



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 12:12 PM JST

PDB ID : 9UG6 / pdb_00009ug6
Title : Crystal structure of HA3 from Clostridium botulinum type B with alpha2,6-sialyllactose
Authors : Amatsu, S.; Kitadokoro, K.
Deposited on : 2025-04-11
Resolution : 2.23 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
buster-report : 1.1.7 (2018)
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

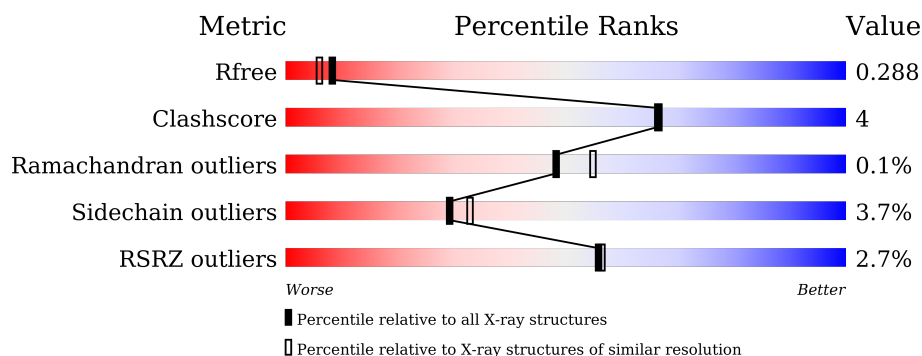
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (2.26-2.22)

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	 3% 79% 12% • 8%
1	B	632	 2% 79% 12% • 8%
1	C	632	 2% 79% 12% • 7%
2	E	2	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27749 atoms, of which 13549 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	581	Total	C	H	N	O	S	0	0	0
			9110	2947	4480	759	918	6			
1	B	583	Total	C	H	N	O	S	0	0	0
			9140	2957	4498	760	919	6			
1	C	587	Total	C	H	N	O	S	0	0	0
			9239	2980	4553	774	926	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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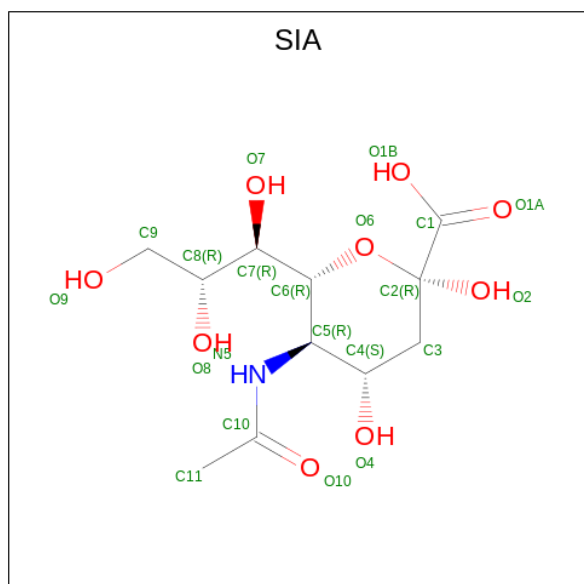
Chain	Residue	Modelled	Actual	Comment	Reference
C	12	PHE	-	expression tag	UNP Q33CP8
C	13	GLN	-	expression tag	UNP Q33CP8
C	14	GLY	-	expression tag	UNP Q33CP8
C	15	PRO	-	expression tag	UNP Q33CP8
C	16	GLY	-	expression tag	UNP Q33CP8
C	17	TYR	-	expression tag	UNP Q33CP8
C	18	GLN	-	expression tag	UNP Q33CP8

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			31	17	1	13			

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			39	11	18	1	9		

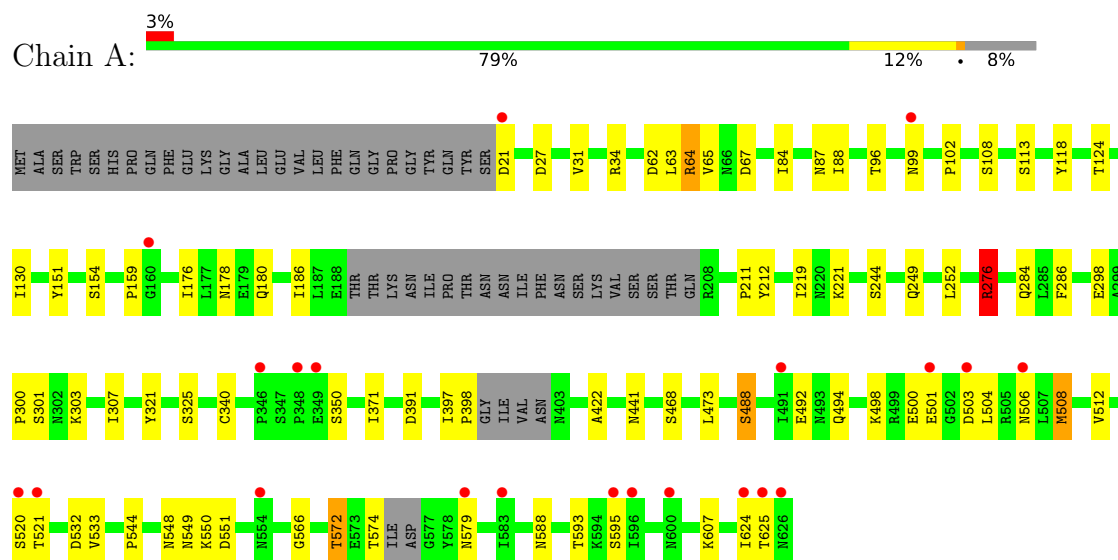
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total 56	O 56	0	0
4	B	73	Total 73	O 73	0	0
4	C	61	Total 61	O 61	0	0

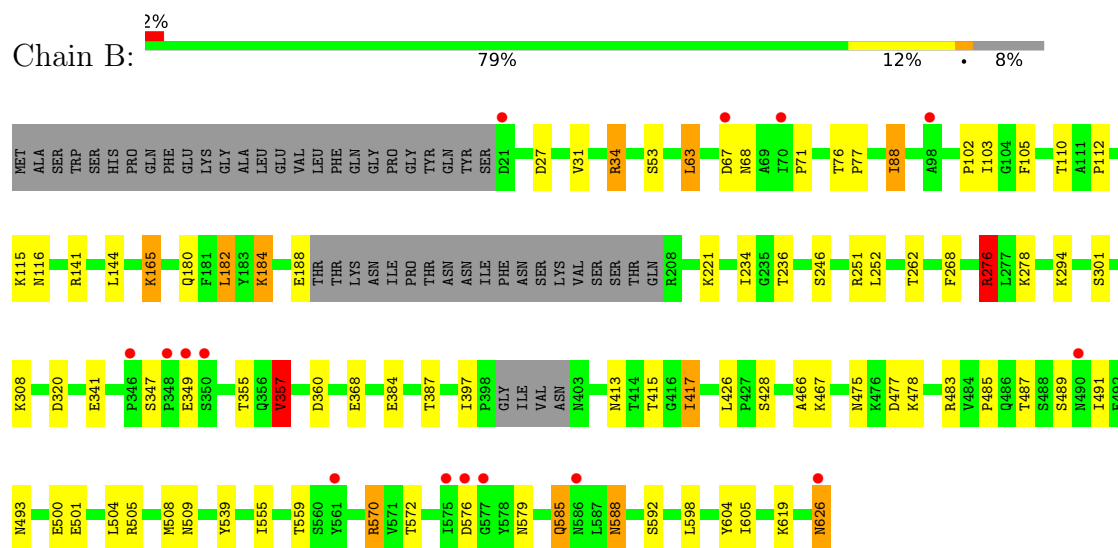
3 Residue-property plots [i](#)

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.

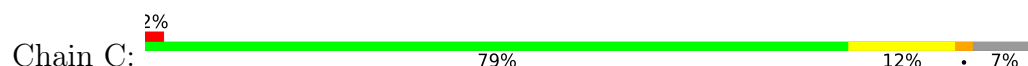
• Molecule 1: HA3

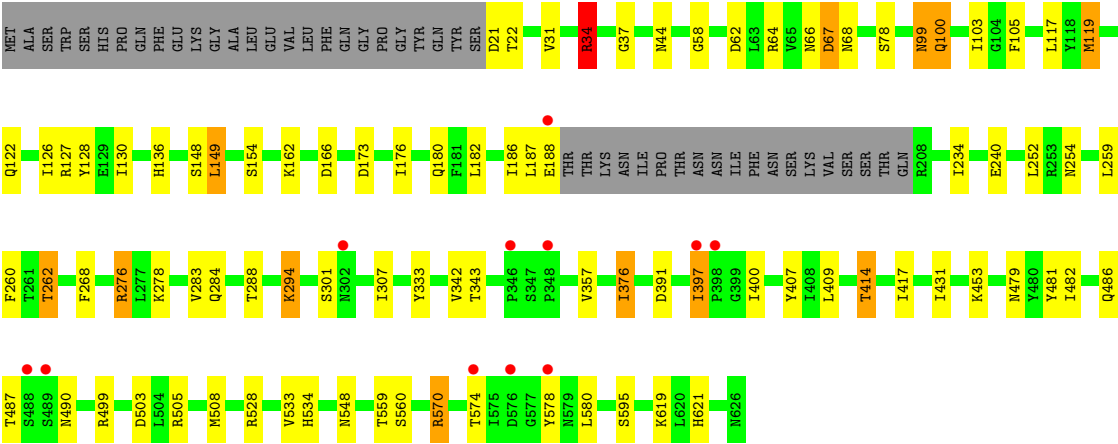


• Molecule 1: HA3



• Molecule 1: HA3





● Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.25Å 145.70Å 159.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.11 – 2.23 42.11 – 2.23	Depositor EDS
% Data completeness (in resolution range)	94.8 (42.11-2.23) 94.7 (42.11-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.229 , 0.287 0.232 , 0.288	Depositor DCC
R_{free} test set	4570 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 18.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27749	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GLC

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	0.67	0/4722	1.25	15/6423 (0.2%)
1	B	0.67	0/4735	1.23	23/6442 (0.4%)
1	C	0.67	1/4780 (0.0%)	1.21	20/6504 (0.3%)
All	All	0.67	1/14237 (0.0%)	1.23	58/19369 (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	2
1	B	0	4
1	C	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	MET	C-O	-6.38	1.16	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	THR	CA-CB-OG1	-10.01	94.59	109.60
1	A	391	ASP	N-CA-C	-9.51	100.53	113.18
1	C	578	TYR	N-CA-CB	-8.80	96.77	110.85
1	A	63	LEU	N-CA-CB	-7.72	98.86	110.90
1	B	508	MET	CA-C-N	7.38	133.30	122.82
1	B	508	MET	C-N-CA	7.38	133.30	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	THR	CA-CB-OG1	-7.25	98.73	109.60
1	C	294	LYS	N-CA-CB	-7.07	99.02	111.39
1	B	165	LYS	N-CA-CB	6.96	120.94	110.22
1	C	343	THR	CA-CB-OG1	-6.88	99.28	109.60
1	B	320	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	391	ASP	N-CA-CB	6.83	122.03	110.49
1	B	67	ASP	N-CA-C	6.62	119.33	111.71
1	A	27	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	268	PHE	N-CA-CB	-6.53	102.57	110.53
1	C	100	GLN	N-CA-CB	-6.46	99.88	110.40
1	A	124	THR	CA-CB-OG1	-6.35	100.07	109.60
1	C	570	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	C	21	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	298	GLU	CB-CG-CD	6.22	123.18	112.60
1	B	182	LEU	N-CA-CB	-6.20	100.98	110.65
1	C	508	MET	CA-C-N	6.15	131.55	122.82
1	C	508	MET	C-N-CA	6.15	131.55	122.82
1	C	268	PHE	CA-CB-CG	6.13	119.93	113.80
1	B	141	ARG	CB-CA-C	-5.91	102.57	110.79
1	C	149	LEU	N-CA-CB	5.91	120.48	110.49
1	B	276	ARG	CB-CG-CD	5.86	124.78	111.30
1	C	166	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	110	THR	CA-CB-OG1	-5.78	100.94	109.60
1	A	159	PRO	CB-CA-C	5.75	118.75	111.39
1	B	570	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	B	262	THR	CA-CB-OG1	-5.71	101.04	109.60
1	C	173	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	576	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	240	GLU	N-CA-CB	5.56	118.22	109.83
1	B	626	ASN	N-CA-CB	5.55	119.94	110.50
1	A	544	PRO	CB-CA-C	-5.51	104.17	111.23
1	B	413	ASN	CB-CA-C	-5.51	101.48	110.85
1	B	63	LEU	N-CA-CB	-5.49	101.82	110.77
1	B	585	GLN	N-CA-CB	5.48	120.08	111.20
1	B	341	GLU	CB-CA-C	5.41	119.60	109.71
1	C	188	GLU	CB-CG-CD	5.38	121.75	112.60
1	C	62	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	262	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	96	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	249	GLN	CB-CA-C	5.29	116.15	110.65
1	A	62	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	509	ASN	CB-CA-C	5.27	120.34	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	LYS	CB-CA-C	5.25	119.77	110.16
1	B	68	ASN	N-CA-C	-5.25	106.47	112.92
1	B	384	GLU	CB-CG-CD	5.23	121.50	112.60
1	A	286	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	357	VAL	N-CA-CB	-5.16	100.39	110.45
1	A	276	ARG	CB-CG-CD	5.15	123.15	111.30
1	C	276	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	27	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	67	ASP	CA-C-O	-5.07	115.05	120.42
1	A	284	GLN	N-CA-CB	5.01	117.26	110.59

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	588	ASN	Peptide
1	A	64	ARG	Sidechain
1	B	251	ARG	Sidechain
1	B	483	ARG	Sidechain
1	B	570	ARG	Sidechain
1	B	588	ASN	Peptide
1	C	127	ARG	Sidechain
1	C	34	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	4630	4480	4480	31	0
1	B	4642	4498	4498	31	0
1	C	4686	4553	4553	37	0
2	E	31	0	25	1	0
3	C	21	18	18	2	0
4	A	56	0	0	0	0
4	B	73	0	0	0	0
4	C	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14200	13549	13574	100	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 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:THR:HA	1:A:624:ILE:HG23	1.74	0.69
1:C:117:LEU:HD21	1:C:154:SER:HB2	1.79	0.62
1:A:548:ASN:HD21	1:A:551:ASP:CG	2.11	0.58
1:C:31:VAL:HG13	1:C:186:ILE:HD11	1.85	0.58
1:A:574:THR:HB	1:A:579:ASN:OD1	2.05	0.57
1:A:397:ILE:O	1:A:398:PRO:C	2.46	0.57
1:C:400:ILE:C	1:C:490:ASN:HB3	2.29	0.57
1:B:477:ASP:O	1:B:478:LYS:HD2	2.05	0.56
1:A:325:SER:HB2	2:E:2:SIA:O4	2.06	0.56
1:C:64:ARG:HD3	1:C:148:SER:O	2.06	0.55
1:A:548:ASN:OD1	1:A:550:LYS:N	2.37	0.55
1:C:44:ASN:ND2	1:C:122:GLN:OE1	2.37	0.55
1:B:76:THR:HB	1:B:77:PRO:HD2	1.88	0.55
1:A:84:ILE:O	1:A:88:ILE:HG12	2.07	0.54
1:A:532:ASP:OD1	1:A:533:VAL:N	2.39	0.54
1:C:278:LYS:HE3	1:C:283:VAL:O	2.07	0.54
1:A:488:SER:O	1:A:488:SER:OG	2.23	0.54
1:B:236:THR:HG23	1:B:308:LYS:HG3	1.90	0.52
1:C:259:LEU:HB2	1:C:333:TYR:HB2	1.92	0.52
1:B:34:ARG:HA	1:B:180:GLN:O	2.10	0.52
1:C:528:ARG:NH2	3:C:701:SIA:O9	2.43	0.52
1:B:559:THR:HA	1:B:619:LYS:O	2.09	0.52
1:B:63:LEU:HD21	1:B:252:LEU:HD12	1.92	0.51
1:B:112:PRO:HG2	1:B:115:LYS:HB2	1.91	0.51
1:A:65:VAL:HG23	1:A:102:PRO:HG3	1.92	0.51
1:C:103:ILE:HG21	1:C:234:ILE:CG2	2.41	0.51
1:B:102:PRO:HG2	1:B:252:LEU:HB2	1.92	0.50
1:B:31:VAL:CG2	1:B:88:ILE:HD12	2.41	0.50
1:C:409:LEU:HD11	1:C:479:ASN:HB3	1.92	0.50
1:A:549:ASN:OD1	1:A:549:ASN:O	2.30	0.50
1:A:34:ARG:HA	1:A:180:GLN:O	2.12	0.50
1:A:108:SER:HB3	1:A:244:SER:HB3	1.93	0.50
1:C:260:PHE:CZ	1:C:262:THR:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:CD1	1:A:176:ILE:HD12	2.47	0.49
1:B:53:SER:HB2	1:B:116:ASN:OD1	2.13	0.49
1:C:34:ARG:HA	1:C:180:GLN:O	2.13	0.49
1:C:31:VAL:HG12	1:C:130:ILE:CD1	2.42	0.49
1:B:588:ASN:O	1:B:592:SER:HB2	2.13	0.48
1:B:103:ILE:HG21	1:B:234:ILE:CG2	2.43	0.48
1:B:71:PRO:HB2	1:B:144:LEU:HD11	1.96	0.48
1:C:376:ILE:HD12	1:C:453:LYS:HA	1.96	0.48
1:C:560:SER:OG	1:C:621:HIS:NE2	2.46	0.48
1:A:549:ASN:O	1:A:549:ASN:CG	2.57	0.47
1:C:414:THR:HB	1:C:499:ARG:NH1	2.29	0.47
1:A:307:ILE:HG13	1:A:340:CYS:SG	2.54	0.47
1:B:182:LEU:HA	1:B:355:THR:O	2.14	0.47
1:A:520:SER:O	1:A:521:THR:HG23	2.14	0.47
1:B:417:ILE:HG22	1:B:500:GLU:HB2	1.96	0.47
1:B:426:LEU:HG	1:B:467:LYS:HG2	1.97	0.47
1:C:400:ILE:O	1:C:490:ASN:HB3	2.15	0.47
3:C:701:SIA:H113	3:C:701:SIA:O7	2.16	0.46
1:A:276:ARG:HH11	1:A:276:ARG:HD2	1.56	0.46
1:B:347:SER:C	1:B:349:GLU:H	2.23	0.46
1:A:572:THR:OG1	1:A:579:ASN:HB2	2.16	0.46
1:A:219:ILE:HA	1:A:371:ILE:O	2.16	0.46
1:C:503:ASP:HB3	1:C:580:LEU:HB2	1.98	0.45
1:C:376:ILE:HD11	1:C:481:TYR:CE2	2.50	0.45
1:A:473:LEU:HB2	1:A:508:MET:HE3	1.98	0.45
1:B:598:LEU:HD22	1:B:604:TYR:CE2	2.51	0.45
1:C:105:PHE:CE1	1:C:149:LEU:O	2.69	0.45
1:B:415:THR:HG23	1:B:475:ASN:HA	1.99	0.45
1:B:485:PRO:O	1:B:487:THR:HG23	2.16	0.45
1:A:31:VAL:HG13	1:A:186:ILE:HD11	1.97	0.44
1:C:397:ILE:HD13	1:C:397:ILE:HA	1.79	0.44
1:A:300:PRO:HG2	1:A:303:LYS:HD3	1.99	0.44
1:B:555:ILE:HG13	1:B:598:LEU:HD12	2.00	0.43
1:C:417:ILE:HD13	1:C:505:ARG:HG2	2.00	0.43
1:B:428:SER:OG	1:B:466:ALA:O	2.29	0.43
1:B:489:SER:OG	1:B:491:ILE:HG22	2.18	0.43
1:B:539:TYR:O	1:B:605:ILE:HA	2.18	0.43
1:C:559:THR:HA	1:C:619:LYS:O	2.18	0.43
1:A:31:VAL:CG1	1:A:87:ASN:HB3	2.48	0.43
1:B:184:LYS:HG3	1:B:357:VAL:HG11	2.00	0.43
1:B:105:PHE:HA	1:B:246:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:OD1	1:C:68:ASN:C	2.60	0.43
1:C:431:ILE:HG13	1:C:482:ILE:HD13	2.01	0.43
1:C:548:ASN:OD1	1:C:548:ASN:C	2.61	0.43
1:B:397:ILE:HD12	1:B:493:ASN:HB3	2.01	0.42
1:A:31:VAL:HG12	1:A:130:ILE:CD1	2.49	0.42
1:C:407:TYR:HA	1:C:482:ILE:O	2.19	0.42
1:C:254:ASN:O	1:C:288:THR:HA	2.18	0.42
1:A:118:TYR:O	1:A:154:SER:HA	2.19	0.42
1:A:422:ALA:HA	1:A:494:GLN:O	2.19	0.42
1:A:498:LYS:HD3	1:A:500:GLU:OE2	2.20	0.42
1:C:37:GLY:O	1:C:176:ILE:HG12	2.20	0.42
1:A:212:TYR:HB2	1:A:321:TYR:CD2	2.54	0.41
1:C:58:GLY:HA3	1:C:119:MET:HE1	2.02	0.41
1:C:105:PHE:CZ	1:C:149:LEU:O	2.73	0.41
1:C:22:THR:HA	1:C:136:HIS:O	2.20	0.41
1:A:468:SER:HA	1:A:512:VAL:O	2.21	0.41
1:B:276:ARG:HH21	1:B:276:ARG:HD2	1.76	0.41
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.91	0.41
1:B:501:GLU:C	1:B:505:ARG:HE	2.29	0.41
1:C:99:ASN:OD1	1:C:100:GLN:HG3	2.21	0.41
1:C:533:VAL:O	1:C:534:HIS:HB2	2.21	0.41
1:B:572:THR:HG23	1:B:579:ASN:HB2	2.03	0.40
1:C:182:LEU:HG	1:C:357:VAL:HG12	2.03	0.40
1:C:126:ILE:HG21	1:C:128:TYR:CZ	2.56	0.40
1:A:566:GLY:HA2	1:A:607:LYS:O	2.21	0.40
1:C:307:ILE:HG22	1:C:342:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	573/632 (91%)	546 (95%)	27 (5%)	0	100	100
1	B	577/632 (91%)	554 (96%)	23 (4%)	0	100	100
1	C	583/632 (92%)	557 (96%)	25 (4%)	1 (0%)	44	49
All	All	1733/1896 (91%)	1657 (96%)	75 (4%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASN

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	515/571 (90%)	493 (96%)	22 (4%)	25	26
1	B	516/571 (90%)	499 (97%)	17 (3%)	33	38
1	C	523/571 (92%)	505 (97%)	18 (3%)	32	37
All	All	1554/1713 (91%)	1497 (96%)	57 (4%)	29	33

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	64	ARG
1	A	67	ASP
1	A	99	ASN
1	A	113	SER
1	A	178	ASN
1	A	211	PRO
1	A	221	LYS
1	A	252	LEU
1	A	276	ARG
1	A	301	SER
1	A	350	SER

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Mol	Chain	Res	Type
1	A	441	ASN
1	A	488	SER
1	A	492	GLU
1	A	501	GLU
1	A	503	ASP
1	A	504	LEU
1	A	506	ASN
1	A	508	MET
1	A	572	THR
1	A	595	SER
1	B	34	ARG
1	B	88	ILE
1	B	165	LYS
1	B	184	LYS
1	B	188	GLU
1	B	221	LYS
1	B	276	ARG
1	B	294	LYS
1	B	301	SER
1	B	357	VAL
1	B	360	ASP
1	B	368	GLU
1	B	387	THR
1	B	417	ILE
1	B	504	LEU
1	B	585	GLN
1	B	626	ASN
1	C	34	ARG
1	C	67	ASP
1	C	78	SER
1	C	99	ASN
1	C	162	LYS
1	C	187	LEU
1	C	252	LEU
1	C	276	ARG
1	C	284	GLN
1	C	294	LYS
1	C	301	SER
1	C	376	ILE
1	C	397	ILE
1	C	414	THR
1	C	486	GLN

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Mol	Chain	Res	Type
1	C	487	THR
1	C	574	THR
1	C	595	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	ASN
1	B	582	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 ⓘ

2 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	E	1	2	12,12,12	2.74	5 (41%)	17,17,17	1.68	5 (29%)
2	SIA	E	2	2	18,19,21	2.96	7 (38%)	20,27,31	2.94	5 (25%)

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	E	1	2	-	0/2/22/22	0/1/1/1
2	SIA	E	2	2	-	0/16/32/38	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	GLC	O1-C1	7.23	1.62	1.39
2	E	2	SIA	C4-C5	-6.70	1.47	1.53
2	E	2	SIA	C3-C4	4.93	1.61	1.52
2	E	2	SIA	O4-C4	4.83	1.53	1.43
2	E	2	SIA	C2-C1	-4.68	1.48	1.52
2	E	2	SIA	C3-C2	4.51	1.60	1.52
2	E	2	SIA	O6-C6	-3.09	1.39	1.44
2	E	1	GLC	C3-C2	2.87	1.59	1.52
2	E	1	GLC	O5-C5	2.71	1.50	1.44
2	E	1	GLC	O4-C4	2.36	1.48	1.43
2	E	1	GLC	O5-C1	2.11	1.48	1.42
2	E	2	SIA	C9-C8	2.08	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	SIA	O6-C2-C3	-10.26	96.35	110.46
2	E	2	SIA	C6-O6-C2	4.25	120.43	111.34
2	E	2	SIA	C4-C3-C2	3.62	116.30	109.81
2	E	1	GLC	O2-C2-C1	-3.15	101.86	109.16
2	E	2	SIA	O7-C7-C6	-2.88	103.28	109.50
2	E	2	SIA	O6-C2-C1	2.86	113.30	107.70
2	E	1	GLC	C1-C2-C3	2.76	116.03	110.31
2	E	1	GLC	O1-C1-O5	2.51	117.92	110.38
2	E	1	GLC	C4-C3-C2	-2.42	106.59	110.82
2	E	1	GLC	O6-C6-C5	-2.22	103.68	111.29

There are no chirality outliers.

There are no torsion outliers.

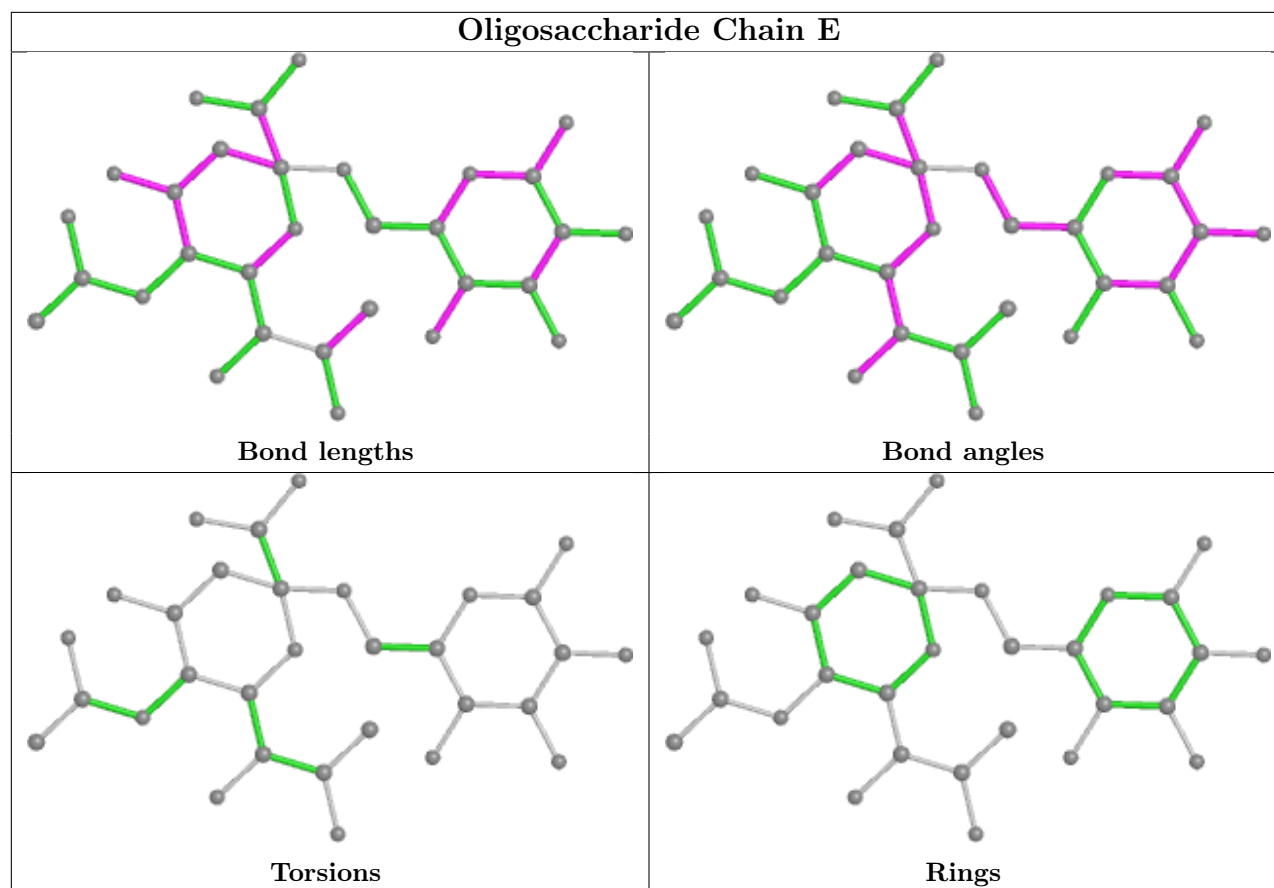
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	SIA	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	C	701	-	21,21,21	0.81	0	25,31,31	1.50	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIA	C	701	-	-	7/20/38/38	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	SIA	O2-C2-C1	-5.38	99.82	110.76
3	C	701	SIA	O2-C2-C3	2.46	112.95	109.40
3	C	701	SIA	O1A-C1-C2	-2.40	119.95	123.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

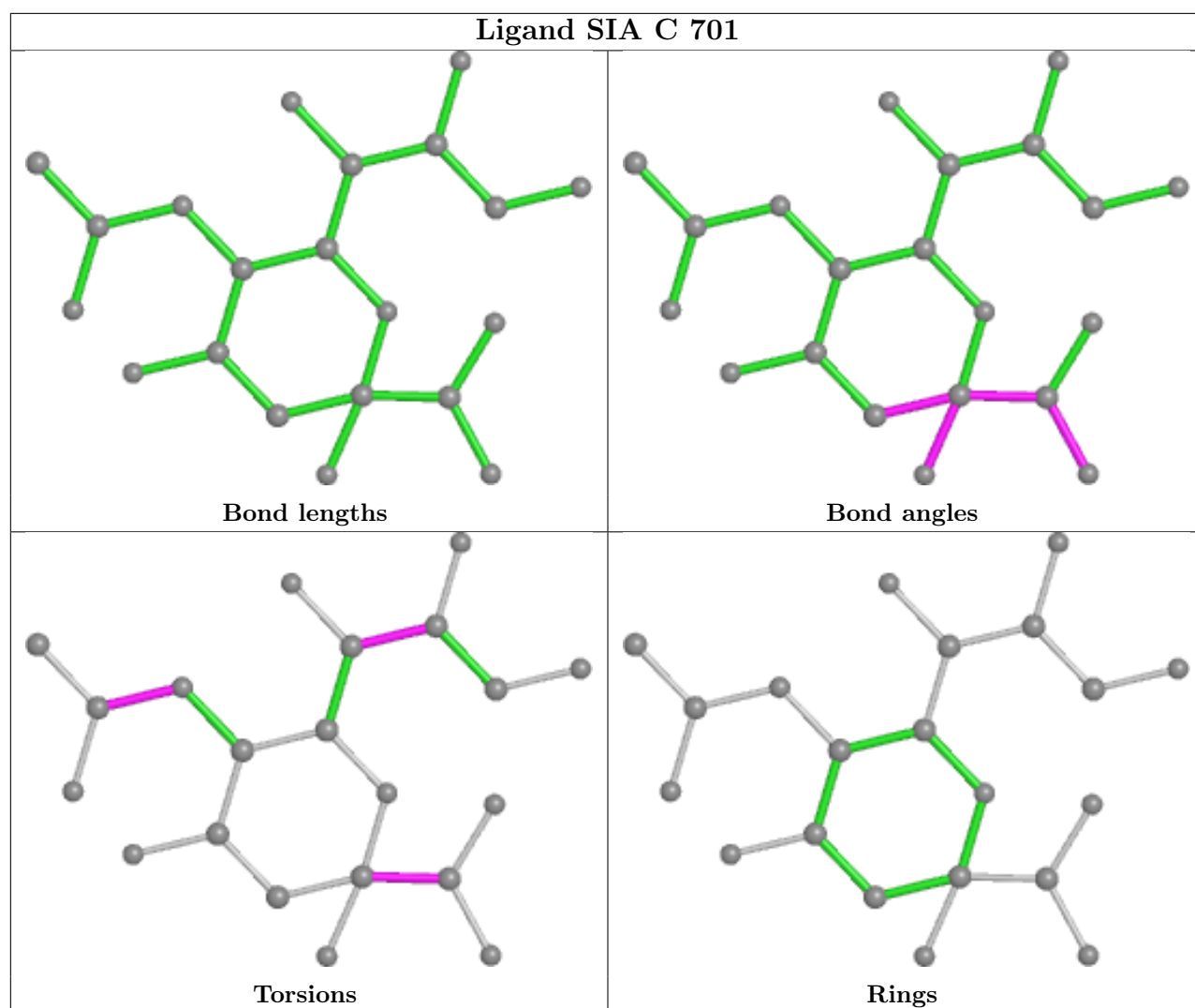
Mol	Chain	Res	Type	Atoms
3	C	701	SIA	C11-C10-N5-C5
3	C	701	SIA	O10-C10-N5-C5
3	C	701	SIA	C6-C7-C8-O8
3	C	701	SIA	C6-C7-C8-C9
3	C	701	SIA	O7-C7-C8-O8
3	C	701	SIA	O1A-C1-C2-O6
3	C	701	SIA	O1A-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	SIA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	581/632 (91%)	0.12	21 (3%) 46 46	16, 24, 35, 53	0
1	B	583/632 (92%)	-0.02	15 (2%) 57 58	14, 24, 35, 42	0
1	C	587/632 (92%)	-0.04	11 (1%) 66 66	18, 24, 34, 43	0
All	All	1751/1896 (92%)	0.02	47 (2%) 56 56	14, 24, 35, 53	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	624	ILE	5.6
1	B	575	ILE	4.2
1	C	488	SER	4.0
1	B	70	ILE	3.9
1	A	501	GLU	3.6
1	B	346	PRO	3.2
1	A	520	SER	3.2
1	A	595	SER	3.2
1	A	160	GLY	3.2
1	B	577	GLY	3.1
1	B	21	ASP	3.1
1	C	489	SER	3.0
1	B	98	ALA	3.0
1	C	574	THR	3.0
1	B	576	ASP	3.0
1	A	491	ILE	2.9
1	C	188	GLU	2.9
1	C	348	PRO	2.9
1	A	506	ASN	2.8
1	B	349	GLU	2.8
1	B	626	ASN	2.8
1	C	398	PRO	2.7
1	A	503	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	99	ASN	2.7
1	B	586	ASN	2.5
1	C	397	ILE	2.5
1	A	21	ASP	2.5
1	A	554	ASN	2.4
1	B	348	PRO	2.4
1	A	348	PRO	2.3
1	B	67	ASP	2.3
1	C	578	TYR	2.3
1	A	626	ASN	2.3
1	B	350	SER	2.3
1	A	579	ASN	2.3
1	B	490	ASN	2.3
1	C	576	ASP	2.3
1	C	302	ASN	2.2
1	A	625	THR	2.2
1	B	561	TYR	2.2
1	A	521	THR	2.1
1	A	583	ILE	2.1
1	C	346	PRO	2.1
1	A	600	ASN	2.1
1	A	346	PRO	2.0
1	A	349	GLU	2.0
1	A	596	ILE	2.0

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

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

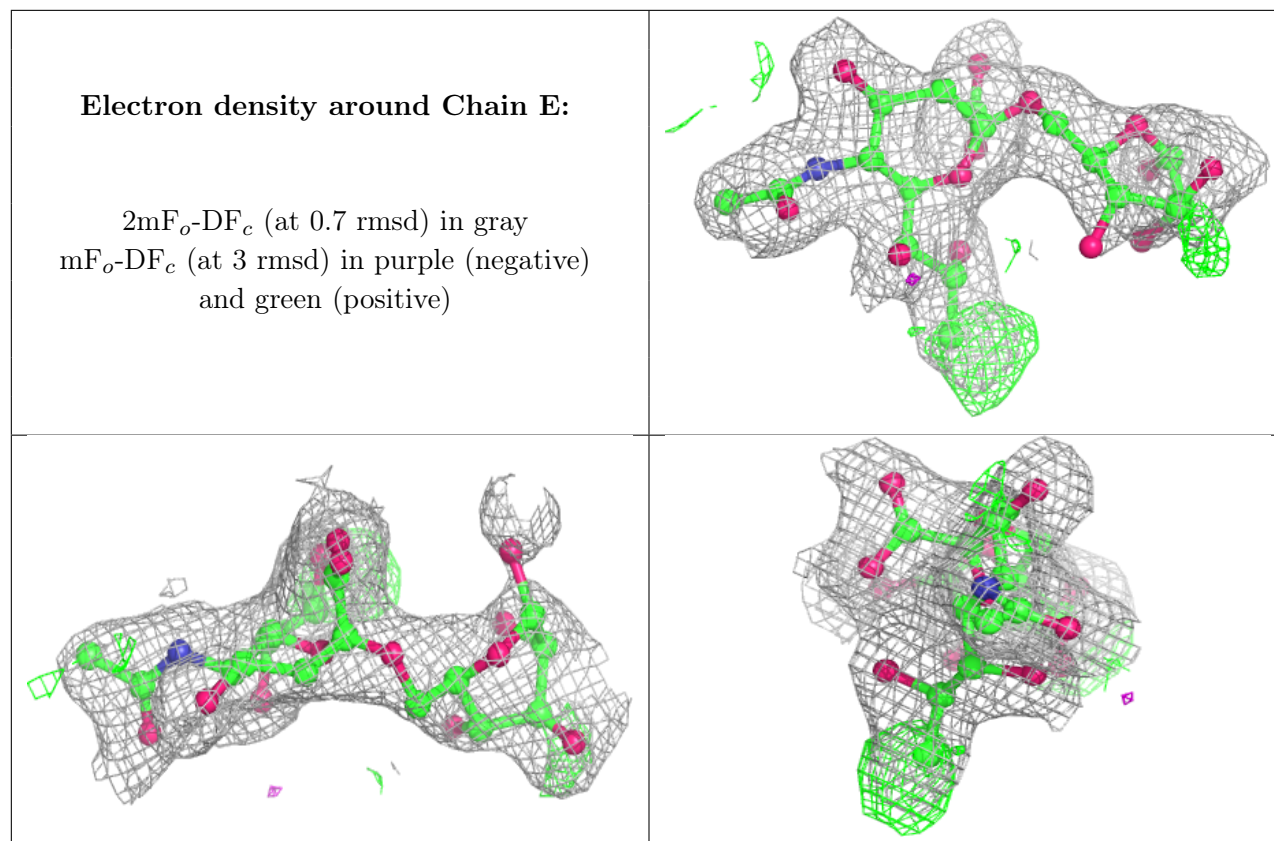
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	1	12/12	-	-	26,34,39,48	0
2	SIA	E	2	19/21	-	-	18,22,24,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

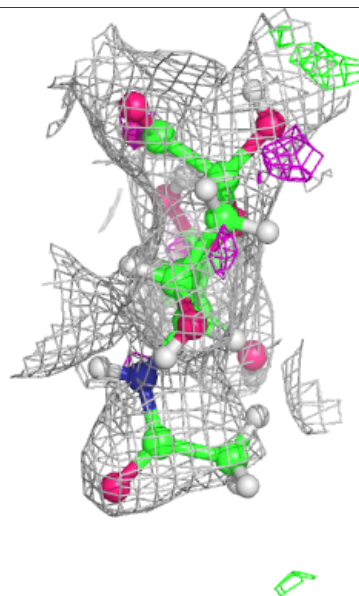
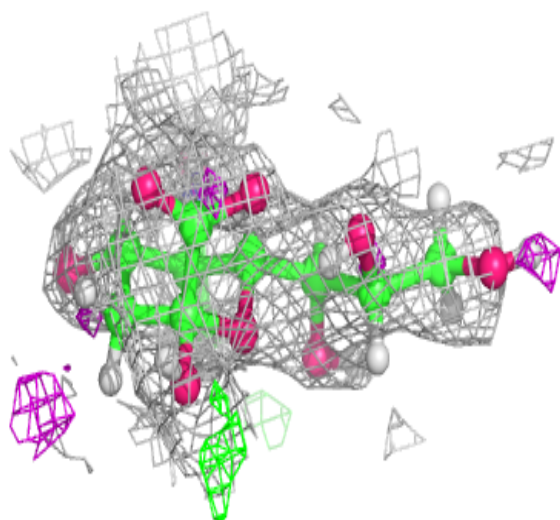
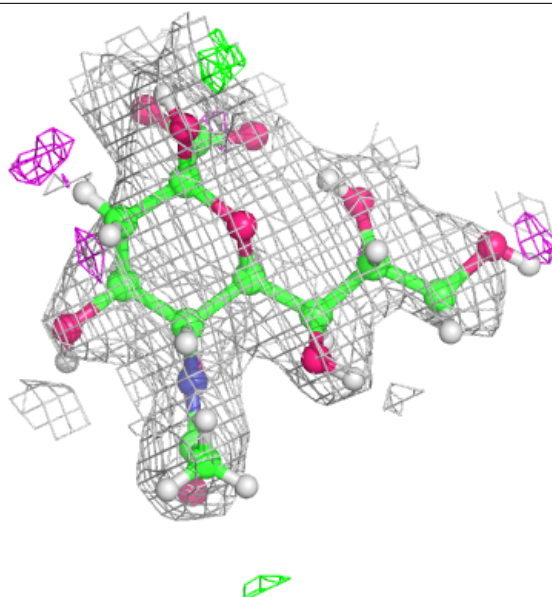
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SIA	C	701	21/21	0.81	0.09	24,31,34,35	0

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

Electron density around SIA C 701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.