

wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2021 – 04:06 am BST

PDB ID : 7AWG

Title : Crystal structure of human butyrylcholinesterase in complex with (2-((1-(ben

zenesulfonyl)-1H-indol-4-yl)oxy)ethyl)(benzyl)amine

Authors: Brazzolotto, X.; Wichur, T.; Wieckowska, A.

Deposited on : 2020-11-08

Resolution : 2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

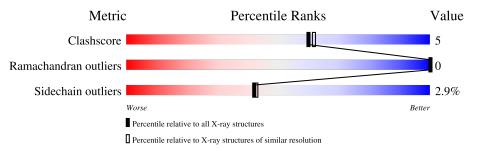
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain							
1	A	529	89%	9%						
2	В	2	50% 50%							
3	С	3	33% 67%							
3	D	3	67% 33%							

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



I	Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	10	GOL	A	613	_	_	X	-



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 4769 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 Cholinesterase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Λ	526	Total	С	N	О	S	0	0	0
1	A	320	4248	2743	713	776	16	U	0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

• Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mo	l Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	2	Total 24	C 14	N 1	O 9	0	0	0

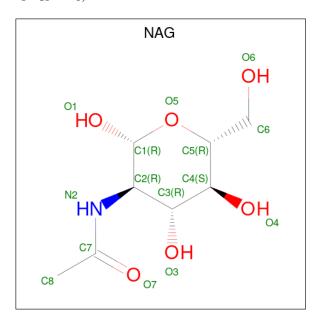
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	С	3	Total C N O 38 22 2 14	0	0	0
3	D	3	Total C N O 38 22 2 14	0	0	0

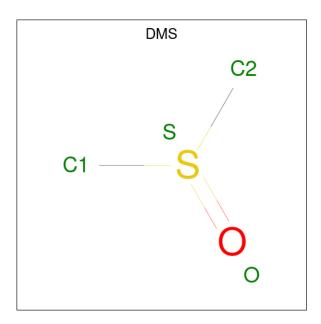
• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

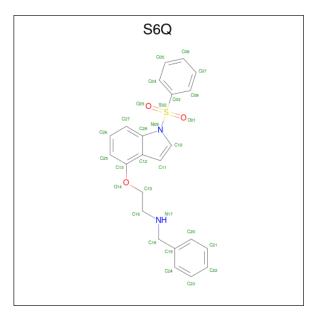
 \bullet Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2		S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0

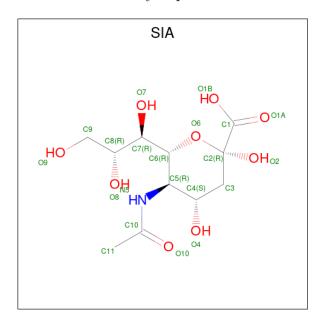
• Molecule 6 is $\{N\}$ -(phenylmethyl)-2-[1-(phenylsulfonyl)indol-4-yl]oxy-ethanami ne (three-letter code: S6Q) (formula: $C_{23}H_{22}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total 29	C 23	N 2	O 3	S 1	0	1

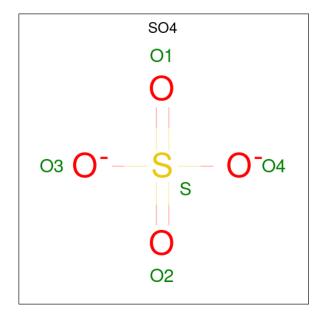


 $\bullet \ \ {\rm Molecule} \ 7 \ {\rm is} \ N\hbox{-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9)$.$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	Δ	1	Total	С	N	О	0	0
'	Λ	1	21	11	1	9	U	0

 \bullet Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0

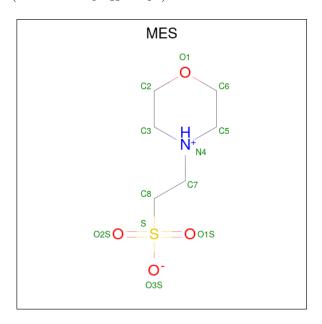
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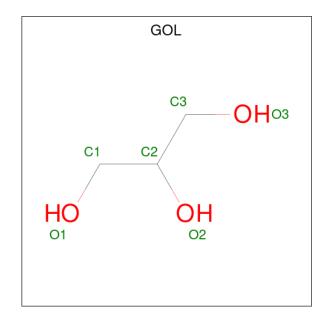
M	ol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	3	A	1	Total 5	O 4	S 1	0	0

• Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



M	ol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
()	A	1	Total 12	C 6	N 1	O 4	S 1	0	0

• Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	246	Total O 246 246	0	0

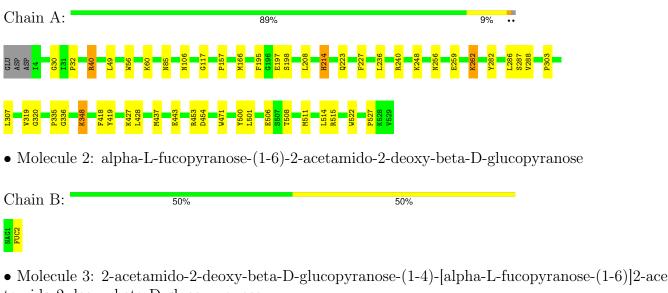


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.





tamido-2-deoxy-beta-D-glucopyranose

Chain C: 67%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-ace tamido-2-deoxy-beta-D-glucopyranose

Chain D: 33%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	I 4 2 2	Depositor	
Cell constants	154.48Å 154.48Å 128.16Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	48.85 - 2.00	Depositor	
% Data completeness	100.0 (48.85-2.00)	Depositor	
(in resolution range)	100.0 (40.00 2.00)	Берозног	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PHENIX 1.19rc4_4035	Depositor	
R, R_{free}	0.173 , 0.197	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4769	wwPDB-VP	
Average B, all atoms (Å ²)	43.0	wwPDB-VP	



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: GOL, S6Q, MES, FUC, DMS, NAG, SO4, 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	$\mathbf{lengths}$	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.45	0/4375	0.63	0/5938	

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 (i)

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	4248	0	4153	39	0
2	В	24	0	22	0	0
3	С	38	0	34	3	0
3	D	38	0	34	1	0
4	A	42	0	39	1	0
5	A	8	0	12	0	0
6	A	29	0	0	2	0
7	A	21	0	18	0	0
8	A	15	0	0	0	0
9	A	12	0	12	3	0
10	A	48	0	63	11	0
11	A	246	0	0	1	0
All	All	4769	0	4387	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 5.

The worst 5 of 41 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	Clash overlap (Å)
1:A:85:ASN:HD22	10:A:612:GOL:H31	1.56	0.71
1:A:427:LYS:HB2	10:A:615:GOL:H32	1.75	0.67
1:A:56:TRP:HE1	10:A:613:GOL:H12	1.60	0.66
1:A:157:PRO:HG3	1:A:236:LEU:HD22	1.84	0.59
1:A:60:LYS:HG3	10:A:613:GOL:H31	1.86	0.57

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	Perce	entiles
1	A	532/529 (101%)	512 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	459/454 (101%)	444 (97%)	15 (3%)	38 3'	7



\sim	c	1 -	• 1	• , 1			• 1	1 .		1 1	1 1	
Э	Οİ	15	residues	with	\mathbf{a}	non-rotameric	Side	chain	are	listed	bel	ow:

Mol	Chain	Res	Type
1	A	262	LYS
1	A	471	TRP
1	A	282	TYR
1	A	506	GLU
1	A	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	176	GLN
1	A	214	HIS

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 (i)

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	l Type Chain Res Link				Во	ond leng	ths	Bond angles			
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	NAG	В	1	2,1	14,14,15	0.44	0	17,19,21	0.42	0	
2	FUC	В	2	2	10,10,11	1.37	2 (20%)	14,14,16	0.83	0	
3	NAG	С	1	3,1	14,14,15	0.52	0	17,19,21	0.51	0	
3	NAG	С	2	3	14,14,15	0.22	0	17,19,21	0.46	0	



Mol	ol Type Chain Res Lin			Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	FUC	С	3	3	10,10,11	1.50	2 (20%)	14,14,16	1.82	4 (28%)	
3	NAG	D	1	3,1	14,14,15	0.40	0	17,19,21	1.16	1 (5%)	
3	NAG	D	2	3	14,14,15	0.25	0	17,19,21	0.64	1 (5%)	
3	FUC	D	3	3	10,10,11	1.08	0	14,14,16	1.09	1 (7%)	

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	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	В	2	2	-	-	0/1/1/1
3	NAG	С	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	4/6/23/26	0/1/1/1
3	FUC	С	3	3	-	-	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{A})$	Ideal(Å)
3	С	3	FUC	O5-C5	3.50	1.51	1.43
2	В	2	FUC	O5-C1	-2.54	1.39	1.43
3	С	3	FUC	C4-C5	2.05	1.57	1.52
2	В	2	FUC	C4-C3	2.01	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	3	FUC	O5-C5-C4	4.43	117.47	109.52
3	С	3	FUC	C1-C2-C3	-3.28	105.63	109.67
3	D	1	NAG	C1-O5-C5	3.07	116.36	112.19
3	С	3	FUC	C1-O5-C5	2.56	118.57	112.78
3	С	3	FUC	C3-C4-C5	2.52	113.69	109.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:



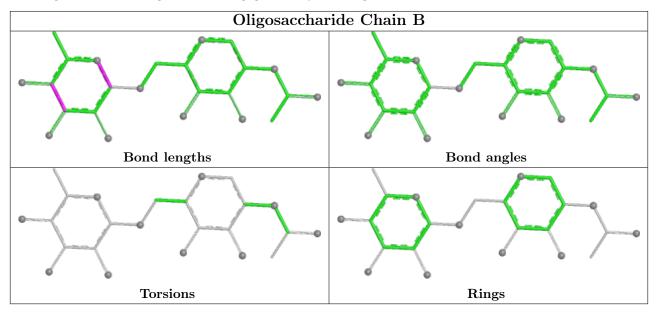
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	С	2	NAG	C8-C7-N2-C2
3	С	2	NAG	O7-C7-N2-C2
3	С	2	NAG	O5-C5-C6-O6

There are no ring outliers.

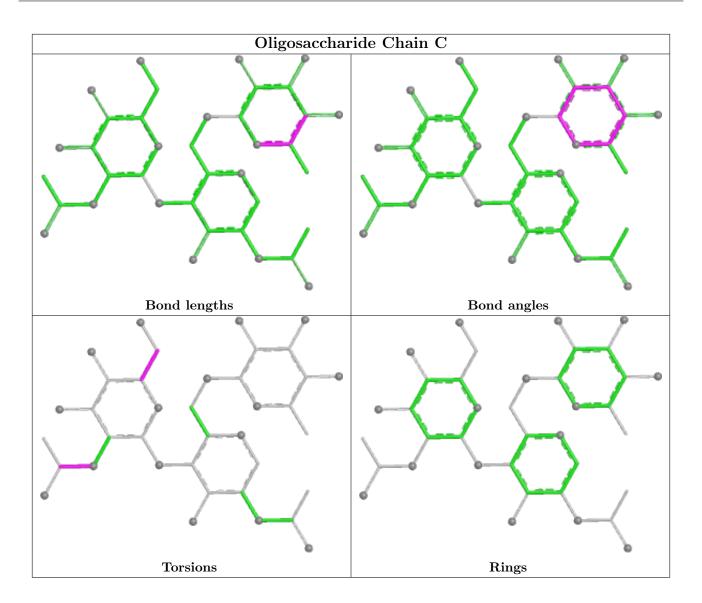
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	2	NAG	3	0
3	D	3	FUC	1	0

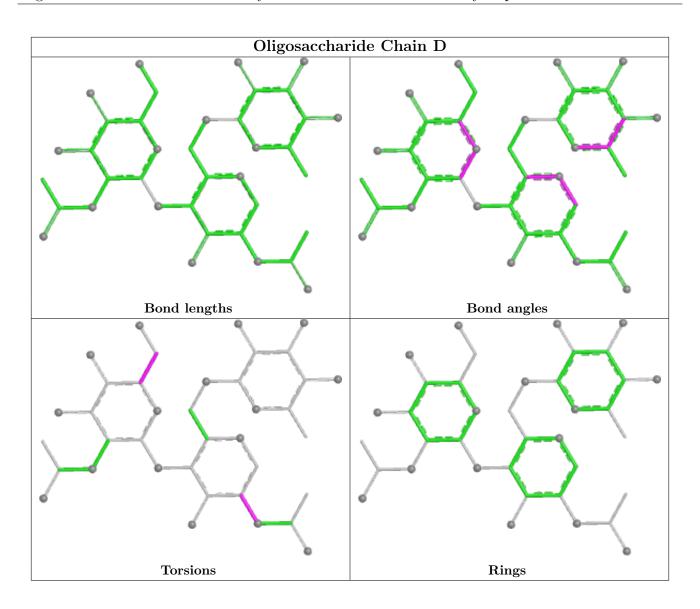
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry (i)

19 ligands 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).

Mal	$\left \begin{array}{c} \mathbf{Mol} \end{array} \right $ Type $\left \begin{array}{c} \mathbf{Chair} \end{array} \right $		Res	Link	\mathbf{B}_{0}	ond leng	${ m ths}$	E	Bond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
10	GOL	A	619	-	5, 5, 5	0.96	0	5,5,5	1.16	0
10	GOL	A	616	-	5,5,5	0.63	0	5,5,5	1.23	0
10	GOL	A	614	-	5,5,5	1.08	0	5,5,5	1.21	0



Mol	Type	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	ond angles		
MIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
7	SIA	A	607	-	18,21,21	2.06	3 (16%)	21,31,31	2.55	9 (42%)		
10	GOL	A	615	-	5,5,5	0.97	0	5,5,5	1.80	1 (20%)		
10	GOL	A	613	-	5,5,5	0.93	0	5,5,5	0.96	0		
4	NAG	A	602	1	14,14,15	0.51	0	17,19,21	0.47	0		
10	GOL	A	618	-	5,5,5	0.68	0	5,5,5	1.03	1 (20%)		
10	GOL	A	617	-	5,5,5	0.92	0	5,5,5	1.08	0		
5	DMS	A	606	-	3,3,3	0.65	0	3,3,3	0.95	0		
4	NAG	A	601	1	14,14,15	0.41	0	17,19,21	0.57	0		
9	MES	A	611	-	12,12,12	2.12	1 (8%)	14,16,16	2.72	7 (50%)		
8	SO4	A	608	-	4,4,4	0.33	0	6,6,6	0.17	0		
8	SO4	A	609	-	4,4,4	0.12	0	6,6,6	0.26	0		
4	NAG	A	603	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)		
8	SO4	A	610	-	4,4,4	0.21	0	6,6,6	0.14	0		
6	S6Q	A	605[A]	_	28,32,32	1.10	4 (14%)	35,44,44	2.23	10 (28%)		
10	GOL	A	612	-	5,5,5	0.90	0	5,5,5	1.04	0		
5	DMS	A	604	-	3,3,3	0.63	0	3,3,3	0.41	0		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	S6Q	A	605[A]	-	-	5/14/20/20	0/4/4/4
10	GOL	A	615	-	-	4/4/4/4	-
10	GOL	A	613	-	-	2/4/4/4	-
10	GOL	A	612	-	-	4/4/4/4	-
10	GOL	A	619	-	-	2/4/4/4	-
4	NAG	A	602	1	-	3/6/23/26	0/1/1/1
10	GOL	A	616	-	-	0/4/4/4	-
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
9	MES	A	611	-	-	4/6/14/14	0/1/1/1
10	GOL	A	614	-	-	4/4/4/4	-
7	SIA	A	607	-	-	6/14/38/38	0/1/1/1
10	GOL	A	618	-		0/4/4/4	-
10	GOL	A	617	-	-	2/4/4/4	-
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1

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



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
7	A	607	SIA	O6-C2	7.07	1.50	1.43
9	A	611	MES	C8-S	-6.97	1.67	1.77
7	A	607	SIA	C3-C2	2.86	1.55	1.51
7	A	607	SIA	C7-C6	2.58	1.56	1.53
6	A	605[A]	S6Q	C10-N09	2.49	1.43	1.38

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
7	A	607	SIA	C6-C5-N5	6.91	122.40	110.91
6	A	605[A]	S6Q	C03-S02-N09	5.69	110.88	104.95
7	A	607	SIA	C5-N5-C10	5.27	135.99	123.18
6	A	605[A]	S6Q	C08-C03-C04	-4.85	113.67	120.44
6	A	605[A]	S6Q	C05-C04-C03	4.60	123.73	118.95

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605[A]	S6Q	C12-C13-O14-C15
6	A	605[A]	S6Q	C25-C13-O14-C15
6	A	605[A]	S6Q	C15-C16-N17-C18
7	A	607	SIA	C5-C6-C7-O7
7	A	607	SIA	O6-C6-C7-O7

There are no ring outliers.

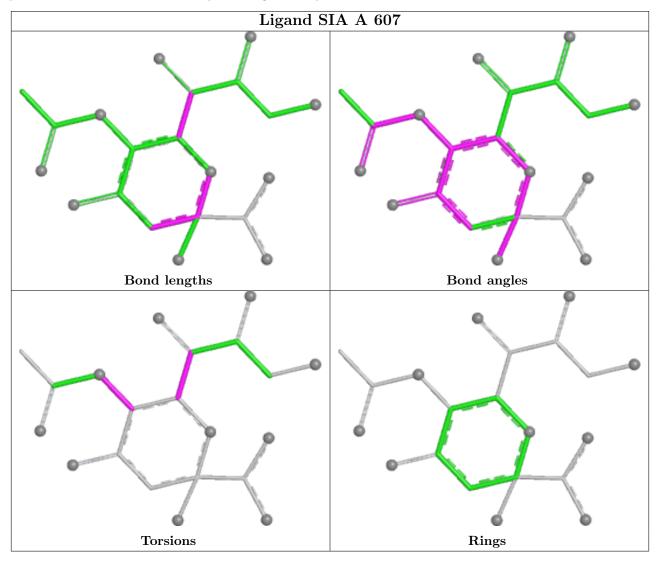
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	619	GOL	1	0
10	A	615	GOL	3	0
10	A	613	GOL	4	0
10	A	618	GOL	1	0
10	A	617	GOL	1	0
4	A	601	NAG	1	0
9	A	611	MES	3	0
6	A	605[A]	S6Q	2	0
10	A	612	GOL	1	0

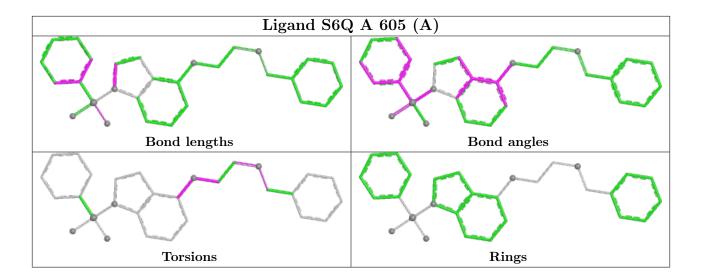
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



also be included. For torsion angles, if less then 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

