W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 08:23 pm GMT

PDB ID	:	7OVW
Title	:	Binding domain of botulinum neurotoxin E in complex with GD1a
Authors	:	Masuyer, G.; Stenmark, P.
Deposited on	:	2021-06-15
Resolution	:	2.20 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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.
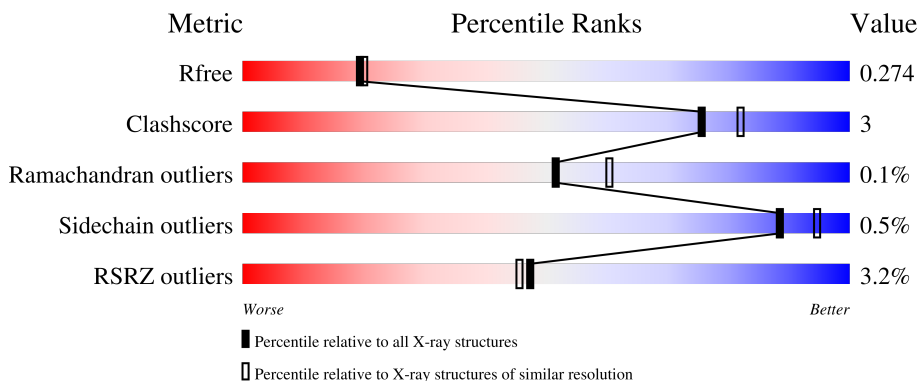
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	468	
1	BBB	468	
2	GGG	5	
3	HHH	4	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13614 atoms, of which 6551 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 Neurotoxin type E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	404	Total 6548	C 2101	H 3223	N 574	O 641	S 9	97	1	0
1	BBB	404	Total 6534	C 2097	H 3217	N 572	O 639	S 9	97	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	785	MET	-	initiating methionine	UNP A5H0J8
AAA	786	GLY	-	expression tag	UNP A5H0J8
AAA	787	SER	-	expression tag	UNP A5H0J8
AAA	788	SER	-	expression tag	UNP A5H0J8
AAA	789	HIS	-	expression tag	UNP A5H0J8
AAA	790	HIS	-	expression tag	UNP A5H0J8
AAA	791	HIS	-	expression tag	UNP A5H0J8
AAA	792	HIS	-	expression tag	UNP A5H0J8
AAA	793	HIS	-	expression tag	UNP A5H0J8
AAA	794	HIS	-	expression tag	UNP A5H0J8
AAA	795	SER	-	expression tag	UNP A5H0J8
AAA	796	SER	-	expression tag	UNP A5H0J8
AAA	797	GLY	-	expression tag	UNP A5H0J8
AAA	798	LEU	-	expression tag	UNP A5H0J8
AAA	799	VAL	-	expression tag	UNP A5H0J8
AAA	800	PRO	-	expression tag	UNP A5H0J8
AAA	801	ARG	-	expression tag	UNP A5H0J8
AAA	802	GLY	-	expression tag	UNP A5H0J8
AAA	803	SER	-	expression tag	UNP A5H0J8
AAA	804	HIS	-	expression tag	UNP A5H0J8
AAA	805	MET	-	expression tag	UNP A5H0J8
AAA	806	ALA	-	expression tag	UNP A5H0J8
AAA	807	SER	-	expression tag	UNP A5H0J8
AAA	808	MET	-	expression tag	UNP A5H0J8
AAA	809	TYR	-	expression tag	UNP A5H0J8

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	810	PRO	-	expression tag	UNP A5H0J8
AAA	811	TYR	-	expression tag	UNP A5H0J8
AAA	812	ASP	-	expression tag	UNP A5H0J8
AAA	813	VAL	-	expression tag	UNP A5H0J8
AAA	814	PRO	-	expression tag	UNP A5H0J8
AAA	815	ASP	-	expression tag	UNP A5H0J8
AAA	816	TYR	-	expression tag	UNP A5H0J8
AAA	817	ALA	-	expression tag	UNP A5H0J8
AAA	818	GLY	-	expression tag	UNP A5H0J8
AAA	819	SER	-	expression tag	UNP A5H0J8
BBB	785	MET	-	initiating methionine	UNP A5H0J8
BBB	786	GLY	-	expression tag	UNP A5H0J8
BBB	787	SER	-	expression tag	UNP A5H0J8
BBB	788	SER	-	expression tag	UNP A5H0J8
BBB	789	HIS	-	expression tag	UNP A5H0J8
BBB	790	HIS	-	expression tag	UNP A5H0J8
BBB	791	HIS	-	expression tag	UNP A5H0J8
BBB	792	HIS	-	expression tag	UNP A5H0J8
BBB	793	HIS	-	expression tag	UNP A5H0J8
BBB	794	HIS	-	expression tag	UNP A5H0J8
BBB	795	SER	-	expression tag	UNP A5H0J8
BBB	796	SER	-	expression tag	UNP A5H0J8
BBB	797	GLY	-	expression tag	UNP A5H0J8
BBB	798	LEU	-	expression tag	UNP A5H0J8
BBB	799	VAL	-	expression tag	UNP A5H0J8
BBB	800	PRO	-	expression tag	UNP A5H0J8
BBB	801	ARG	-	expression tag	UNP A5H0J8
BBB	802	GLY	-	expression tag	UNP A5H0J8
BBB	803	SER	-	expression tag	UNP A5H0J8
BBB	804	HIS	-	expression tag	UNP A5H0J8
BBB	805	MET	-	expression tag	UNP A5H0J8
BBB	806	ALA	-	expression tag	UNP A5H0J8
BBB	807	SER	-	expression tag	UNP A5H0J8
BBB	808	MET	-	expression tag	UNP A5H0J8
BBB	809	TYR	-	expression tag	UNP A5H0J8
BBB	810	PRO	-	expression tag	UNP A5H0J8
BBB	811	TYR	-	expression tag	UNP A5H0J8
BBB	812	ASP	-	expression tag	UNP A5H0J8
BBB	813	VAL	-	expression tag	UNP A5H0J8
BBB	814	PRO	-	expression tag	UNP A5H0J8
BBB	815	ASP	-	expression tag	UNP A5H0J8
BBB	816	TYR	-	expression tag	UNP A5H0J8

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	817	ALA	-	expression tag	UNP A5H0J8
BBB	818	GLY	-	expression tag	UNP A5H0J8
BBB	819	SER	-	expression tag	UNP A5H0J8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	GGG	5	129	37	61	2	29	16	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.
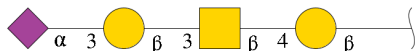
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	HHH	4	106	31	50	2	23	12	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	AAA	169	169	169	0	0
4	BBB	128	128	128	0	0

3 Residue-property plots ⓘ

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.
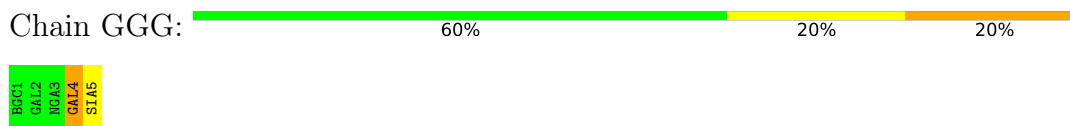
• Molecule 1: Neurotoxin type E

Chain AAA:

• Molecule 1: Neurotoxin type E

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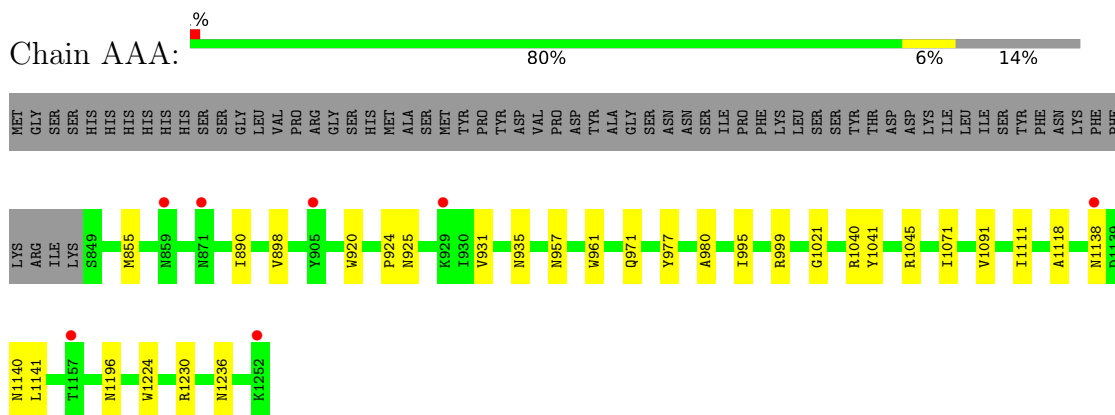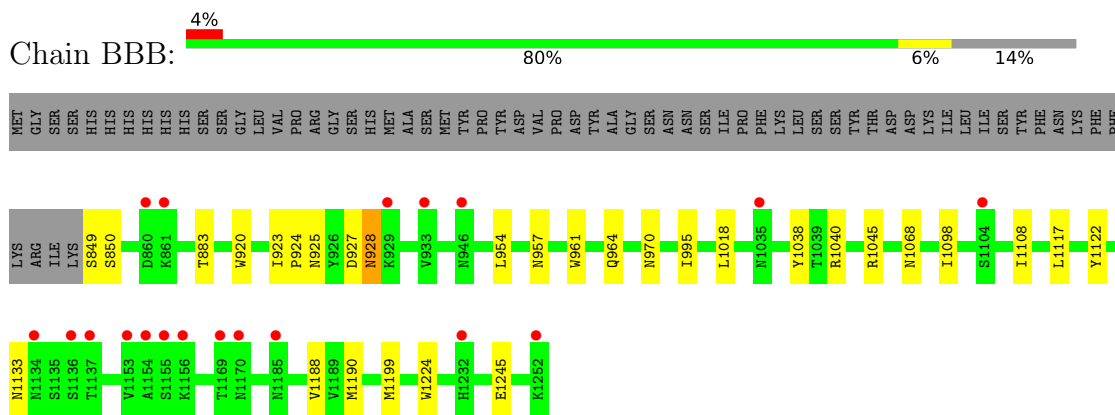
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain GGG:

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

Chain HHH:

50%   50%

GAL1 NGA2 GAL3 SIA4
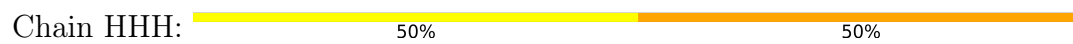
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.37Å 84.92Å 79.90Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	53.77 – 2.20 53.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (53.77-2.20) 95.2 (53.71-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.271 0.221 , 0.274	Depositor DCC
R_{free} test set	2081 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.2	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13614	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	AAA	0.63	0/3395	0.72	0/4603
1	BBB	0.64	0/3387	0.72	0/4592
All	All	0.64	0/6782	0.72	0/9195

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	3325	3223	3215	21	0
1	BBB	3317	3217	3210	19	0
2	GGG	68	61	58	1	0
3	HHH	56	50	47	3	0
4	AAA	169	0	0	1	0
4	BBB	128	0	0	1	0
All	All	7063	6551	6530	41	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 3.

All (41) 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:BBB:925:ASN:HD21	1:BBB:957:ASN:HD21	1.12	0.98
1:AAA:925:ASN:HD21	1:AAA:957:ASN:HD21	1.28	0.81
1:BBB:924:PRO:O	1:BBB:1040:ARG:NH2	2.30	0.64
1:AAA:1230:ARG:H	1:AAA:1236:ASN:HD21	1.45	0.64
1:AAA:925:ASN:HD21	1:AAA:957:ASN:ND2	1.96	0.63
1:BBB:925:ASN:HD21	1:BBB:957:ASN:ND2	1.91	0.60
1:AAA:961:TRP:CE2	1:AAA:995:ILE:HG21	2.39	0.57
1:AAA:999:ARG:NH2	1:AAA:1021:GLY:O	2.38	0.55
3:HHH:4:SIA:H112	3:HHH:4:SIA:O4	2.06	0.55
1:AAA:925:ASN:ND2	1:AAA:957:ASN:HD21	2.04	0.53
1:AAA:1111:ILE:HD11	1:BBB:1018:LEU:HD12	1.92	0.51
1:BBB:920:TRP:HB2	1:BBB:1045:ARG:HG2	1.93	0.51
1:AAA:924:PRO:O	1:AAA:1040:ARG:NH2	2.40	0.50
1:AAA:1091:VAL:HG21	1:AAA:1196:ASN:HD22	1.78	0.49
1:BBB:961:TRP:CE2	1:BBB:995:ILE:HG21	2.48	0.48
1:AAA:855:MET:HE1	1:AAA:898:VAL:HG11	1.96	0.48
1:BBB:883:THR:HG21	4:BBB:1344:HOH:O	2.14	0.47
1:BBB:1190:MET:CE	1:BBB:1199:MET:HG2	2.45	0.47
1:AAA:980:ALA:HB3	1:AAA:1118:ALA:HB2	1.97	0.46
1:BBB:1122:TYR:CE1	1:BBB:1245:GLU:HA	2.51	0.46
1:BBB:928:ASN:HD22	1:BBB:928:ASN:N	2.14	0.46
1:BBB:1038:TYR:OH	1:BBB:1040:ARG:NH1	2.48	0.46
1:AAA:1196:ASN:ND2	4:AAA:1307:HOH:O	2.49	0.45
1:AAA:920:TRP:HB2	1:AAA:1045:ARG:HG2	1.97	0.45
1:AAA:1224:TRP:CE3	2:GGG:4:GAL:H5	2.52	0.45
3:HHH:4:SIA:O8	3:HHH:4:SIA:N5	2.48	0.45
1:AAA:1140[A]:ASN:OD1	1:AAA:1140[A]:ASN:N	2.51	0.44
1:AAA:925:ASN:HA	1:AAA:931:VAL:HG11	2.00	0.44
1:BBB:923:ILE:HD12	1:BBB:954:LEU:HD13	2.00	0.44
1:AAA:855:MET:CE	1:AAA:898:VAL:HG11	2.48	0.44
1:AAA:890:ILE:O	1:AAA:1041:TYR:HA	2.18	0.44
1:BBB:1224:TRP:CE3	3:HHH:3:GAL:H5	2.53	0.44
1:AAA:971:GLN:HA	1:AAA:971:GLN:NE2	2.33	0.43
1:BBB:1188:VAL:HG12	1:BBB:1190:MET:CE	2.48	0.42
1:BBB:849:SER:OG	1:BBB:850:SER:N	2.51	0.42
1:BBB:1117:LEU:N	1:BBB:1117:LEU:HD12	2.34	0.42
1:BBB:964:GLN:HE21	1:BBB:970:ASN:HB3	1.84	0.41
1:AAA:957:ASN:HA	1:AAA:977:TYR:CZ	2.55	0.41
1:BBB:1098:ILE:HD11	1:BBB:1108:ILE:HD12	2.02	0.41
1:BBB:927:ASP:O	1:BBB:928:ASN:HB2	2.22	0.40
1:AAA:1071:ILE:HD13	1:AAA:1141:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	AAA	403/468 (86%)	384 (95%)	19 (5%)	0	100	100
1	BBB	402/468 (86%)	384 (96%)	17 (4%)	1 (0%)	47	55
All	All	805/936 (86%)	768 (95%)	36 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	1068	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	AAA	376/433 (87%)	374 (100%)	2 (0%)	88	94
1	BBB	375/433 (87%)	373 (100%)	2 (0%)	88	94
All	All	751/866 (87%)	747 (100%)	4 (0%)	88	94

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

Mol	Chain	Res	Type
1	AAA	935	ASN
1	AAA	1138	ASN

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Mol	Chain	Res	Type
1	BBB	928	ASN
1	BBB	1133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

9 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	BGC	GGG	1	2	12,12,12	0.48	0	17,17,17	0.49	0
2	GAL	GGG	2	2	11,11,12	0.37	0	15,15,17	0.93	0
2	NGA	GGG	3	2	14,14,15	0.41	0	17,19,21	0.55	0
2	GAL	GGG	4	2	11,11,12	0.29	0	15,15,17	0.85	1 (6%)
2	SIA	GGG	5	2	20,20,21	0.77	1 (5%)	24,28,31	1.13	3 (12%)
3	GAL	HHH	1	3	11,11,12	0.51	0	15,15,17	0.91	1 (6%)
3	NGA	HHH	2	3	14,14,15	0.39	0	17,19,21	1.39	3 (17%)
3	GAL	HHH	3	3	11,11,12	0.39	0	15,15,17	1.03	2 (13%)
3	SIA	HHH	4	3	20,20,21	0.74	1 (5%)	24,28,31	1.31	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
2	BGC	GGG	1	2	-	0/2/22/22	0/1/1/1
2	GAL	GGG	2	2	-	1/2/19/22	0/1/1/1
2	NGA	GGG	3	2	-	1/6/23/26	0/1/1/1
2	GAL	GGG	4	2	-	0/2/19/22	0/1/1/1
2	SIA	GGG	5	2	-	5/18/34/38	0/1/1/1
3	GAL	HHH	1	3	-	2/2/19/22	0/1/1/1
3	NGA	HHH	2	3	-	2/6/23/26	0/1/1/1
3	GAL	HHH	3	3	-	0/2/19/22	0/1/1/1
3	SIA	HHH	4	3	-	7/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	GGG	5	SIA	O1B-C1	-3.00	1.20	1.30
3	HHH	4	SIA	O1B-C1	-2.92	1.21	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	HHH	4	SIA	C8-C7-C6	3.87	120.36	113.03
3	HHH	2	NGA	C2-N2-C7	2.84	126.95	122.90
3	HHH	2	NGA	O5-C5-C6	2.78	111.56	107.20
3	HHH	2	NGA	C8-C7-N2	2.64	120.57	116.10
2	GGG	5	SIA	O1B-C1-C2	2.62	120.51	113.03
3	HHH	3	GAL	C1-O5-C5	2.58	115.69	112.19
3	HHH	1	GAL	O5-C5-C6	2.42	110.99	107.20
2	GGG	5	SIA	C8-C7-C6	2.35	117.48	113.03
3	HHH	4	SIA	O1B-C1-C2	2.34	119.70	113.03
2	GGG	5	SIA	C6-C5-N5	2.17	114.51	110.91
3	HHH	4	SIA	O6-C2-C1	2.14	111.90	107.70
2	GGG	4	GAL	O5-C5-C6	2.14	110.55	107.20
3	HHH	3	GAL	C1-C2-C3	2.12	112.27	109.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	GGG	5	SIA	C5-C6-C7-C8
2	GGG	5	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	GGG	5	SIA	O6-C6-C7-C8
3	HHH	4	SIA	C4-C5-N5-C10
3	HHH	4	SIA	C5-C6-C7-C8
3	HHH	4	SIA	C5-C6-C7-O7
3	HHH	4	SIA	O6-C6-C7-C8
3	HHH	4	SIA	O6-C6-C7-O7
3	HHH	4	SIA	C11-C10-N5-C5
3	HHH	4	SIA	O10-C10-N5-C5
3	HHH	1	GAL	O5-C5-C6-O6
3	HHH	1	GAL	C4-C5-C6-O6
3	HHH	2	NGA	C8-C7-N2-C2
3	HHH	2	NGA	O7-C7-N2-C2
2	GGG	2	GAL	O5-C5-C6-O6
2	GGG	5	SIA	C4-C5-N5-C10
2	GGG	3	NGA	C4-C5-C6-O6
2	GGG	5	SIA	C6-C5-N5-C10

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	HHH	3	GAL	1	0
3	HHH	4	SIA	2	0
2	GGG	4	GAL	1	0

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

Oligosaccharide Chain GGG

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain HHH

Bond lengths

Bond angles

Torsions

Rings
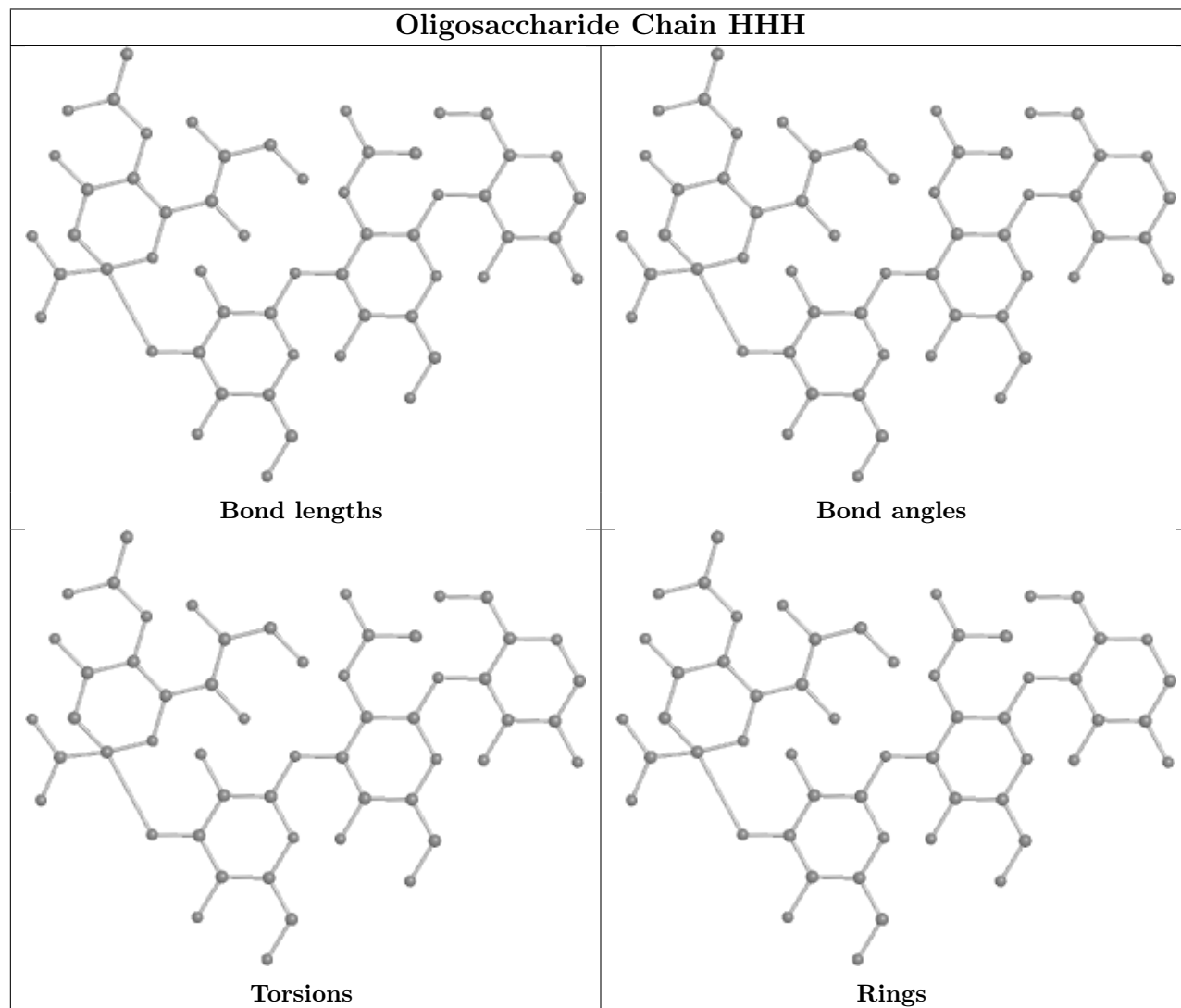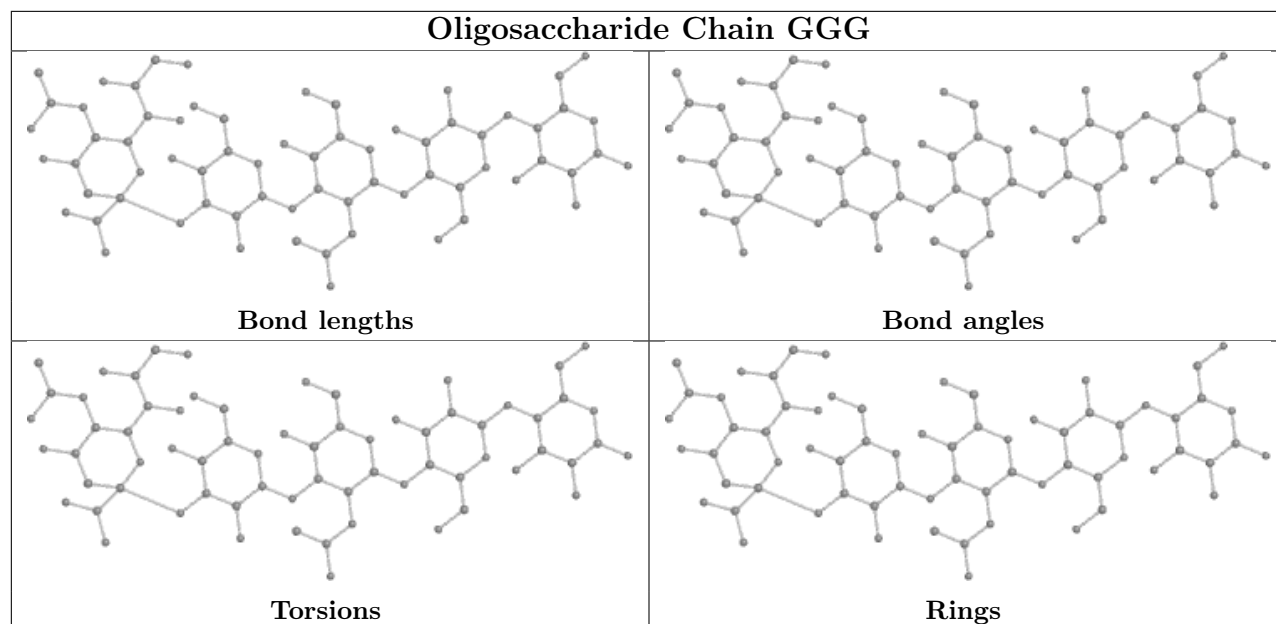
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	404/468 (86%)	0.06	7 (1%)	70	68	27, 39, 60, 90	0
1	BBB	404/468 (86%)	0.23	19 (4%)	31	30	29, 42, 69, 107	0
All	All	808/936 (86%)	0.14	26 (3%)	47	45	27, 40, 66, 107	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	1137	THR	5.6
1	BBB	1136	SER	4.7
1	BBB	1155	SER	4.6
1	BBB	1252	LYS	4.3
1	AAA	905	TYR	3.7
1	BBB	1185	ASN	3.4
1	BBB	860	ASP	3.3
1	AAA	1252	LYS	3.2
1	BBB	929	LYS	3.2
1	BBB	946	ASN	3.1
1	AAA	871	ASN	2.9
1	BBB	1170	ASN	2.8
1	BBB	1232	HIS	2.7
1	AAA	929	LYS	2.7
1	BBB	1156	LYS	2.6
1	AAA	859	ASN	2.6
1	AAA	1138	ASN	2.6
1	BBB	1035	ASN	2.6
1	AAA	1157	THR	2.6
1	BBB	1134	ASN	2.5
1	BBB	1154	ALA	2.4
1	BBB	933	VAL	2.4
1	BBB	1169	THR	2.4
1	BBB	1153	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	1104	SER	2.2
1	BBB	861	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GAL	HHH	1	11/12	0.81	0.11	56,58,61,62	3
2	GAL	GGG	2	11/12	0.82	0.18	60,69,75,76	3
2	BGC	GGG	1	12/12	0.83	0.22	81,91,95,99	4
3	SIA	HHH	4	20/21	0.85	0.18	44,56,63,63	4
2	SIA	GGG	5	20/21	0.89	0.16	40,46,53,54	4
3	NGA	HHH	2	14/15	0.91	0.15	49,53,62,65	2
2	NGA	GGG	3	14/15	0.94	0.13	45,52,56,60	2
3	GAL	HHH	3	11/12	0.95	0.13	46,46,48,51	3
2	GAL	GGG	4	11/12	0.95	0.13	35,38,40,41	3

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 GGG:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
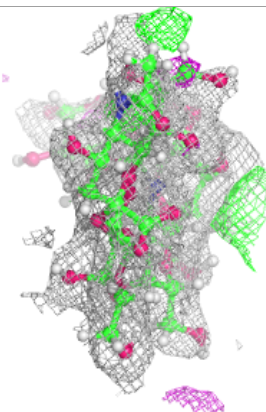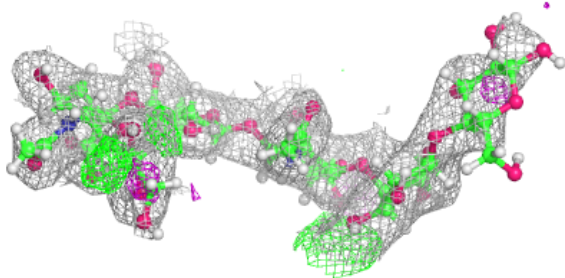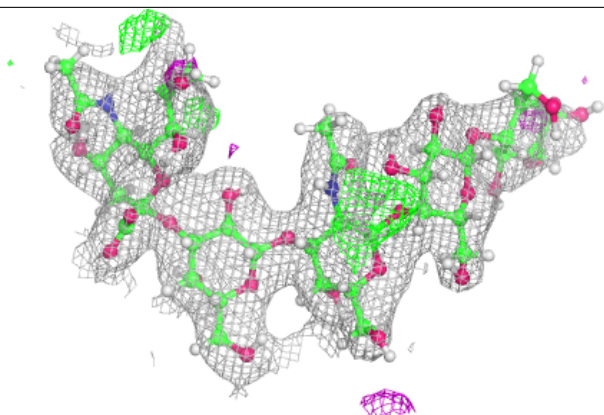
Electron density around Chain HHH:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
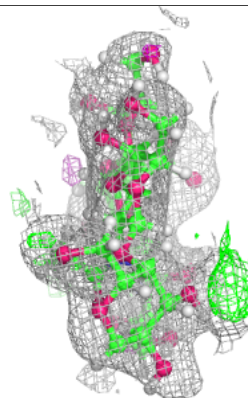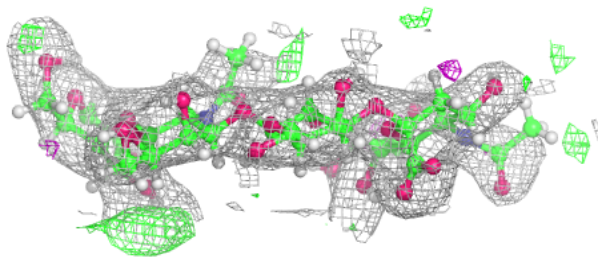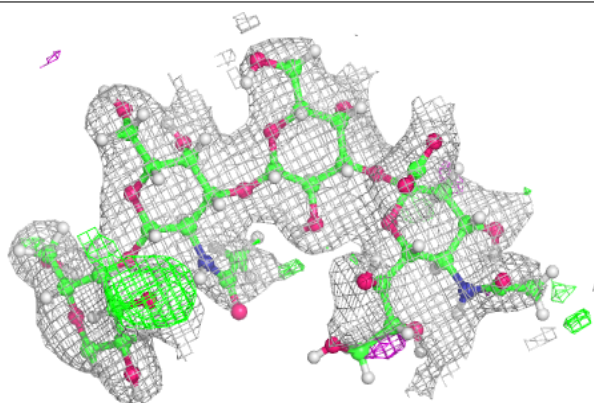
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.