



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 12:10 PM JST

PDB ID : 9UG5 / pdb_00009ug5
Title : Crystal structure of HA3 from Clostridium botulinum type B with alpha2,3-sialyllactose
Authors : Amatsu, S.; Kitadokoro, K.
Deposited on : 2025-04-11
Resolution : 3.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

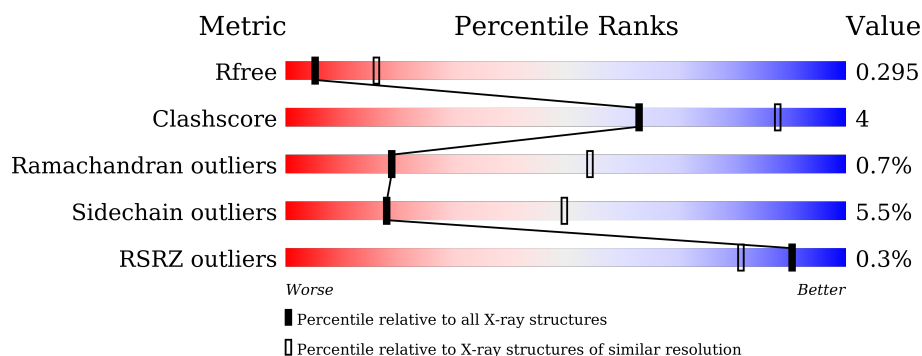
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	632	<div> <div>74%</div> <div>13%</div> <div>•</div> <div>12%</div> </div>
1	B	632	<div> <div>78%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>
1	C	632	<div> <div>77%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>
2	D	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
2	E	3	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13678 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 HA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4397	2803	712	876	6			
1	B	579	Total	C	N	O	S	0	0	0
			4572	2918	745	903	6			
1	C	581	Total	C	N	O	S	0	0	0
			4607	2933	754	914	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q33CP8
A	-4	ALA	-	expression tag	UNP Q33CP8
A	-3	SER	-	expression tag	UNP Q33CP8
A	-2	TRP	-	expression tag	UNP Q33CP8
A	-1	SER	-	expression tag	UNP Q33CP8
A	0	HIS	-	expression tag	UNP Q33CP8
A	1	PRO	-	expression tag	UNP Q33CP8
A	2	GLN	-	expression tag	UNP Q33CP8
A	3	PHE	-	expression tag	UNP Q33CP8
A	4	GLU	-	expression tag	UNP Q33CP8
A	5	LYS	-	expression tag	UNP Q33CP8
A	6	GLY	-	expression tag	UNP Q33CP8
A	7	ALA	-	expression tag	UNP Q33CP8
A	8	LEU	-	expression tag	UNP Q33CP8
A	9	GLU	-	expression tag	UNP Q33CP8
A	10	VAL	-	expression tag	UNP Q33CP8
A	11	LEU	-	expression tag	UNP Q33CP8
A	12	PHE	-	expression tag	UNP Q33CP8
A	13	GLN	-	expression tag	UNP Q33CP8
A	14	GLY	-	expression tag	UNP Q33CP8
A	15	PRO	-	expression tag	UNP Q33CP8
A	16	GLY	-	expression tag	UNP Q33CP8
A	17	TYR	-	expression tag	UNP Q33CP8

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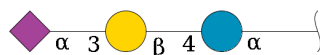
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLN	-	expression tag	UNP Q33CP8
B	-5	MET	-	initiating methionine	UNP Q33CP8
B	-4	ALA	-	expression tag	UNP Q33CP8
B	-3	SER	-	expression tag	UNP Q33CP8
B	-2	TRP	-	expression tag	UNP Q33CP8
B	-1	SER	-	expression tag	UNP Q33CP8
B	0	HIS	-	expression tag	UNP Q33CP8
B	1	PRO	-	expression tag	UNP Q33CP8
B	2	GLN	-	expression tag	UNP Q33CP8
B	3	PHE	-	expression tag	UNP Q33CP8
B	4	GLU	-	expression tag	UNP Q33CP8
B	5	LYS	-	expression tag	UNP Q33CP8
B	6	GLY	-	expression tag	UNP Q33CP8
B	7	ALA	-	expression tag	UNP Q33CP8
B	8	LEU	-	expression tag	UNP Q33CP8
B	9	GLU	-	expression tag	UNP Q33CP8
B	10	VAL	-	expression tag	UNP Q33CP8
B	11	LEU	-	expression tag	UNP Q33CP8
B	12	PHE	-	expression tag	UNP Q33CP8
B	13	GLN	-	expression tag	UNP Q33CP8
B	14	GLY	-	expression tag	UNP Q33CP8
B	15	PRO	-	expression tag	UNP Q33CP8
B	16	GLY	-	expression tag	UNP Q33CP8
B	17	TYR	-	expression tag	UNP Q33CP8
B	18	GLN	-	expression tag	UNP Q33CP8
C	-5	MET	-	initiating methionine	UNP Q33CP8
C	-4	ALA	-	expression tag	UNP Q33CP8
C	-3	SER	-	expression tag	UNP Q33CP8
C	-2	TRP	-	expression tag	UNP Q33CP8
C	-1	SER	-	expression tag	UNP Q33CP8
C	0	HIS	-	expression tag	UNP Q33CP8
C	1	PRO	-	expression tag	UNP Q33CP8
C	2	GLN	-	expression tag	UNP Q33CP8
C	3	PHE	-	expression tag	UNP Q33CP8
C	4	GLU	-	expression tag	UNP Q33CP8
C	5	LYS	-	expression tag	UNP Q33CP8
C	6	GLY	-	expression tag	UNP Q33CP8
C	7	ALA	-	expression tag	UNP Q33CP8
C	8	LEU	-	expression tag	UNP Q33CP8
C	9	GLU	-	expression tag	UNP Q33CP8
C	10	VAL	-	expression tag	UNP Q33CP8
C	11	LEU	-	expression tag	UNP Q33CP8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	PHE	-	expression tag	UNP Q33CP8
C	13	GLN	-	expression tag	UNP Q33CP8
C	14	GLY	-	expression tag	UNP Q33CP8
C	15	PRO	-	expression tag	UNP Q33CP8
C	16	GLY	-	expression tag	UNP Q33CP8
C	17	TYR	-	expression tag	UNP Q33CP8
C	18	GLN	-	expression tag	UNP Q33CP8

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	E	3	Total	C	N	O	0	0	0
			43	23	1	19			

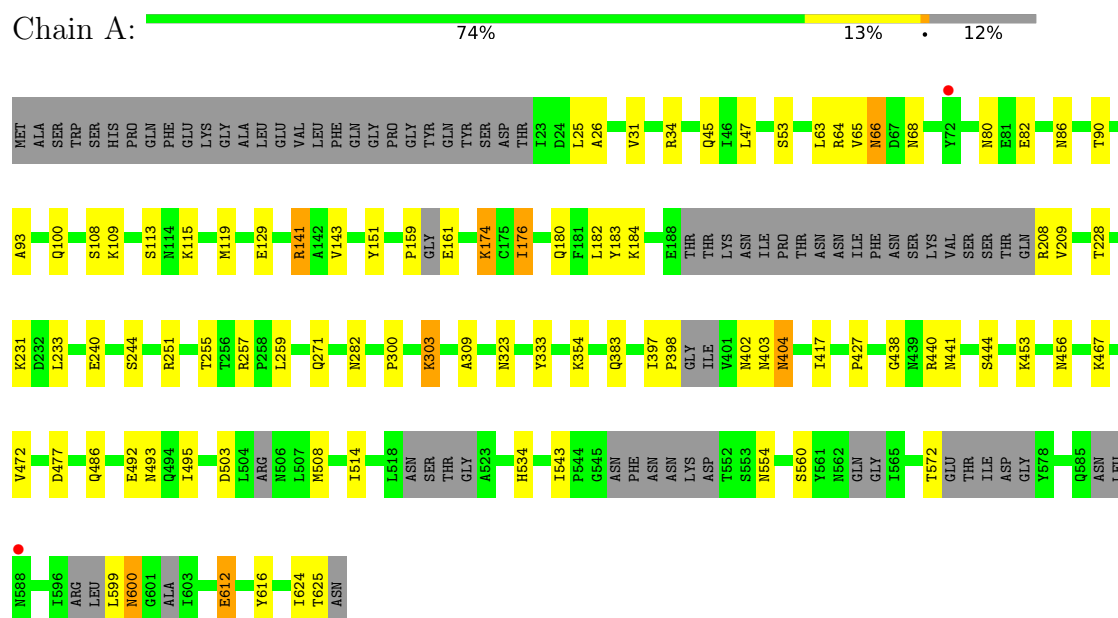
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	4	Total	O	0	0
			4	4		
3	C	5	Total	O	0	0
			5	5		

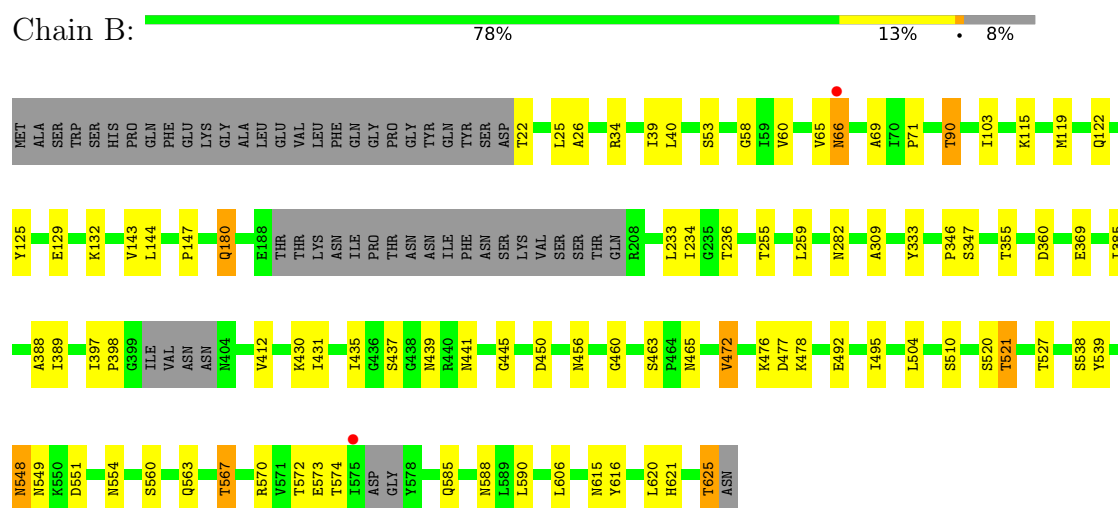
3 Residue-property plots [i](#)

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: HA3

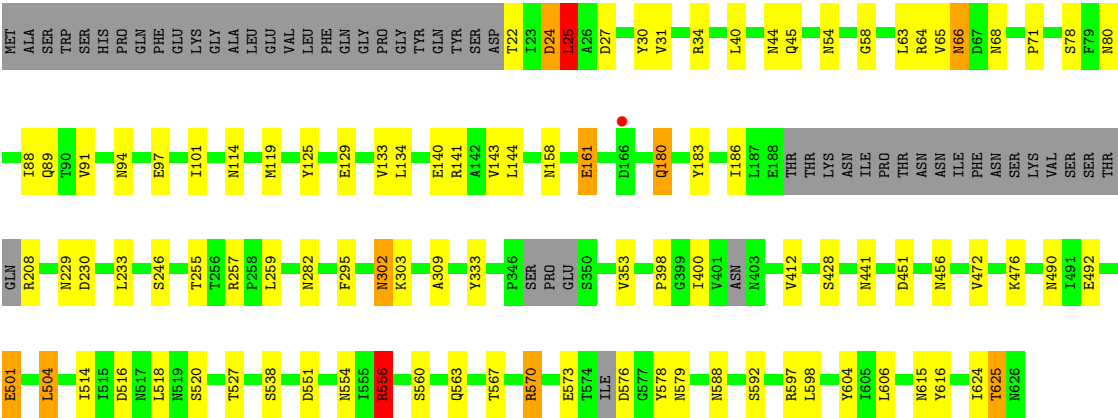


• Molecule 1: HA3



• Molecule 1: HA3

Chain C: 77% 13% 8%



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 33% 33% 33%



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain E: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.97Å 144.09Å 158.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 3.00 44.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (44.32-3.00) 90.0 (44.32-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.224 , 0.303 0.229 , 0.295	Depositor DCC
R_{free} test set	1749 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13678	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: GLC, GAL, SIA

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	0.52	0/4477	0.98	4/6087 (0.1%)
1	B	0.52	0/4663	0.99	7/6345 (0.1%)
1	C	0.53	0/4697	1.00	8/6393 (0.1%)
All	All	0.52	0/13837	0.99	19/18825 (0.1%)

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	2
1	C	0	3
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	ASN	CB-CA-C	-7.57	96.36	109.07
1	C	229	ASN	CB-CA-C	6.49	125.42	116.34
1	B	521	THR	CA-CB-OG1	-6.43	99.95	109.60
1	A	240	GLU	CB-CA-C	5.96	120.50	109.54
1	C	551	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	516	ASP	CA-C-N	5.63	128.28	120.29
1	C	516	ASP	C-N-CA	5.63	128.28	120.29
1	B	551	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	501	GLU	N-CA-CB	5.46	116.46	110.35
1	C	27	ASP	CB-CA-C	5.44	121.24	110.42
1	C	45	GLN	CB-CA-C	-5.37	102.48	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASP	CA-CB-CG	5.30	117.91	112.60
1	B	450	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	600	ASN	CA-CB-CG	5.25	117.84	112.60
1	A	440	ARG	N-CA-CB	-5.23	106.72	111.59
1	C	180	GLN	N-CA-CB	-5.16	102.58	111.55
1	B	180	GLN	N-CA-CB	-5.15	102.59	111.55
1	B	90	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	174	LYS	CB-CG-CD	5.10	123.02	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	251	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	556	ARG	Sidechain
1	C	570	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4397	0	4198	31	3
1	B	4572	0	4412	36	3
1	C	4607	0	4428	37	5
2	D	43	0	37	2	0
2	E	43	0	37	1	0
3	A	7	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
All	All	13678	0	13112	103	6

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 4.

All (103) 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:C:54:ASN:HB3	1:C:114:ASN:H	1.56	0.70
1:C:556:ARG:NH1	1:C:592:SER:O	2.28	0.66
1:B:465:ASN:HB2	2:D:1:GLC:H61	1.81	0.62
1:C:598:LEU:HD22	1:C:604:TYR:CE2	2.35	0.62
1:C:31:VAL:HG13	1:C:186:ILE:HD11	1.82	0.60
1:C:133:VAL:O	1:C:134:LEU:HD12	2.05	0.56
1:C:34:ARG:HA	1:C:180:GLN:O	2.06	0.56
1:B:527:THR:H	2:D:3:SIA:C1	2.19	0.56
1:A:441:ASN:OD1	1:A:441:ASN:N	2.37	0.55
1:A:402:ASN:O	1:A:403:ASN:C	2.50	0.55
1:A:398:PRO:HA	1:A:492:GLU:OE1	2.07	0.55
1:A:34:ARG:HA	1:A:180:GLN:O	2.07	0.54
1:B:34:ARG:HA	1:B:180:GLN:O	2.07	0.54
1:C:24:ASP:O	1:C:25:LEU:C	2.51	0.54
1:A:159:PRO:O	1:A:161:GLU:N	2.41	0.54
1:B:441:ASN:N	1:B:441:ASN:OD1	2.39	0.54
1:C:441:ASN:N	1:C:441:ASN:OD1	2.40	0.53
1:B:397:ILE:O	1:B:398:PRO:C	2.51	0.53
1:C:64:ARG:HA	1:C:68:ASN:OD1	2.09	0.53
1:C:71:PRO:HB2	1:C:144:LEU:HD11	1.91	0.52
1:B:397:ILE:HD11	1:B:495:ILE:HG13	1.92	0.52
1:A:151:TYR:CD1	1:A:176:ILE:HD12	2.45	0.52
1:C:101:ILE:O	1:C:101:ILE:HG13	2.10	0.52
1:B:437:SER:HB2	1:B:478:LYS:HA	1.92	0.52
1:B:69:ALA:HA	1:B:147:PRO:HG2	1.90	0.52
1:A:612:GLU:O	1:A:612:GLU:HG2	2.11	0.51
1:B:567:THR:HA	1:B:585:GLN:HA	1.92	0.51
1:C:31:VAL:HG21	1:C:91:VAL:HG21	1.93	0.51
1:A:228:THR:O	1:A:231:LYS:HG3	2.11	0.49
1:B:554:ASN:HB3	1:B:625:THR:HB	1.94	0.49
1:A:417:ILE:HD12	1:A:508:MET:HG3	1.94	0.49
1:C:563:GLN:OE1	1:C:588:ASN:HB2	2.12	0.49
1:B:560:SER:HB3	1:B:621:HIS:NE2	2.27	0.48
1:B:65:VAL:O	1:B:66:ASN:C	2.56	0.48
1:A:599:LEU:HD23	1:A:599:LEU:C	2.39	0.48
1:A:65:VAL:O	1:A:66:ASN:C	2.57	0.47
1:C:97:GLU:HB3	1:C:257:ARG:NH1	2.29	0.47
1:C:58:GLY:HA3	1:C:119:MET:HE1	1.96	0.47
1:C:65:VAL:O	1:C:66:ASN:C	2.57	0.47
1:B:103:ILE:HG21	1:B:234:ILE:HG23	1.95	0.47
1:B:39:ILE:HB	1:B:122:GLN:NE2	2.29	0.47
1:A:233:LEU:HD12	1:A:309:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:THR:H	2:E:3:SIA:C1	2.28	0.46
1:C:34:ARG:NH1	1:C:129:GLU:OE2	2.48	0.46
1:A:129:GLU:HG2	1:A:143:VAL:HG22	1.97	0.46
1:B:388:ALA:HB3	1:B:445:GLY:HA2	1.98	0.46
1:C:40:LEU:HD13	1:C:125:TYR:CD1	2.50	0.46
1:A:34:ARG:NH1	1:A:129:GLU:OE2	2.47	0.46
1:C:30:TYR:HE1	1:C:133:VAL:CG1	2.29	0.46
1:C:31:VAL:HG13	1:C:186:ILE:CD1	2.45	0.46
1:B:385:ILE:HG21	1:B:389:ILE:HD11	1.98	0.46
1:B:233:LEU:HD12	1:B:309:ALA:O	2.16	0.45
1:B:34:ARG:NH1	1:B:129:GLU:OE2	2.48	0.45
1:B:563:GLN:HA	1:B:590:LEU:HB2	1.98	0.45
1:A:323:ASN:HA	1:A:616:TYR:CE2	2.51	0.45
1:A:129:GLU:OE1	1:A:141:ARG:NH2	2.49	0.45
1:C:233:LEU:HD12	1:C:309:ALA:O	2.16	0.45
1:B:58:GLY:C	1:B:119:MET:HE1	2.43	0.44
1:A:300:PRO:HG2	1:A:303:LYS:HE3	1.99	0.44
1:C:25:LEU:HB2	1:C:30:TYR:CZ	2.53	0.44
1:C:554:ASN:HB3	1:C:625:THR:HB	1.99	0.44
1:A:109:LYS:CB	1:A:119:MET:HE1	2.48	0.44
1:B:129:GLU:HG2	1:B:143:VAL:HG22	1.99	0.44
1:A:64:ARG:HA	1:A:68:ASN:OD1	2.17	0.44
1:A:86:ASN:O	1:A:90:THR:HG23	2.18	0.43
1:A:53:SER:O	1:A:115:LYS:O	2.36	0.43
1:B:53:SER:O	1:B:115:LYS:O	2.36	0.43
1:B:71:PRO:HB2	1:B:144:LEU:HD11	1.99	0.43
1:A:259:LEU:HB2	1:A:333:TYR:HB2	2.00	0.43
1:B:430:LYS:HA	1:B:460:GLY:HA3	2.00	0.43
1:B:431:ILE:HG21	1:B:472:VAL:HG11	2.01	0.43
1:A:438:GLY:HA3	1:A:477:ASP:O	2.18	0.43
1:C:129:GLU:HG2	1:C:143:VAL:HG22	1.99	0.43
1:A:403:ASN:O	1:A:404:ASN:C	2.62	0.43
1:C:259:LEU:HB2	1:C:333:TYR:HB2	2.00	0.43
1:C:518:LEU:HD13	1:C:624:ILE:HD11	1.99	0.43
1:A:397:ILE:HD13	1:A:495:ILE:HD11	2.01	0.42
1:A:534:HIS:CD2	1:B:588:ASN:HB3	2.53	0.42
1:A:612:GLU:N	1:A:612:GLU:OE1	2.52	0.42
1:C:89:GLN:HG2	1:C:94:ASN:HA	2.02	0.42
1:A:108:SER:HB3	1:A:244:SER:HB3	2.01	0.42
1:B:435:ILE:HG12	1:B:456:ASN:HB2	2.01	0.42
1:A:427:PRO:HD3	1:A:493:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HA	1:A:231:LYS:HA	2.01	0.42
1:B:539:TYR:CD2	1:B:620:LEU:HD22	2.55	0.42
1:C:412:VAL:HG23	1:C:476:LYS:HA	2.01	0.41
1:C:538:SER:HA	1:C:606:LEU:O	2.21	0.41
1:B:60:VAL:HG23	1:B:119:MET:HE3	2.03	0.41
1:C:246:SER:HA	1:C:295:PHE:O	2.21	0.41
1:B:40:LEU:HD13	1:B:125:TYR:CD1	2.55	0.41
1:C:230:ASP:HB3	1:C:233:LEU:HB2	2.02	0.41
1:C:302:ASN:HD22	1:C:303:LYS:N	2.19	0.41
1:B:615:ASN:OD1	1:B:616:TYR:N	2.53	0.41
1:C:504:LEU:HB2	1:C:578:TYR:OH	2.21	0.41
1:B:259:LEU:HB2	1:B:333:TYR:HB2	2.01	0.41
1:B:346:PRO:O	1:B:347:SER:C	2.63	0.41
1:C:78:SER:OG	1:C:140:GLU:CD	2.64	0.40
1:B:412:VAL:HG23	1:B:476:LYS:HA	2.03	0.40
1:A:31:VAL:O	1:A:183:TYR:HA	2.21	0.40
1:B:538:SER:HA	1:B:606:LEU:O	2.22	0.40
1:B:548:ASN:O	1:B:549:ASN:CB	2.69	0.40
1:C:31:VAL:O	1:C:183:TYR:HA	2.21	0.40
1:C:615:ASN:OD1	1:C:616:TYR:N	2.54	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ASN:OD1	1:C:158:ASN:OD1[3_554]	2.07	0.13
1:C:80:ASN:ND2	1:C:520:SER:OG[3_444]	2.10	0.10
1:A:45:GLN:OE1	1:B:369:GLU:OE2[2_555]	2.14	0.06
1:B:570:ARG:NH2	1:C:161:GLU:OE1[3_554]	2.14	0.06
1:A:82:GLU:OE2	1:C:604:TYR:OH[2_555]	2.16	0.04
1:A:80:ASN:OD1	1:C:597:ARG:O[2_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	534/632 (84%)	506 (95%)	23 (4%)	5 (1%)	14	49
1	B	571/632 (90%)	537 (94%)	31 (5%)	3 (0%)	25	61
1	C	571/632 (90%)	537 (94%)	31 (5%)	3 (0%)	25	61
All	All	1676/1896 (88%)	1580 (94%)	85 (5%)	11 (1%)	19	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASN
1	A	503	ASP
1	B	66	ASN
1	B	439	ASN
1	A	25	LEU
1	A	66	ASN
1	C	25	LEU
1	A	26	ALA
1	B	26	ALA
1	A	404	ASN
1	C	398	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/571 (85%)	452 (93%)	32 (7%)	14	43
1	B	504/571 (88%)	483 (96%)	21 (4%)	25	59
1	C	509/571 (89%)	479 (94%)	30 (6%)	16	47
All	All	1497/1713 (87%)	1414 (94%)	83 (6%)	18	50

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	63	LEU
1	A	100	GLN
1	A	113	SER
1	A	174	LYS
1	A	176	ILE
1	A	182	LEU
1	A	184	LYS
1	A	208	ARG
1	A	209	VAL
1	A	255	THR
1	A	257	ARG
1	A	271	GLN
1	A	282	ASN
1	A	303	LYS
1	A	354	LYS
1	A	383	GLN
1	A	444	SER
1	A	453	LYS
1	A	456	ASN
1	A	467	LYS
1	A	472	VAL
1	A	486	GLN
1	A	514	ILE
1	A	543	ILE
1	A	554	ASN
1	A	560	SER
1	A	572	THR
1	A	600	ASN
1	A	612	GLU
1	A	624	ILE
1	A	625	THR
1	B	22	THR
1	B	25	LEU
1	B	90	THR
1	B	132	LYS
1	B	236	THR
1	B	255	THR
1	B	282	ASN
1	B	355	THR
1	B	463	SER
1	B	472	VAL
1	B	477	ASP

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Mol	Chain	Res	Type
1	B	492	GLU
1	B	504	LEU
1	B	510	SER
1	B	520	SER
1	B	521	THR
1	B	567	THR
1	B	572	THR
1	B	573	GLU
1	B	574	THR
1	B	625	THR
1	C	22	THR
1	C	24	ASP
1	C	25	LEU
1	C	44	ASN
1	C	63	LEU
1	C	88	ILE
1	C	161	GLU
1	C	208	ARG
1	C	255	THR
1	C	282	ASN
1	C	302	ASN
1	C	353	VAL
1	C	400	ILE
1	C	428	SER
1	C	451	ASP
1	C	456	ASN
1	C	472	VAL
1	C	490	ASN
1	C	492	GLU
1	C	501	GLU
1	C	504	LEU
1	C	514	ILE
1	C	556	ARG
1	C	560	SER
1	C	567	THR
1	C	570	ARG
1	C	573	GLU
1	C	576	ASP
1	C	579	ASN
1	C	625	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	A	328	ASN
1	A	365	ASN
1	A	383	GLN
1	A	404	ASN
1	B	80	ASN
1	B	180	GLN
1	B	328	ASN
1	B	424	ASN
1	B	617	ASN
1	C	302	ASN
1	C	328	ASN
1	C	617	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	D	1	2	12,12,12	0.16	0	17,17,17	0.43	0
2	GAL	D	2	2	11,11,12	0.49	0	15,15,17	0.66	0
2	SIA	D	3	2	20,20,21	0.75	1 (5%)	24,28,31	0.87	1 (4%)
2	GLC	E	1	2	12,12,12	0.23	0	17,17,17	0.37	0
2	GAL	E	2	2	11,11,12	0.61	0	15,15,17	0.46	0
2	SIA	E	3	2	20,20,21	0.79	1 (5%)	24,28,31	0.72	1 (4%)

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	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	2/2/19/22	0/1/1/1
2	SIA	E	3	2	-	6/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	SIA	O1B-C1	-3.25	1.19	1.30
2	D	3	SIA	O1B-C1	-2.93	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SIA	O1B-C1-C2	2.87	121.23	113.03
2	E	3	SIA	O1B-C1-C2	2.12	119.07	113.03

There are no chirality outliers.

All (11) torsion outliers are listed below:

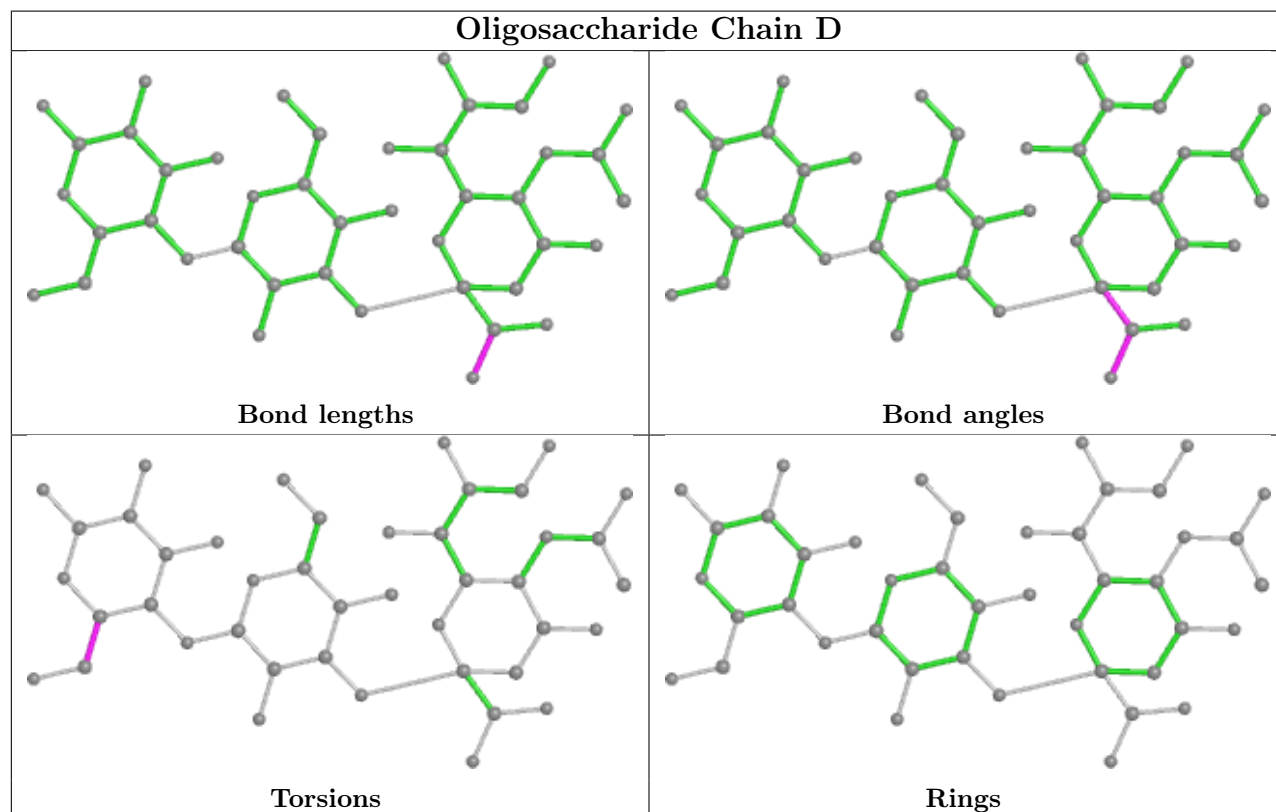
Mol	Chain	Res	Type	Atoms
2	E	1	GLC	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	E	2	GAL	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	E	3	SIA	C6-C7-C8-O8
2	E	3	SIA	C11-C10-N5-C5
2	E	3	SIA	O10-C10-N5-C5
2	E	3	SIA	C6-C7-C8-C9
2	E	3	SIA	O7-C7-C8-O8
2	E	3	SIA	O7-C7-C8-C9

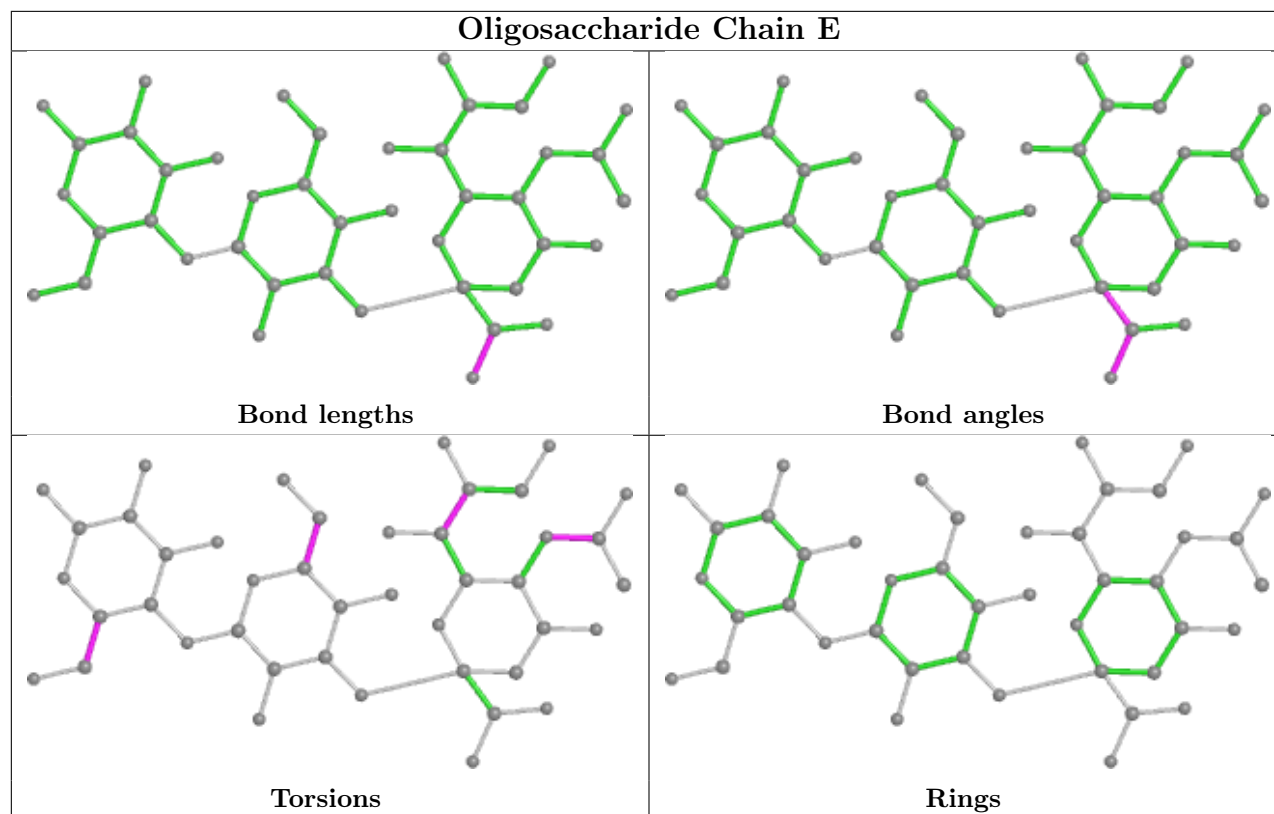
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	SIA	1	0
2	D	3	SIA	1	0
2	D	1	GLC	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](#)

There are no ligands in this entry.

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	558/632 (88%)	-0.26	2 (0%) 89 77	36, 67, 115, 151	0
1	B	579/632 (91%)	-0.40	2 (0%) 90 81	36, 57, 91, 127	0
1	C	581/632 (91%)	-0.42	1 (0%) 92 84	35, 57, 88, 113	0
All	All	1718/1896 (90%)	-0.36	5 (0%) 90 81	35, 59, 103, 151	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	TYR	2.8
1	C	166	ASP	2.7
1	B	66	ASN	2.5
1	B	575	ILE	2.2
1	A	588	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

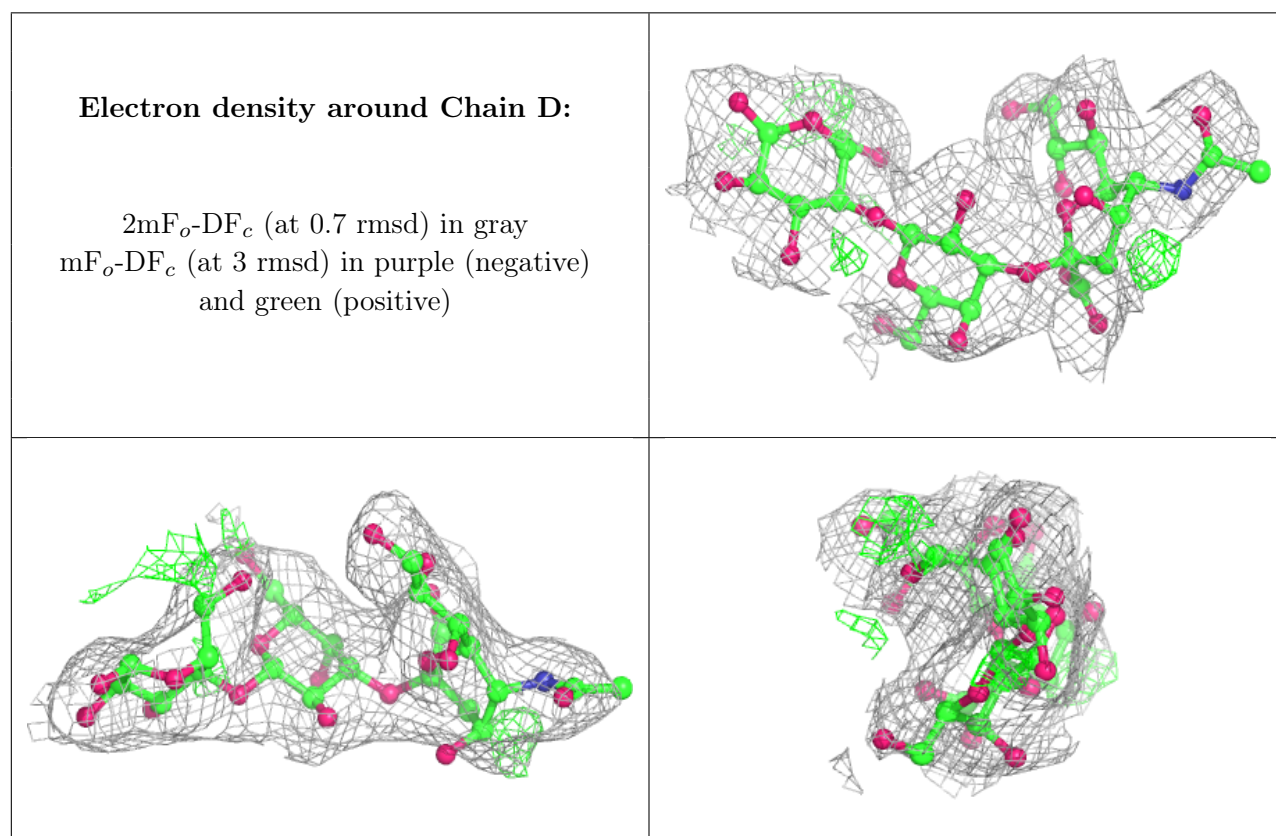
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	1	12/12	0.69	0.11	65,87,91,96	0
2	SIA	D	3	20/21	0.84	0.11	55,61,70,90	0
2	GLC	E	1	12/12	0.85	0.10	51,61,72,75	0

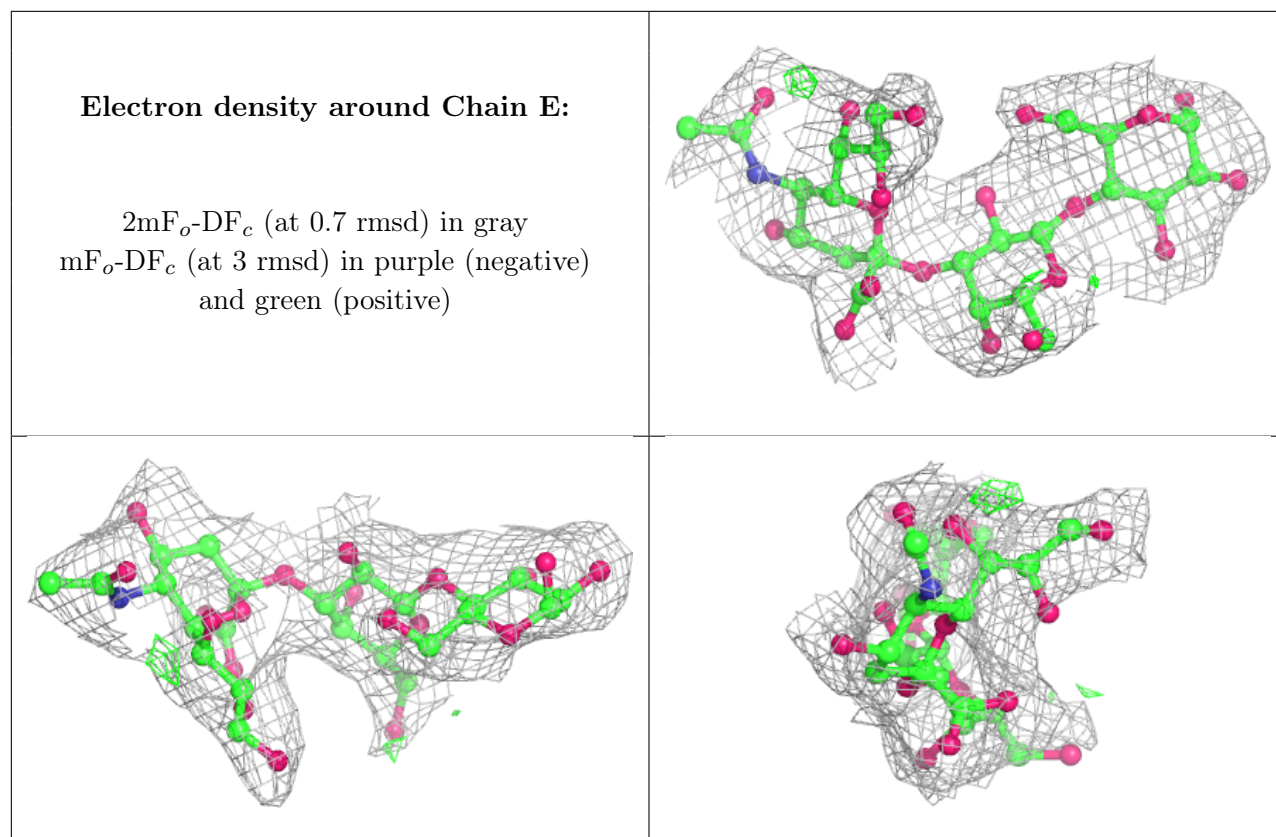
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GAL	D	2	11/12	0.87	0.08	58,67,73,77	0
2	SIA	E	3	20/21	0.87	0.10	53,61,71,73	0
2	GAL	E	2	11/12	0.88	0.08	53,59,66,67	0

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.