Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2021 – 04:06 am BST

PDB ID	:	7AWG
Title	:	Crystal structure of human butyrylcholinesterase in complex with (2-((1-(benzenesulfonyl)-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 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 (i) symbol.

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

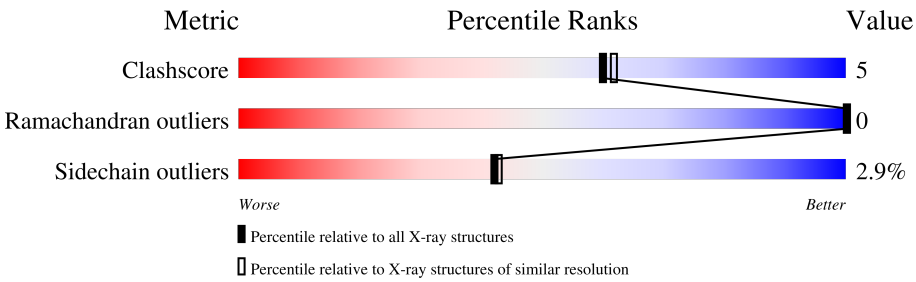
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 (#Entries)	Similar resolution (#Entries, resolution range(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	B	2	50% 50%
3	C	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:

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
			Total	C	N	O	S			
1	A	526	4248	2743	713	776	16	0	8	0

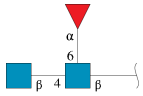
There are 4 discrepancies between the modelled and reference sequences:

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-beta-D-glucopyranose.

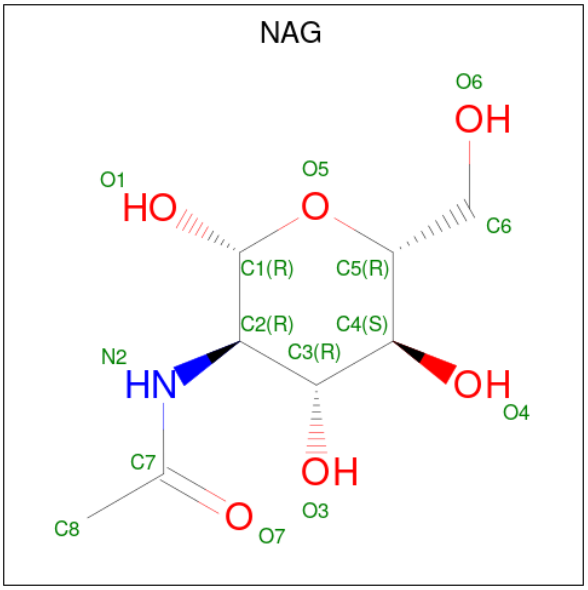
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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



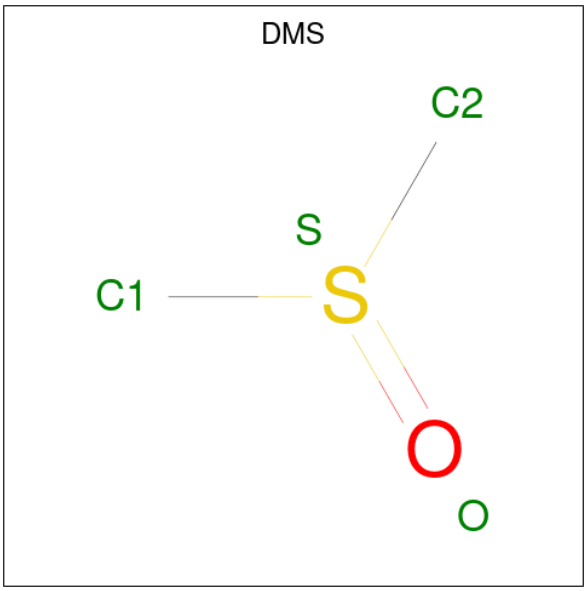
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0
			Total	C	N	O			
3	D	3	38	22	2	14	0	0	0

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



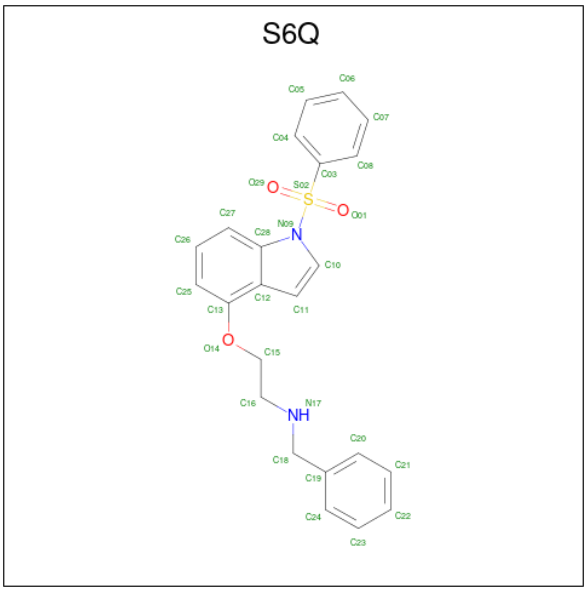
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

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



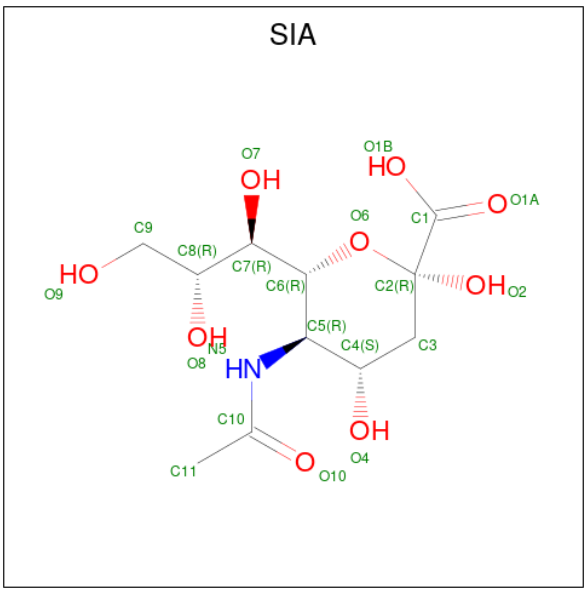
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	4	2	1	1	0	0
			Total	C	O	S		
5	A	1	4	2	1	1	0	0

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



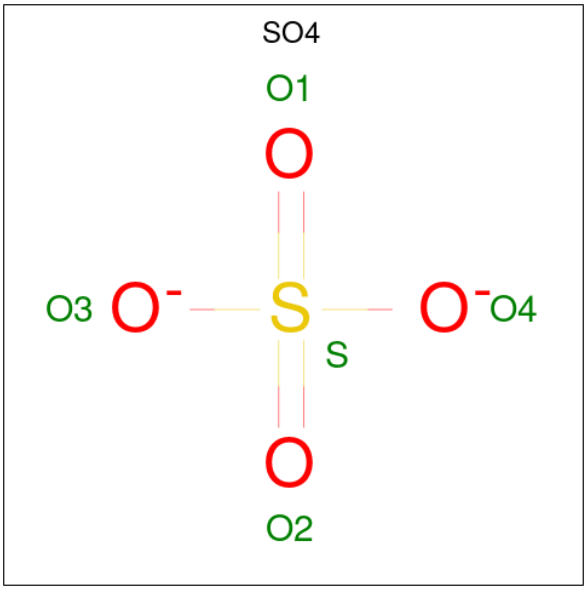
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	29	23	2	3	1	0	1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	21	11	1	9	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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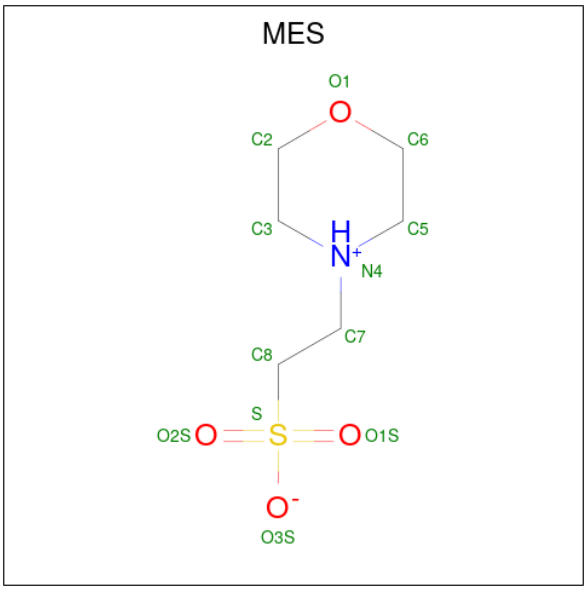
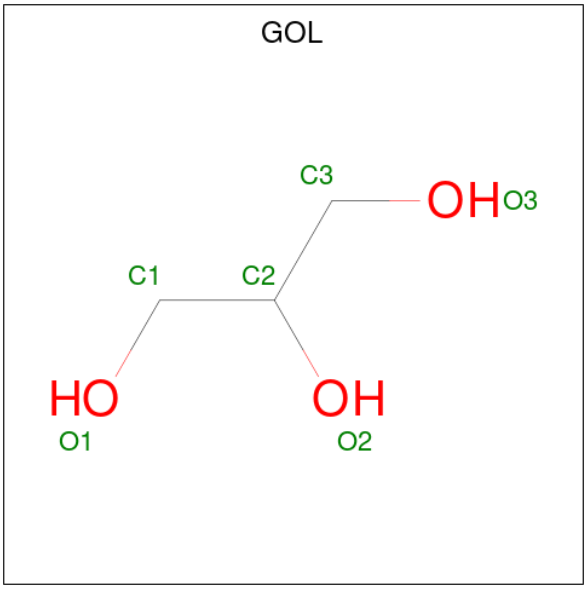
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
8	A	1	5	4	1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	A	1	12	6	1	4	1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 11 is water.

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

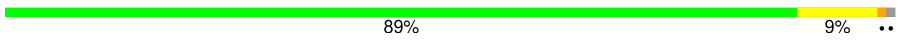
3 Residue-property plots (i)

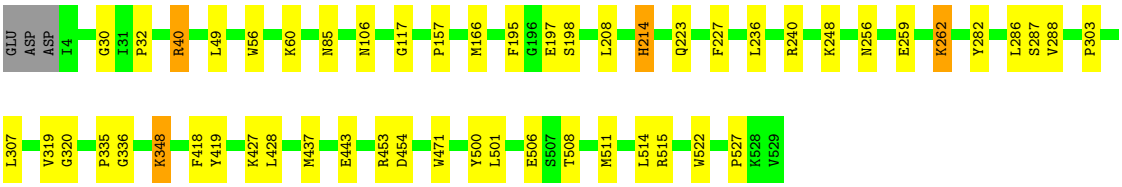
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

• Molecule 1: Cholinesterase

Chain A:



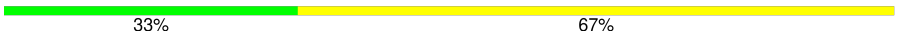


• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain C:



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

Chain D:

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 a, b, c, α, β, γ	154.48Å 154.48Å 128.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (48.85-2.00)	Depositor
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 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	B	24	0	22	0	0
3	C	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.

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: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
10:A:617:GOL:O1	10:A:617:GOL:O3	2.21	0.57
1:A:32:PRO:HB2	1:A:49:LEU:HD11	1.89	0.54
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.73	0.54
1:A:56:TRP:NE1	10:A:613:GOL:H12	2.23	0.53
1:A:514:LEU:HD12	9:A:611:MES:H32	1.90	0.53
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.44	0.53
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.74	0.52
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.46	0.51
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.47	0.50
1:A:522:TRP:O	1:A:527:PRO:HD3	2.12	0.50
1:A:319:VAL:O	1:A:418:PHE:HA	2.12	0.50
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.42	0.49
1:A:336:GLY:H	3:C:2:NAG:C8	2.26	0.49
1:A:427:LYS:CB	10:A:615:GOL:H32	2.41	0.49
1:A:30:GLY:HA3	10:A:613:GOL:H2	1.95	0.48
1:A:336:GLY:H	3:C:2:NAG:H83	1.78	0.48
1:A:40:ARG:HD2	1:A:40:ARG:H	1.79	0.47
1:A:256:ASN:HB3	1:A:259:GLU:HB2	1.97	0.47
9:A:611:MES:H51	9:A:611:MES:H82	1.61	0.47
1:A:208:LEU:O	1:A:214:HIS:HE1	1.99	0.46
1:A:248:LYS:HD2	3:D:3:FUC:H61	1.98	0.46
1:A:286[A]:LEU:HB3	6:A:605[A]:S6Q:C26	2.45	0.46
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.51	0.45
1:A:443:GLU:OE1	10:A:615:GOL:O1	2.33	0.45
1:A:286[A]:LEU:HD12	10:A:618:GOL:H12	1.98	0.45
1:A:501:LEU:HD11	1:A:508:THR:HG23	1.99	0.45
1:A:437:MET:HB3	11:A:852:HOH:O	2.17	0.43
1:A:197:GLU:HA	1:A:223:GLN:O	2.18	0.43
1:A:515:ARG:H	9:A:611:MES:H21	1.84	0.43
1:A:117:GLY:HA3	6:A:605[A]:S6Q:C27	2.49	0.43
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.70	0.42
1:A:259:GLU:O	1:A:262:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:ND2	4:A:601:NAG:H83	2.36	0.41
1:A:454:ASP:OD2	1:A:454:ASP:O	2.38	0.41
1:A:335:PRO:HA	3:C:2:NAG:H81	2.03	0.41
1:A:288:VAL:HB	10:A:619:GOL:H32	2.02	0.41

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	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 37

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	166	MET

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Mol	Chain	Res	Type
1	A	195	PHE
1	A	198[A]	SER
1	A	198[B]	SER
1	A	214	HIS
1	A	240	ARG
1	A	262	LYS
1	A	282	TYR
1	A	287[A]	SER
1	A	287[B]	SER
1	A	348	LYS
1	A	428	LEU
1	A	471	TRP
1	A	506	GLU

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.44	0	17,19,21	0.42	0
2	FUC	B	2	2	10,10,11	1.37	2 (20%)	14,14,16	0.83	0
3	NAG	C	1	3,1	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	C	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	FUC	C	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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	FUC	C	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	Z	Observed(Å)	Ideal(Å)
3	C	3	FUC	O5-C5	3.50	1.51	1.43
2	B	2	FUC	O5-C1	-2.54	1.39	1.43
3	C	3	FUC	C4-C5	2.05	1.57	1.52
2	B	2	FUC	C4-C3	2.01	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	FUC	O5-C5-C4	4.43	117.47	109.52
3	C	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	C	3	FUC	C1-O5-C5	2.56	118.57	112.78
3	C	3	FUC	C3-C4-C5	2.52	113.69	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	FUC	O5-C5-C4	2.06	113.21	109.52
3	D	2	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (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	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7

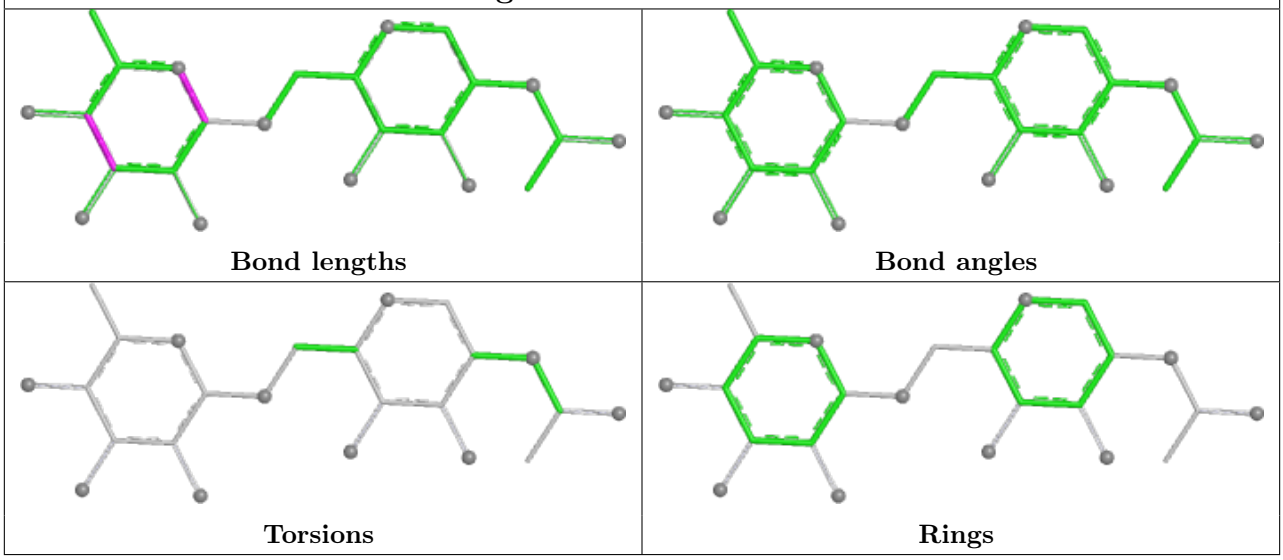
There are no ring outliers.

2 monomers are involved in 4 short contacts:

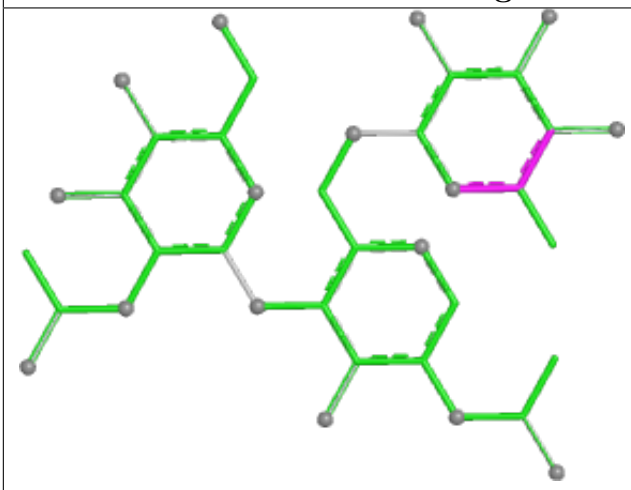
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	3	0
3	D	3	FUC	1	0

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

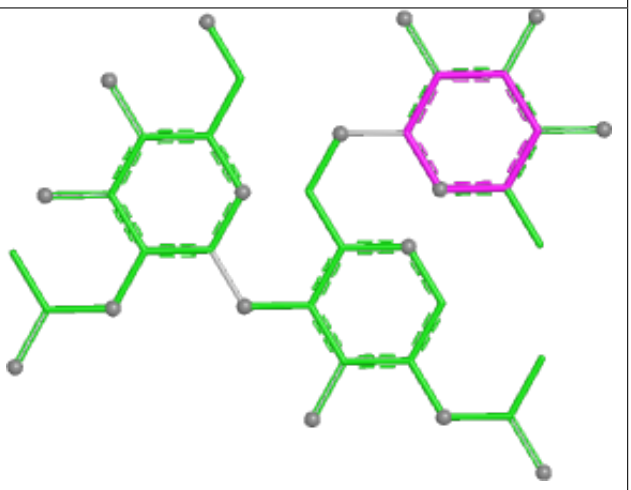
Oligosaccharide Chain B



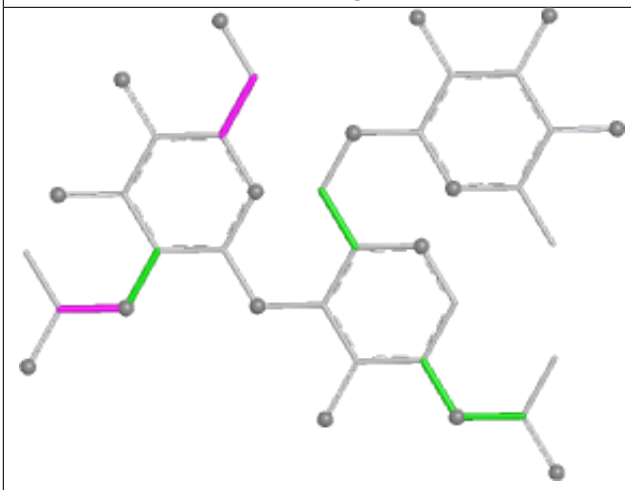
Oligosaccharide Chain C



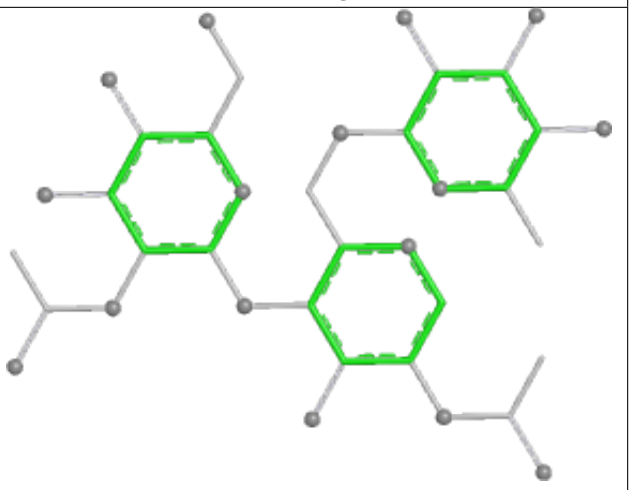
Bond lengths



Bond angles

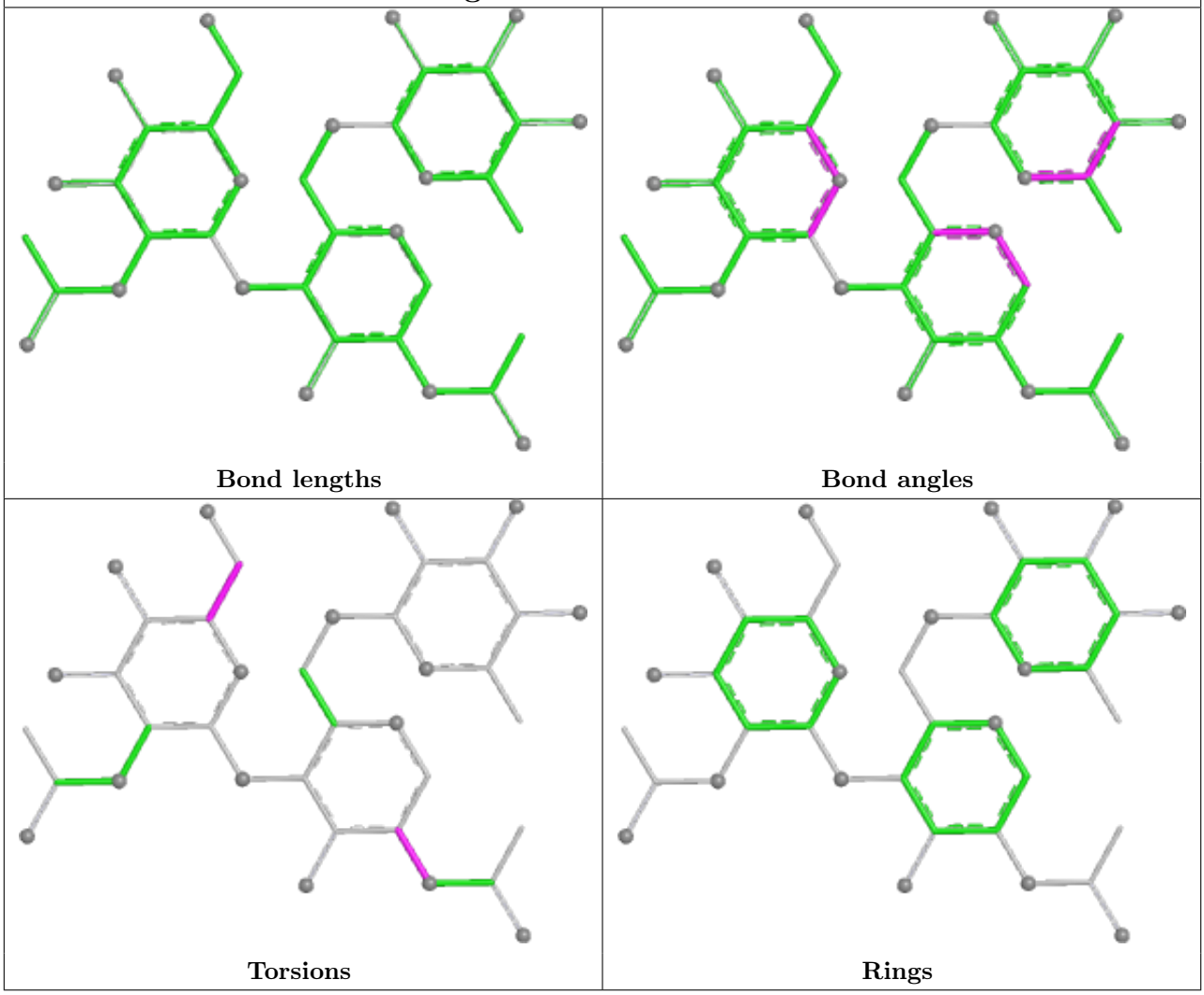


Torsions



Rings

Oligosaccharide Chain D



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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					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	Bond lengths			Bond angles		
					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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
6	A	605[A]	S6Q	C04-C03	2.24	1.42	1.38
6	A	605[A]	S6Q	O29-S02	-2.08	1.41	1.43
6	A	605[A]	S6Q	C08-C03	2.04	1.42	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	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
6	A	605[A]	S6Q	C08-C03-S02	4.39	124.64	119.77
9	A	611	MES	O1S-S-C8	4.33	112.13	106.92
9	A	611	MES	C5-N4-C3	4.27	118.45	108.83
6	A	605[A]	S6Q	C07-C08-C03	4.21	123.32	118.95
9	A	611	MES	C7-N4-C5	3.93	121.28	111.23
9	A	611	MES	C6-C5-N4	-3.71	104.48	110.10
7	A	607	SIA	C3-C4-C5	-3.54	104.54	109.98
7	A	607	SIA	O6-C6-C5	-3.53	106.34	109.78
9	A	611	MES	C7-N4-C3	3.46	120.08	111.23
6	A	605[A]	S6Q	O14-C13-C12	3.45	124.66	115.01
6	A	605[A]	S6Q	C25-C13-C12	-3.10	115.72	121.15
10	A	615	GOL	C3-C2-C1	-3.05	99.85	111.70
9	A	611	MES	C2-C3-N4	-2.77	105.90	110.10
7	A	607	SIA	O10-C10-N5	2.70	126.91	121.95
9	A	611	MES	O3S-S-C8	2.67	110.09	105.77
4	A	603	NAG	C1-O5-C5	2.56	115.67	112.19
6	A	605[A]	S6Q	C11-C12-C28	-2.49	104.06	106.18
7	A	607	SIA	O4-C4-C3	2.36	115.40	109.91
6	A	605[A]	S6Q	O14-C13-C25	-2.20	119.61	124.46
7	A	607	SIA	C4-C5-N5	2.19	114.70	110.38
6	A	605[A]	S6Q	O01-S02-C03	2.11	112.39	107.62
10	A	618	GOL	C3-C2-C1	-2.06	103.70	111.70
7	A	607	SIA	C4-C5-C6	-2.03	103.95	109.10
7	A	607	SIA	O2-C2-O6	-2.01	105.27	109.85

There are no chirality outliers.

All (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
9	A	611	MES	C8-C7-N4-C5
9	A	611	MES	C7-C8-S-O2S
9	A	611	MES	C7-C8-S-O3S
10	A	613	GOL	C1-C2-C3-O3
10	A	614	GOL	C1-C2-C3-O3
10	A	619	GOL	C1-C2-C3-O3
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
10	A	612	GOL	O1-C1-C2-C3
10	A	612	GOL	C1-C2-C3-O3
10	A	614	GOL	O1-C1-C2-C3
10	A	615	GOL	O1-C1-C2-C3
10	A	615	GOL	C1-C2-C3-O3
10	A	617	GOL	C1-C2-C3-O3
4	A	602	NAG	C1-C2-N2-C7
10	A	612	GOL	O1-C1-C2-O2
10	A	613	GOL	O2-C2-C3-O3
10	A	614	GOL	O1-C1-C2-O2
10	A	619	GOL	O2-C2-C3-O3
7	A	607	SIA	C6-C5-N5-C10
10	A	614	GOL	O2-C2-C3-O3
10	A	612	GOL	O2-C2-C3-O3
10	A	615	GOL	O2-C2-C3-O3
4	A	602	NAG	O5-C5-C6-O6
9	A	611	MES	C7-C8-S-O1S
7	A	607	SIA	C5-C6-C7-C8
7	A	607	SIA	O6-C6-C7-C8
4	A	602	NAG	C3-C2-N2-C7
10	A	615	GOL	O1-C1-C2-O2
7	A	607	SIA	C4-C5-N5-C10
10	A	617	GOL	O2-C2-C3-O3
6	A	605[A]	S6Q	C19-C18-N17-C16
6	A	605[A]	S6Q	C16-C15-O14-C13

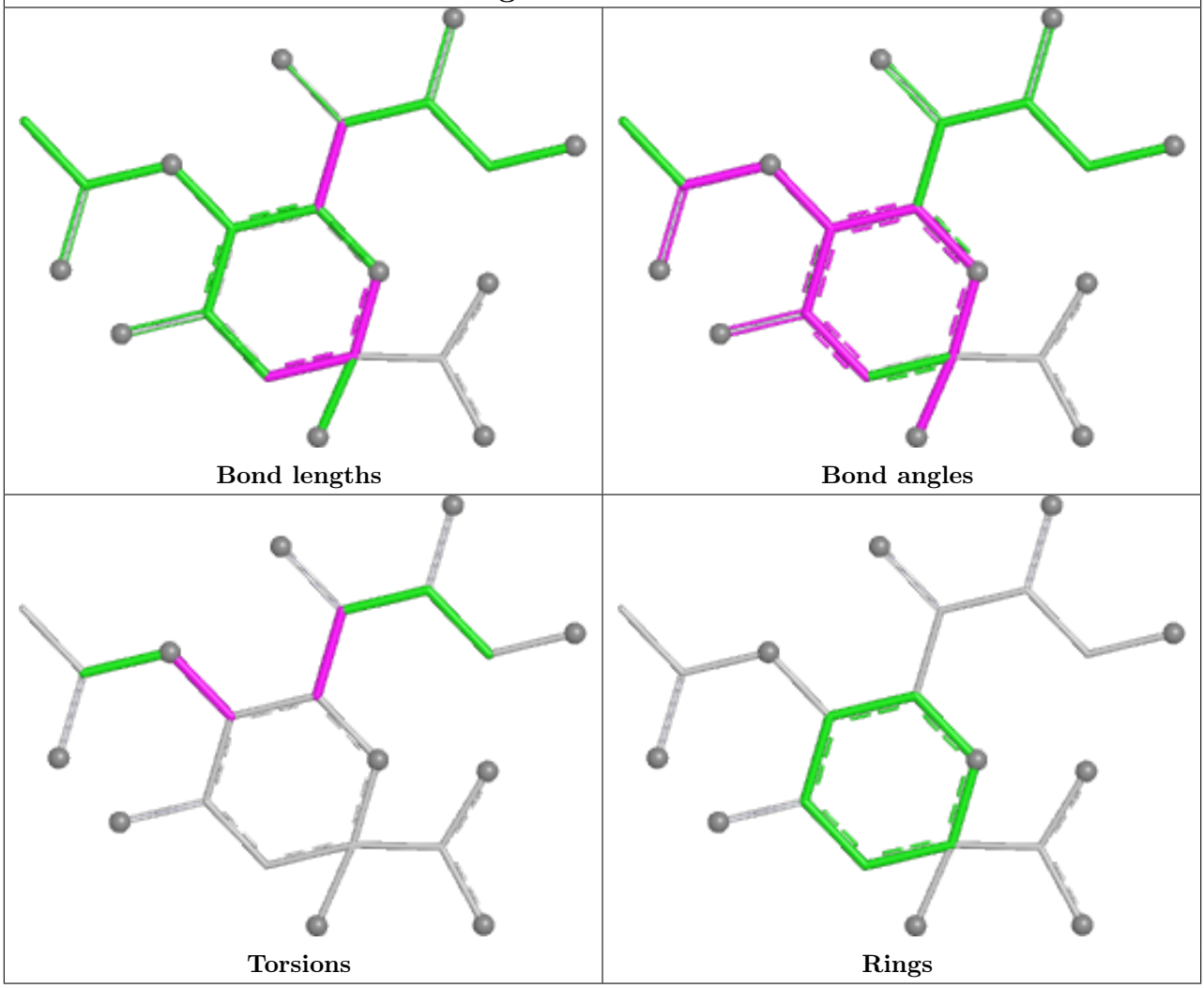
There are no ring outliers.

9 monomers are involved in 17 short contacts:

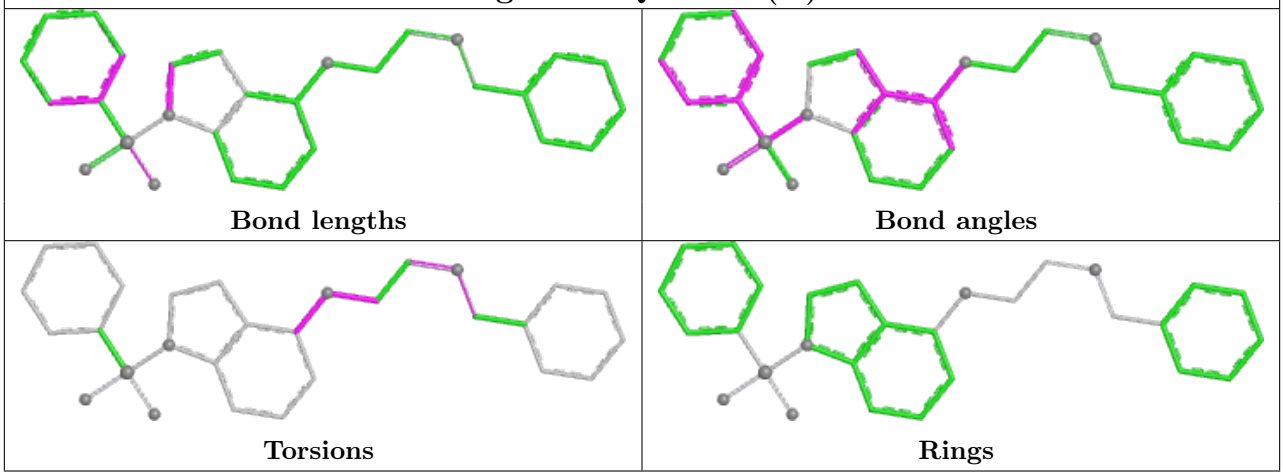
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	619	GOL	1	0
10	A	615	GOL	3	0
10	A	613	GOL	4	0
10	A	618	GOL	1	0
10	A	617	GOL	1	0
4	A	601	NAG	1	0
9	A	611	MES	3	0
6	A	605[A]	S6Q	2	0
10	A	612	GOL	1	0

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.

Ligand SIA A 607



Ligand S6Q A 605 (A)



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.