



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 2, 2025 – 02:01 am GMT

PDB ID : 8RVG
Title : Structure of the binding domain of BoNT/A mutant Y1117V in complex with the GD1a ganglioside receptor
Authors : Masuyer, G.; Stenmark, P.
Deposited on : 2024-02-01
Resolution : 1.90 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

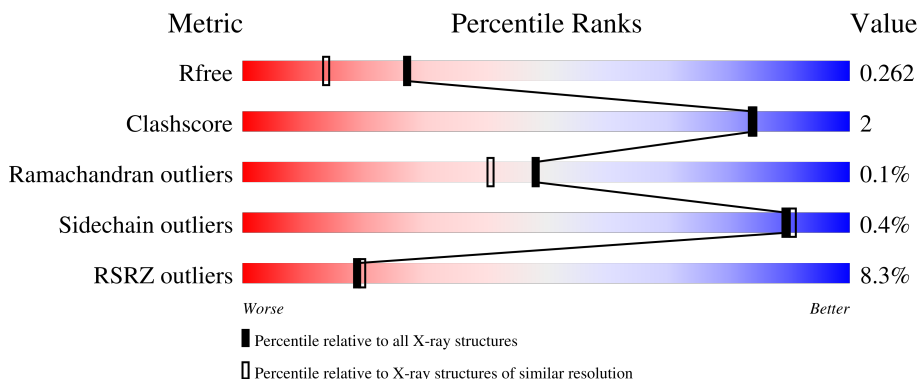
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	444	
1	B	444	
2	G	4	
2	H	4	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7268 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 Botulinum neurotoxin A heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	3	0
			3446	2197	589	645	15			
1	B	413	Total	C	N	O	S	0	1	0
			3397	2169	581	633	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	MET	-	initiating methionine	UNP P0DPI0
A	855	GLY	-	expression tag	UNP P0DPI0
A	856	SER	-	expression tag	UNP P0DPI0
A	857	SER	-	expression tag	UNP P0DPI0
A	858	HIS	-	expression tag	UNP P0DPI0
A	859	HIS	-	expression tag	UNP P0DPI0
A	860	HIS	-	expression tag	UNP P0DPI0
A	861	HIS	-	expression tag	UNP P0DPI0
A	862	HIS	-	expression tag	UNP P0DPI0
A	863	HIS	-	expression tag	UNP P0DPI0
A	864	SER	-	expression tag	UNP P0DPI0
A	865	SER	-	expression tag	UNP P0DPI0
A	866	GLY	-	expression tag	UNP P0DPI0
A	867	LEU	-	expression tag	UNP P0DPI0
A	868	VAL	-	expression tag	UNP P0DPI0
A	869	PRO	-	expression tag	UNP P0DPI0
A	870	ARG	-	expression tag	UNP P0DPI0
A	871	GLY	-	expression tag	UNP P0DPI0
A	872	SER	-	expression tag	UNP P0DPI0
A	873	HIS	-	expression tag	UNP P0DPI0
A	874	MET	-	expression tag	UNP P0DPI0
A	875	ASP	-	expression tag	UNP P0DPI0
A	1117	VAL	TYR	engineered mutation	UNP P0DPI0
A	1297	GLN	-	expression tag	UNP P0DPI0
B	854	MET	-	initiating methionine	UNP P0DPI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	855	GLY	-	expression tag	UNP P0DPI0
B	856	SER	-	expression tag	UNP P0DPI0
B	857	SER	-	expression tag	UNP P0DPI0
B	858	HIS	-	expression tag	UNP P0DPI0
B	859	HIS	-	expression tag	UNP P0DPI0
B	860	HIS	-	expression tag	UNP P0DPI0
B	861	HIS	-	expression tag	UNP P0DPI0
B	862	HIS	-	expression tag	UNP P0DPI0
B	863	HIS	-	expression tag	UNP P0DPI0
B	864	SER	-	expression tag	UNP P0DPI0
B	865	SER	-	expression tag	UNP P0DPI0
B	866	GLY	-	expression tag	UNP P0DPI0
B	867	LEU	-	expression tag	UNP P0DPI0
B	868	VAL	-	expression tag	UNP P0DPI0
B	869	PRO	-	expression tag	UNP P0DPI0
B	870	ARG	-	expression tag	UNP P0DPI0
B	871	GLY	-	expression tag	UNP P0DPI0
B	872	SER	-	expression tag	UNP P0DPI0
B	873	HIS	-	expression tag	UNP P0DPI0
B	874	MET	-	expression tag	UNP P0DPI0
B	875	ASP	-	expression tag	UNP P0DPI0
B	1117	VAL	TYR	engineered mutation	UNP P0DPI0
B	1297	GLN	-	expression tag	UNP P0DPI0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			56	31	2	23			
2	H	4	Total	C	N	O	0	0	0
			56	31	2	23			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		

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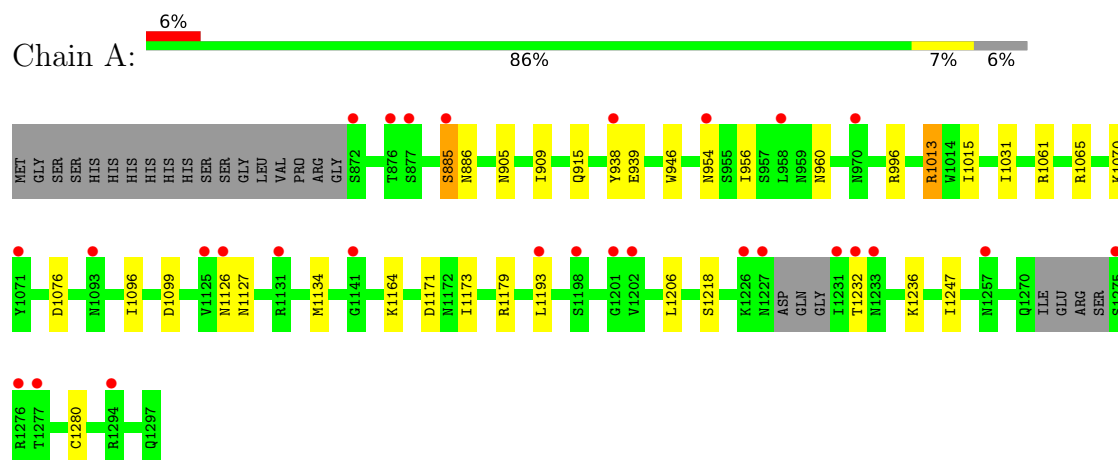
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	134	Total 134	O 134	0	0

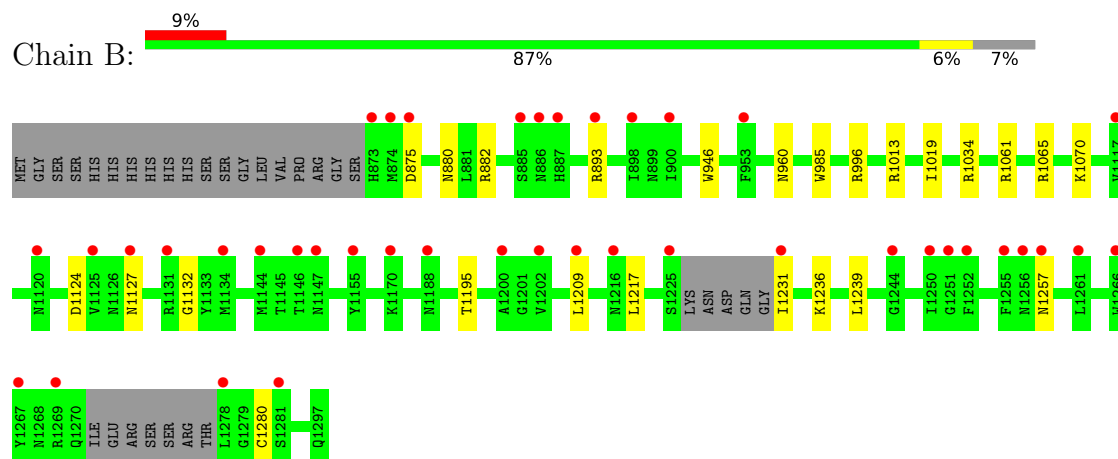
3 Residue-property plots

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: Botulinum neurotoxin A heavy chain



- Molecule 1: Botulinum neurotoxin A heavy chain



- 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



- 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

Chain H:  50% 50%

GAL1
NGA2
GAL3
STAA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 104.42Å 112.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.01 – 1.90 55.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.01-1.90) 99.7 (55.01-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.218 , 0.260 0.222 , 0.262	Depositor DCC
R_{free} test set	3381 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5510e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NGA, 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	0.54	0/3520	0.78	6/4760 (0.1%)
1	B	0.50	0/3467	0.72	2/4686 (0.0%)
All	All	0.52	0/6987	0.75	8/9446 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1013	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	1179	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	1134	MET	CA-CB-CG	-6.01	103.08	113.30
1	B	996	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	1013	ARG	NE-CZ-NH1	5.70	123.15	120.30

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	A	3446	0	3375	19	1
1	B	3397	0	3350	11	1
2	G	56	0	47	0	0
2	H	56	0	47	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	179	0	0	1	0
3	B	134	0	0	0	0
All	All	7268	0	6819	30	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 2.

The worst 5 of 30 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1236:LYS:NZ	1:B:1280:CYS:SG	2.44	0.90
1:A:885:SER:OG	1:A:886:ASN:N	2.05	0.87
1:A:1193:LEU:HD21	1:A:1206:LEU:HD13	1.81	0.63
1:A:960:ASN:HD21	1:A:1061:ARG:H	1.46	0.61
1:A:909:ILE:HG21	1:A:1173:ILE:HD11	1.82	0.60

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)
1:A:938[A]:TYR:CE1	1:B:1124:ASP:OD1[2_555]	2.12	0.08

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	416/444 (94%)	393 (94%)	23 (6%)	0	100	100
1	B	408/444 (92%)	396 (97%)	11 (3%)	1 (0%)	44	36
All	All	824/888 (93%)	789 (96%)	34 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1257	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/408 (94%)	381 (100%)	2 (0%)	86	88
1	B	379/408 (93%)	378 (100%)	1 (0%)	91	92
All	All	762/816 (93%)	759 (100%)	3 (0%)	89	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	885	SER
1	A	1065	ARG
1	B	1065	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	960	ASN
1	B	1046	ASN
1	B	1093	ASN
1	B	1073	ASN
1	A	1172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GAL	G	1	2	11,11,12	0.41	0	15,15,17	1.03	1 (6%)
2	NGA	G	2	2	14,14,15	0.24	0	17,19,21	0.99	1 (5%)
2	GAL	G	3	2	11,11,12	0.37	0	15,15,17	1.08	1 (6%)
2	SIA	G	4	2	20,20,21	0.54	0	24,28,31	1.22	3 (12%)
2	GAL	H	1	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NGA	H	2	2	14,14,15	0.43	0	17,19,21	0.70	0
2	GAL	H	3	2	11,11,12	0.44	0	15,15,17	1.21	2 (13%)
2	SIA	H	4	2	20,20,21	0.83	0	24,28,31	1.62	5 (20%)

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	GAL	G	1	2	-	2/2/19/22	0/1/1/1
2	NGA	G	2	2	-	1/6/23/26	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	SIA	G	4	2	-	2/18/34/38	0/1/1/1
2	GAL	H	1	2	-	2/2/19/22	0/1/1/1
2	NGA	H	2	2	-	0/6/23/26	0/1/1/1
2	GAL	H	3	2	-	0/2/19/22	0/1/1/1
2	SIA	H	4	2	-	8/18/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	SIA	C6-O6-C2	3.11	117.99	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	SIA	C8-C7-C6	3.04	118.80	113.03
2	H	3	GAL	O5-C5-C6	2.89	111.74	107.20
2	H	4	SIA	C11-C10-N5	2.82	120.88	116.10
2	H	4	SIA	O6-C2-C1	2.81	113.21	107.70

There are no chirality outliers.

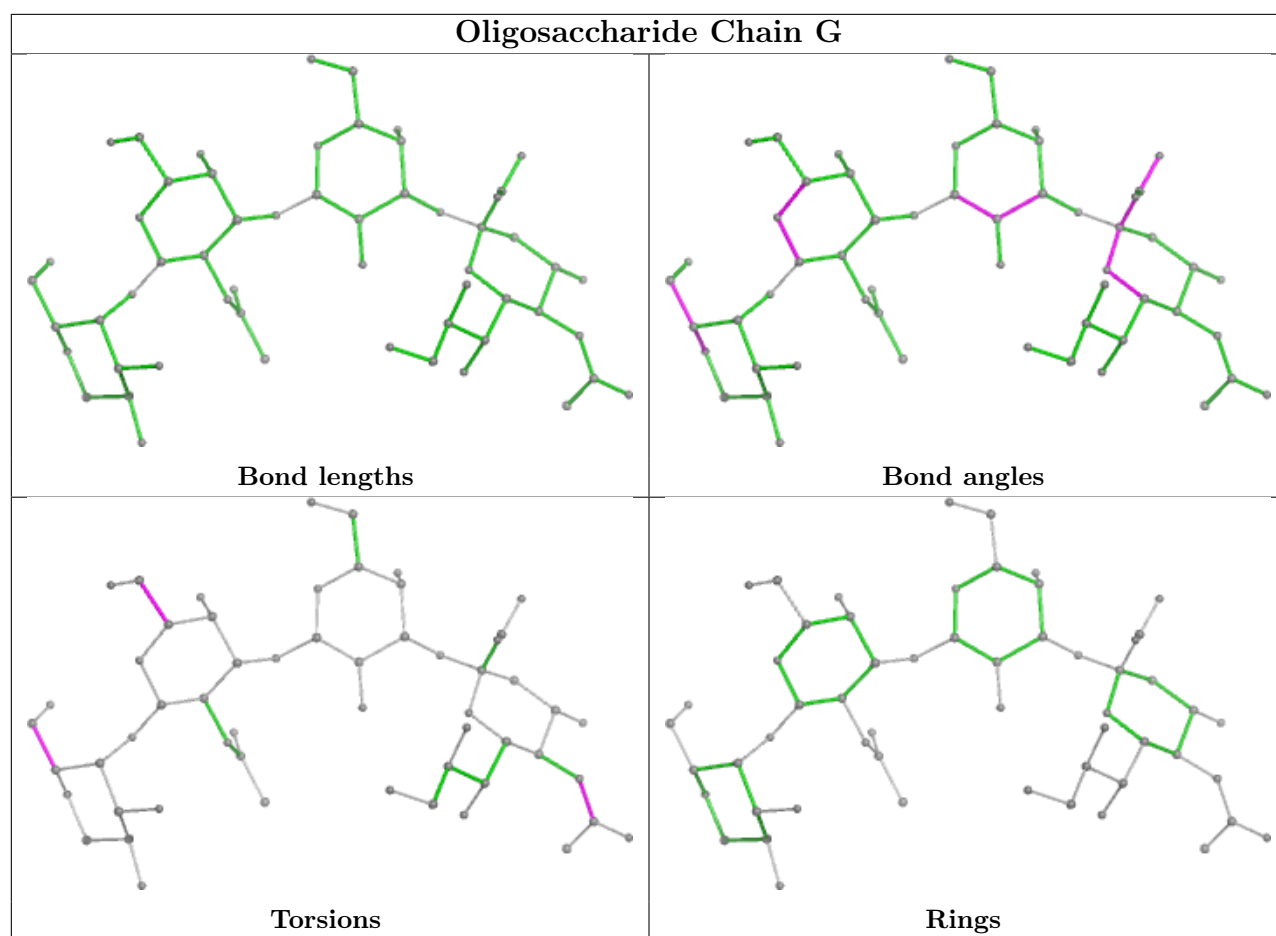
5 of 15 torsion outliers are listed below:

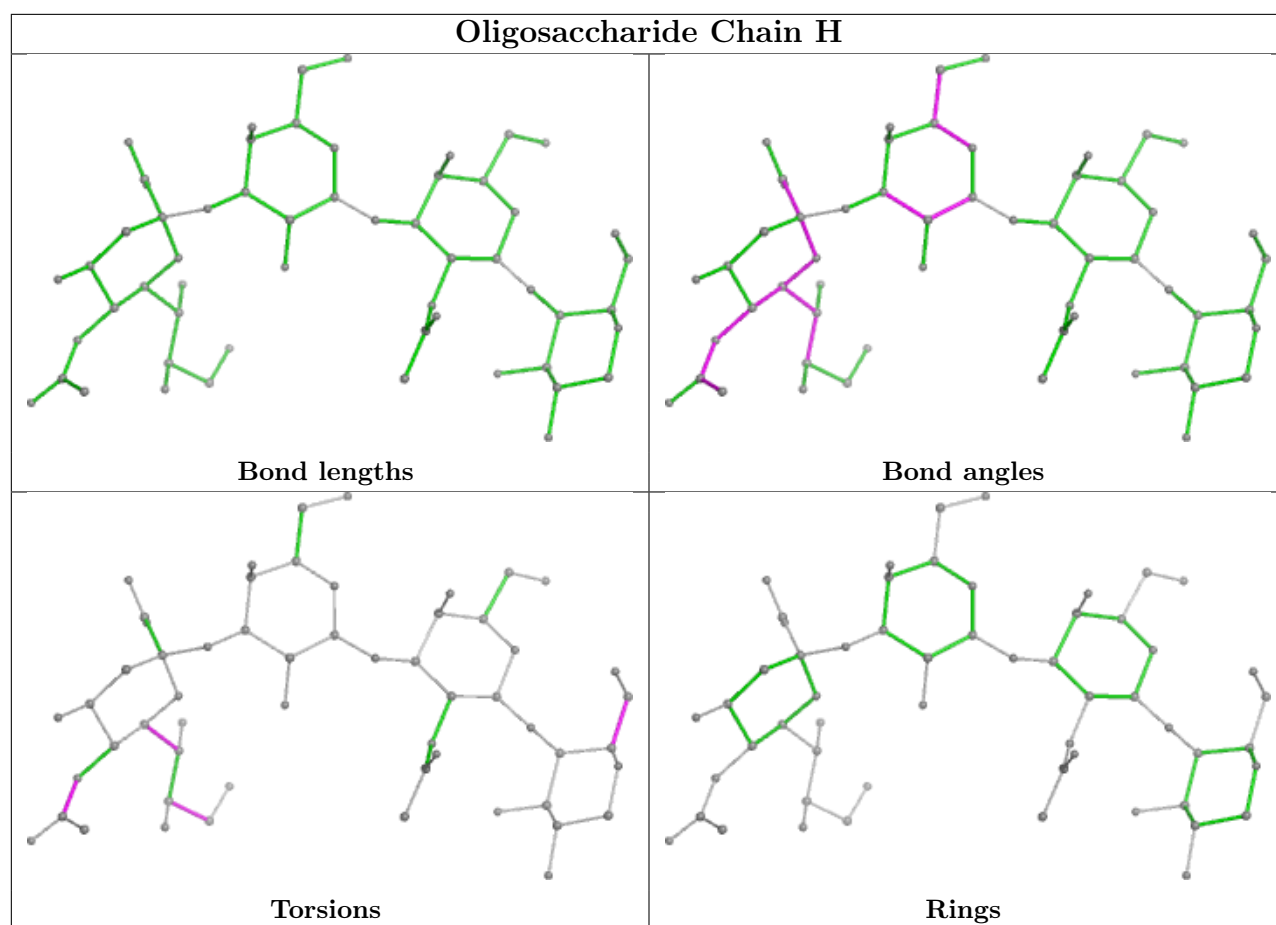
Mol	Chain	Res	Type	Atoms
2	H	4	SIA	C5-C6-C7-C8
2	H	4	SIA	C5-C6-C7-O7
2	H	4	SIA	O6-C6-C7-C8
2	H	4	SIA	O6-C6-C7-O7
2	G	4	SIA	C11-C10-N5-C5

There are no ring outliers.

No monomer is involved in short contacts.

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	419/444 (94%)	0.40	28 (6%)	25 26	12, 24, 38, 53	3 (0%)
1	B	413/444 (93%)	0.83	41 (9%)	14 15	17, 28, 45, 64	1 (0%)
All	All	832/888 (93%)	0.61	69 (8%)	19 20	12, 26, 42, 64	4 (0%)

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1256	ASN	6.0
1	A	1277	THR	4.7
1	B	1251	GLY	4.5
1	A	1231	ILE	4.4
1	A	1232	THR	4.4

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.