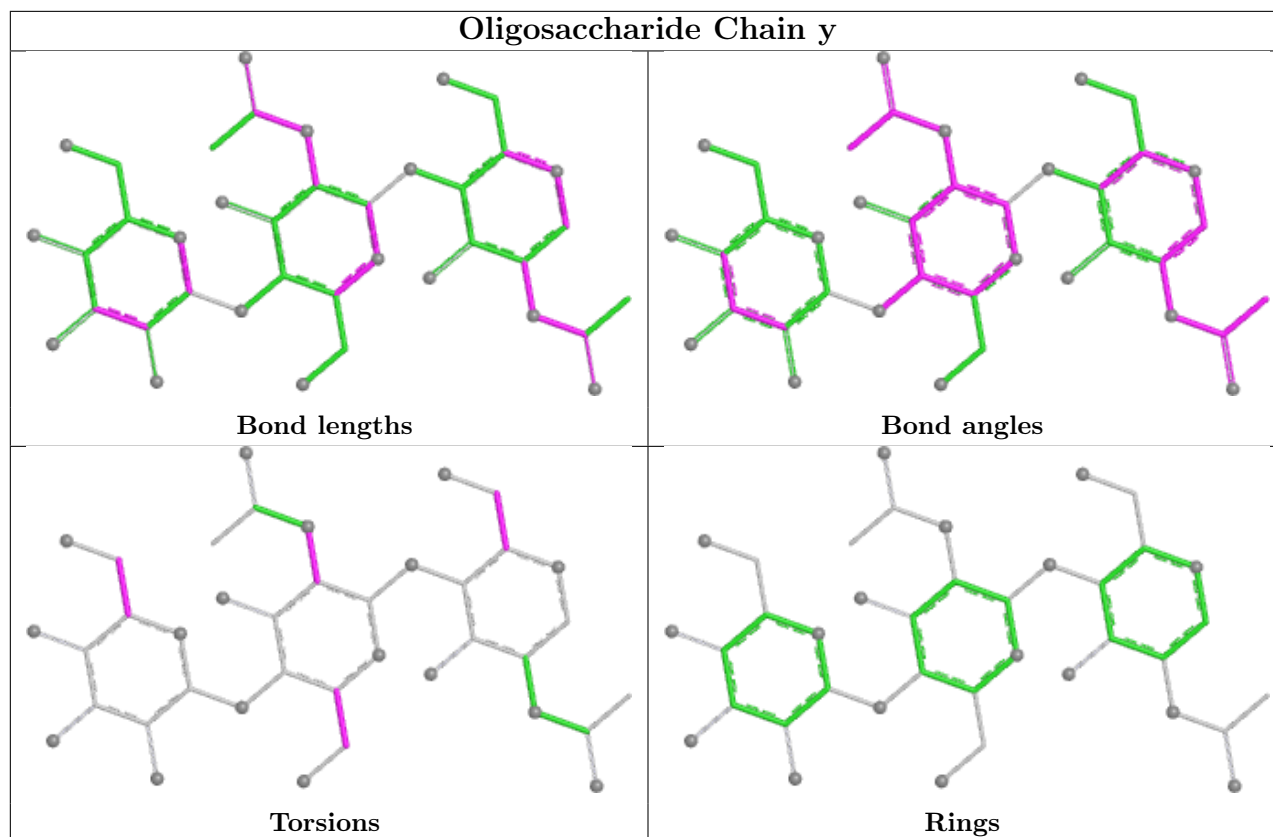
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	2	0

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](#)

Of 41 ligands modelled in this entry, 4 are modelled with single atom - leaving 37 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	NAG	N	605	1	14,14,15	1.97	3 (21%)	17,19,21	1.46	4 (23%)
6	NAG	N	606	1	14,14,15	2.10	5 (35%)	17,19,21	1.93	4 (23%)
6	NAG	M	606	1	14,14,15	1.98	3 (21%)	17,19,21	1.23	2 (11%)
8	EDO	C	611	-	3,3,3	0.43	0	2,2,2	0.35	0
6	NAG	M	605	1	14,14,15	1.97	3 (21%)	17,19,21	1.05	1 (5%)
6	NAG	C	601	1	14,14,15	2.19	5 (35%)	17,19,21	2.34	5 (29%)
6	NAG	C	603	1	14,14,15	2.01	5 (35%)	17,19,21	1.51	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	604	1	14,14,15	1.95	3 (21%)	17,19,21	1.58	4 (23%)
9	SO4	C	612	-	4,4,4	0.23	0	6,6,6	0.08	0
6	NAG	N	610	1	14,14,15	2.03	3 (21%)	17,19,21	1.36	3 (17%)
9	SO4	M	607	-	4,4,4	0.23	0	6,6,6	0.10	0
6	NAG	N	604	1	14,14,15	2.03	5 (35%)	17,19,21	1.44	3 (17%)
6	NAG	N	601	1	14,14,15	2.06	4 (28%)	17,19,21	2.09	6 (35%)
6	NAG	M	601	1	14,14,15	2.00	3 (21%)	17,19,21	1.67	4 (23%)
6	NAG	N	603	1	14,14,15	2.11	5 (35%)	17,19,21	1.54	3 (17%)
6	NAG	N	609	1	14,14,15	1.96	3 (21%)	17,19,21	1.10	2 (11%)
6	NAG	C	602	1	14,14,15	1.94	3 (21%)	17,19,21	1.22	2 (11%)
8	EDO	C	610	-	3,3,3	0.43	0	2,2,2	0.34	0
6	NAG	N	607	1	14,14,15	2.02	4 (28%)	17,19,21	1.20	2 (11%)
8	EDO	H	302	-	3,3,3	0.42	0	2,2,2	0.33	0
8	EDO	H	301	-	3,3,3	0.42	0	2,2,2	0.34	0
6	NAG	N	602	1	14,14,15	2.02	3 (21%)	17,19,21	1.34	3 (17%)
6	NAG	M	602	1	14,14,15	2.05	4 (28%)	17,19,21	1.22	1 (5%)
8	EDO	D	607	-	3,3,3	0.42	0	2,2,2	0.34	0
6	NAG	M	603	1	14,14,15	1.95	3 (21%)	17,19,21	1.02	1 (5%)
6	NAG	N	608	1	14,14,15	2.12	4 (28%)	17,19,21	1.44	3 (17%)
8	EDO	N	611	-	3,3,3	0.43	0	2,2,2	0.35	0
6	NAG	D	605	1	14,14,15	2.00	5 (35%)	17,19,21	1.08	1 (5%)
9	SO4	D	608	-	4,4,4	0.22	0	6,6,6	0.08	0
6	NAG	C	607	1	14,14,15	1.93	3 (21%)	17,19,21	1.12	2 (11%)
6	NAG	C	604	1	14,14,15	2.01	5 (35%)	17,19,21	1.81	6 (35%)
6	NAG	D	602	1	14,14,15	2.14	4 (28%)	17,19,21	1.83	4 (23%)
6	NAG	D	601	1	14,14,15	1.96	3 (21%)	17,19,21	1.46	4 (23%)
6	NAG	D	603	1	14,14,15	1.99	4 (28%)	17,19,21	1.53	4 (23%)
6	NAG	C	606	1	14,14,15	1.99	3 (21%)	17,19,21	1.14	2 (11%)
6	NAG	C	605	1	14,14,15	1.97	4 (28%)	17,19,21	1.76	4 (23%)
6	NAG	D	604	1	14,14,15	1.97	3 (21%)	17,19,21	1.54	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	605	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	606	1	-	0/6/23/26	0/1/1/1
6	NAG	M	606	1	-	1/6/23/26	0/1/1/1
8	EDO	C	611	-	-	0/1/1/1	-
6	NAG	M	605	1	-	0/6/23/26	0/1/1/1
6	NAG	C	601	1	-	6/6/23/26	0/1/1/1
6	NAG	C	603	1	-	0/6/23/26	0/1/1/1
6	NAG	M	604	1	-	2/6/23/26	0/1/1/1
6	NAG	N	610	1	-	0/6/23/26	0/1/1/1
6	NAG	N	604	1	-	0/6/23/26	0/1/1/1
6	NAG	N	601	1	-	4/6/23/26	0/1/1/1
6	NAG	M	601	1	-	6/6/23/26	0/1/1/1
6	NAG	N	603	1	-	2/6/23/26	0/1/1/1
6	NAG	N	609	1	-	0/6/23/26	0/1/1/1
6	NAG	C	602	1	-	0/6/23/26	0/1/1/1
8	EDO	C	610	-	-	0/1/1/1	-
6	NAG	N	607	1	-	1/6/23/26	0/1/1/1
8	EDO	H	302	-	-	0/1/1/1	-
8	EDO	H	301	-	-	0/1/1/1	-
6	NAG	N	602	1	-	2/6/23/26	0/1/1/1
6	NAG	M	602	1	-	0/6/23/26	0/1/1/1
8	EDO	D	607	-	-	0/1/1/1	-
6	NAG	M	603	1	-	0/6/23/26	0/1/1/1
6	NAG	N	608	1	-	2/6/23/26	0/1/1/1
8	EDO	N	611	-	-	0/1/1/1	-
6	NAG	D	605	1	-	0/6/23/26	0/1/1/1
6	NAG	C	607	1	-	0/6/23/26	0/1/1/1
6	NAG	C	604	1	-	1/6/23/26	0/1/1/1
6	NAG	D	602	1	-	0/6/23/26	0/1/1/1
6	NAG	D	601	1	-	2/6/23/26	0/1/1/1
6	NAG	D	603	1	-	1/6/23/26	0/1/1/1
6	NAG	C	606	1	-	2/6/23/26	0/1/1/1
6	NAG	C	605	1	-	1/6/23/26	0/1/1/1
6	NAG	D	604	1	-	1/6/23/26	0/1/1/1

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	602	NAG	O5-C1	4.71	1.51	1.43
6	C	601	NAG	O5-C1	4.71	1.51	1.43
6	N	606	NAG	O5-C1	4.66	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	603	NAG	O5-C1	4.63	1.51	1.43
6	N	608	NAG	O5-C1	4.62	1.51	1.43

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C1-O5-C5	5.64	119.75	112.19
6	N	606	NAG	C1-O5-C5	5.29	119.27	112.19
6	M	601	NAG	C8-C7-N2	4.95	124.33	116.12
6	N	601	NAG	C8-C7-N2	4.87	124.19	116.12
6	C	601	NAG	C8-C7-N2	4.68	123.88	116.12

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	601	NAG	C1-C2-N2-C7
6	N	603	NAG	O5-C5-C6-O6
6	D	601	NAG	O5-C5-C6-O6
6	N	608	NAG	O5-C5-C6-O6
6	M	601	NAG	O5-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	605	NAG	1	0
6	M	606	NAG	1	0
6	C	601	NAG	3	0
6	C	603	NAG	1	0
6	N	604	NAG	1	0
6	N	601	NAG	1	0
6	C	602	NAG	1	0
6	M	602	NAG	1	0
9	D	608	SO4	1	0
6	D	601	NAG	1	0
6	C	606	NAG	1	0

5.7 Other polymers [i](#)

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	C	326/373 (87%)	0.51	8 (2%) 58 33	30, 62, 95, 128	0
1	D	329/373 (88%)	0.41	9 (2%) 56 31	26, 60, 89, 114	0
1	M	328/373 (87%)	0.44	5 (1%) 72 44	27, 60, 93, 106	0
1	N	329/373 (88%)	0.52	8 (2%) 59 33	29, 62, 92, 117	0
2	G	209/225 (92%)	0.72	15 (7%) 21 13	36, 65, 130, 141	0
2	U	207/225 (92%)	0.79	24 (11%) 9 7	35, 60, 164, 172	0
3	H	209/225 (92%)	0.47	9 (4%) 40 21	29, 59, 117, 137	0
3	Q	212/225 (94%)	0.44	3 (1%) 73 45	35, 62, 100, 114	0
4	I	209/211 (99%)	0.80	19 (9%) 15 9	37, 87, 143, 152	0
4	L	208/211 (98%)	0.56	6 (2%) 53 29	31, 73, 123, 127	0
4	R	205/211 (97%)	0.50	6 (2%) 53 29	32, 74, 108, 121	0
4	V	200/211 (94%)	0.85	22 (11%) 10 7	32, 81, 169, 186	0
All	All	2971/3236 (91%)	0.56	134 (4%) 38 20	26, 64, 137, 186	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	134	CYS	6.4
2	U	140	CYS	5.2
2	U	152	VAL	4.8
4	I	111	ALA	4.7
4	L	202	SER	4.2

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(Å ²)	Q<0.9
2	PCA	G	1	8/9	0.69	0.17	64,67,78,79	0
2	PCA	U	1	8/9	0.71	0.14	70,77,82,91	0

6.3 Carbohydrates [\(i\)](#)

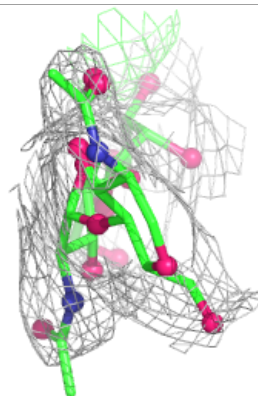
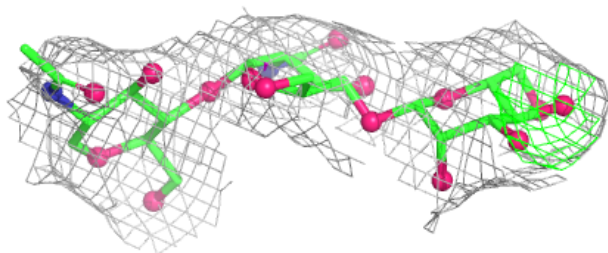
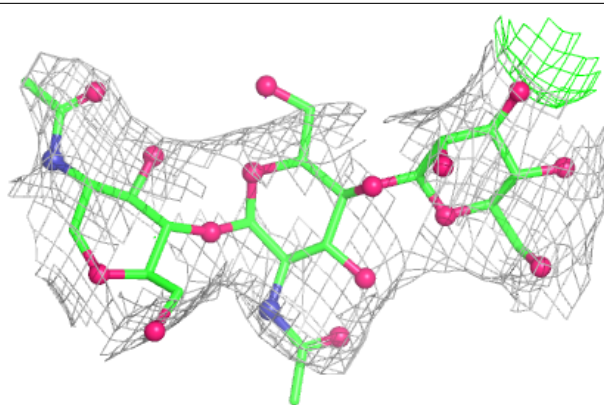
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	O	3	11/12	0.70	0.12	49,56,70,84	0
5	NAG	O	2	14/15	0.84	0.17	54,65,74,83	0
5	NAG	O	1	14/15	0.89	0.11	46,54,62,67	0
5	NAG	c	1	14/15	-	-	46,50,64,66	0
5	NAG	c	2	14/15	-	-	60,68,82,85	0
5	BMA	c	3	11/12	-	-	55,70,80,84	0
5	NAG	m	1	14/15	-	-	51,64,72,74	0
5	NAG	m	2	14/15	-	-	59,74,81,86	0
5	BMA	m	3	11/12	-	-	50,62,72,74	0
5	NAG	y	1	14/15	-	-	54,66,77,78	0
5	NAG	y	2	14/15	-	-	58,70,79,86	0
5	BMA	y	3	11/12	-	-	56,61,78,87	0

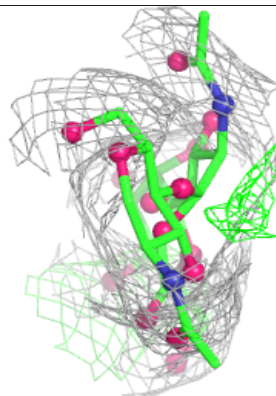
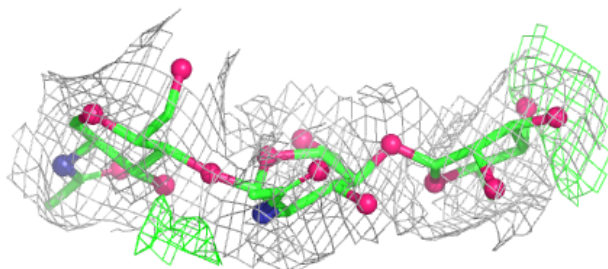
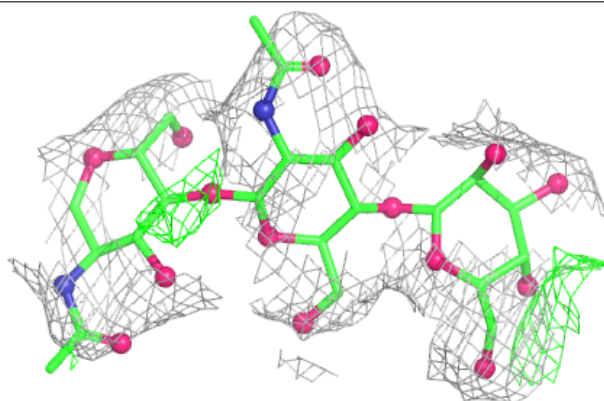
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain O:

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

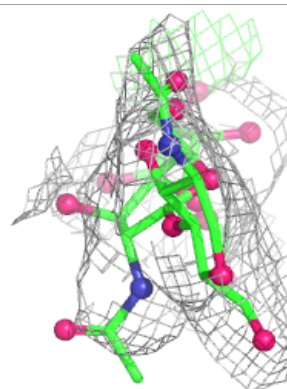
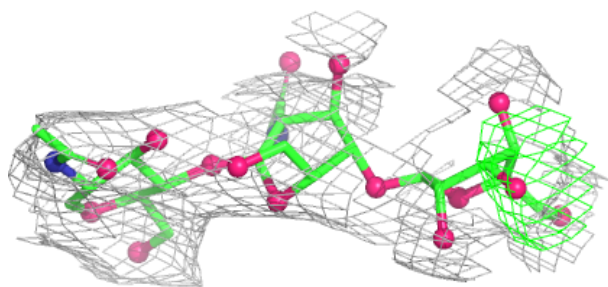
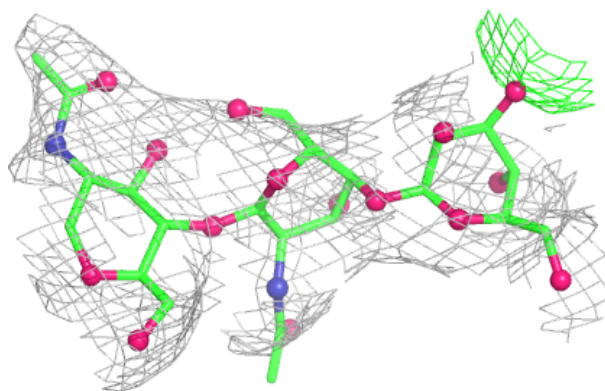
**Electron density around Chain c:**

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

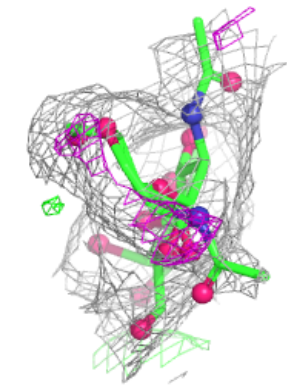
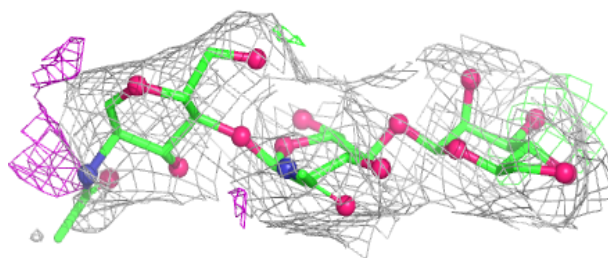
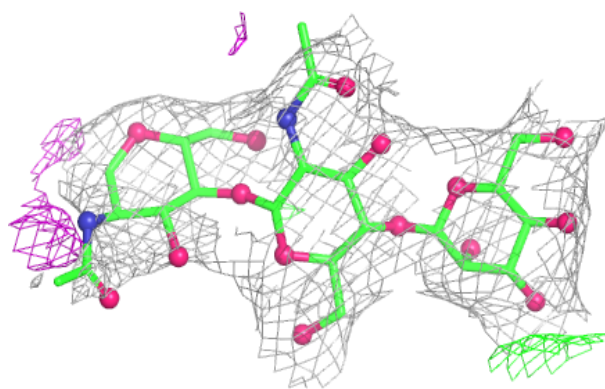


Electron density around Chain m:

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

**Electron density around Chain y:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	C	610	4/4	0.36	0.22	69,72,73,77	0
6	NAG	M	604	14/15	0.42	0.17	107,114,130,130	0
6	NAG	M	605	14/15	0.43	0.15	92,99,109,110	0
6	NAG	N	603	14/15	0.47	0.15	84,98,107,107	0
6	NAG	M	603	14/15	0.50	0.23	94,125,140,144	0
6	NAG	N	608	14/15	0.55	0.12	146,163,168,171	0
6	NAG	N	604	14/15	0.58	0.13	70,85,93,98	0
6	NAG	C	603	14/15	0.59	0.14	101,109,118,132	0
6	NAG	N	605	14/15	0.59	0.15	84,108,134,140	0
6	NAG	D	602	14/15	0.61	0.17	82,98,108,115	0
6	NAG	N	607	14/15	0.63	0.16	94,110,128,133	0
8	EDO	N	611	4/4	0.63	0.19	69,70,75,80	0
8	EDO	H	301	4/4	0.64	0.17	50,53,64,66	0
6	NAG	C	602	14/15	0.66	0.11	96,105,110,127	0
6	NAG	D	603	14/15	0.67	0.15	103,123,132,136	0
6	NAG	C	605	14/15	0.67	0.13	76,85,89,90	0
6	NAG	N	610	14/15	0.68	0.13	65,105,110,113	0
6	NAG	M	602	14/15	0.69	0.14	90,97,106,109	0
6	NAG	D	604	14/15	0.71	0.13	82,88,97,98	0
6	NAG	C	606	14/15	0.71	0.11	85,94,104,110	0
8	EDO	C	611	4/4	0.72	0.25	50,62,69,75	0
6	NAG	C	604	14/15	0.73	0.13	106,116,130,135	0
6	NAG	N	602	14/15	0.75	0.10	89,97,108,123	0
6	NAG	D	605	14/15	0.76	0.12	62,86,95,96	0
7	NH4	C	608	1/1	0.78	0.17	24,24,24,24	0
6	NAG	D	601	14/15	0.79	0.16	62,77,84,92	0
6	NAG	N	601	14/15	0.79	0.16	68,80,85,88	0
6	NAG	M	601	14/15	0.80	0.14	81,88,101,108	0
6	NAG	C	607	14/15	0.82	0.09	93,107,114,117	0
6	NAG	N	609	14/15	0.82	0.13	82,93,99,102	0
6	NAG	N	606	14/15	0.83	0.12	74,91,109,110	0
6	NAG	C	601	14/15	0.83	0.13	58,69,73,75	0
8	EDO	D	607	4/4	0.85	0.21	42,55,57,62	0
6	NAG	M	606	14/15	0.86	0.10	64,80,90,101	0
9	SO4	C	612	5/5	0.86	0.15	79,94,107,113	0
9	SO4	M	607	5/5	0.87	0.10	66,68,83,88	0
7	NH4	D	606	1/1	0.89	0.16	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EDO	H	302	4/4	0.90	0.08	33,37,38,38	0
7	NH4	I	301	1/1	0.92	0.24	21,21,21,21	0
9	SO4	D	608	5/5	0.93	0.07	62,63,66,70	0
7	NH4	C	609	1/1	0.94	0.20	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.