

wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2021 - 04:05 am BST

PDB ID	:	7AWI
Title	:	Crystal structure of human butyrylcholinesterase in complex with tert-butyl
		3-(((2-((1-benzyl-1H-indol-4-yl)oxy)ethyl)amino)methyl]piperidine-1-carboxyl
		ate
Authors	:	Brazzolotto, X.; Goral, I.; Wieckowska, A.
Deposited on		
Resolution	:	2.30 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:

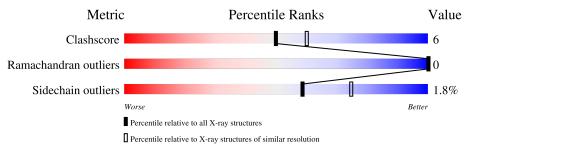
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\# \textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	А	529	84%	14%	••
2	В	2	100%		_
3	С	3	67% 333	%	
3	D	3	100%		



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4547 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		At	oms			ZeroOcc	AltConf	Trace
1	А	526	Total 4235	C 2735	N 714	O 770	S 16	0	6	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
А	455	GLN	ASN	engineered mutation	UNP P06276
А	481	GLN	ASN	engineered mutation	UNP P06276
А	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.



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

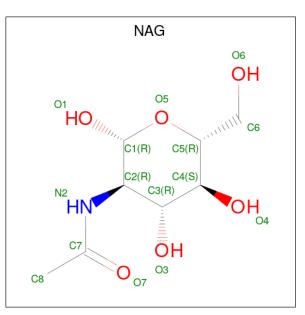
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.





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

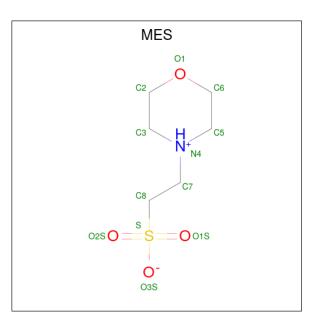
• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



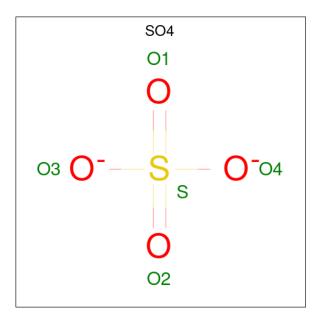
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C N O 14 8 1 5	0	0
4	А	1	Total C N O 14 8 1 5	0	0
4	А	1	Total C N O 14 8 1 5	0	0

• Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).





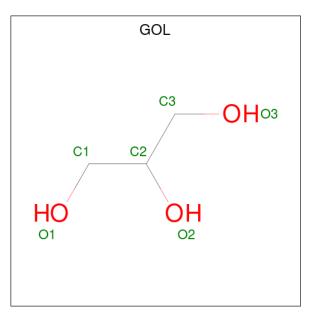
Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	Δ	1	Total	С	Ν	0	\mathbf{S}	0	0
5	А	1	12	6	1	4	1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

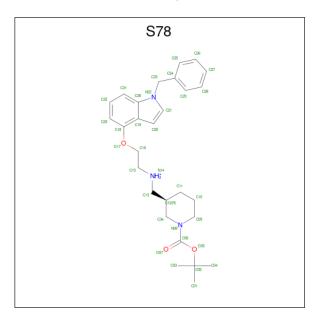


• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 8 is 2-((1-benzyl-1H-indol-4-yl)oxy)-N-((1-(tert-butoxycarbonyl)piperidin-3-yl)me thyl)ethan-1-aminium (three-letter code: S78) (formula: C₂₈H₃₈N₃O₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
8	А	1	Total 34	C 28	N 3	0 3	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	97	Total O 97 97	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.

Chain A:	84%	14% ••
GEU ASP ASP ASP ASP ASP N10 N10 N10 A34 A34 A34 A34 A34	K61 W52 853 853 853 853 853 154 1110 1110 1112 1125 1125 1125 1125 1125	H214 H221 L222 F227 F227 F226 L244 L244 K248 K248 K248 K248 K248 K248 K248 K
1284 5287 5287 5387 5303 5310 6310 6310 6310	K313 137 1317 1317 1317 1319 (3319 (332) 1322 1325 1325 1325 1325 1344 1344 1344 1344 1344 1344 1344 134	R381 P382 P382 P385 P385 P385 P385 P431 P431 P431 P431 P431 M471 M471
F474 A475 P480 P480 F500 L501 L501 L500 B507 S507 T508 R509	1510 1514 1514 1527 1528 1529 1529	
• Molecule 2: alp	ha-L-fucopyranose-(1-6)-2-acetamic	do-2-deoxy-beta-D-glucopyranose
Chain B:	100%	
NAG1 FUC2		

• Molecule 1: Cholinesterase

 • 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:	67%	33%
NAG1 POC3 FUC3		

• 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:

100%

NAG1 NAG2 FUC3



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	154.09Å 154.09Å 127.47Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 - 2.30	Depositor
% Data completeness	99.9 (48.73-2.30)	Depositor
(in resolution range)	55.5 (40.10 2.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.195 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4547	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	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, S78, FUC, SO4, NAG, MES

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	А	0.43	0/4365	0.60	0/5924

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	А	4235	0	4140	49	0
2	В	24	0	22	0	0
3	С	38	0	34	2	0
3	D	38	0	34	0	0
4	А	42	0	39	1	0
5	А	12	0	12	2	0
6	А	15	0	0	0	0
7	А	12	0	16	0	0
8	А	34	0	0	0	0
9	А	97	0	0	2	0
All	All	4547	0	4297	51	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 6.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PRO:HG3	1:A:236:LEU:HD12	1.52	0.92
1:A:378:ASP:HB3	1:A:381:ARG:HG3	1.79	0.63
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.63	0.63
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.38	0.59
1:A:319:VAL:O	1:A:418:PHE:HA	2.04	0.57

The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	А	530/529~(100%)	509~(96%)	21 (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	А	456/454~(100%)	447 (98%)	9~(2%)	55 72

5 of 9 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	511[A]	MET
1	А	511[B]	MET
1	А	195	PHE
1	А	248	LYS
1	А	287	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	35	GLN

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	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	14,14,15	0.71	0	17,19,21	0.57	0
2	FUC	В	2	2	10,10,11	1.22	0	14,14,16	0.71	0
3	NAG	С	1	1,3	14,14,15	0.43	0	17,19,21	0.48	0
3	NAG	С	2	3	$14,\!14,\!15$	0.41	0	$17,\!19,\!21$	0.56	0
3	FUC	С	3	3	10,10,11	1.04	0	$14,\!14,\!16$	0.86	0
3	NAG	D	1	1,3	14,14,15	0.46	0	17,19,21	1.18	2 (11%)
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	0.66	1 (5%)
3	FUC	D	3	3	10,10,11	1.40	2 (20%)	14,14,16	1.52	3 (21%)



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	1,2	-	2/6/23/26	0/1/1/1
2	FUC	В	2	2	-	-	0/1/1/1
3	NAG	С	1	1,3	-	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	1,3	-	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	D	3	FUC	C1-C2	2.50	1.57	1.52
3	D	3	FUC	C4-C5	2.27	1.57	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	1	NAG	C1-O5-C5	3.06	116.34	112.19
3	D	3	FUC	C1-C2-C3	2.94	113.28	109.67
3	D	3	FUC	O5-C5-C4	2.81	114.57	109.52
3	D	1	NAG	C1-C2-N2	2.21	114.26	110.49
3	D	2	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

5 of 9 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

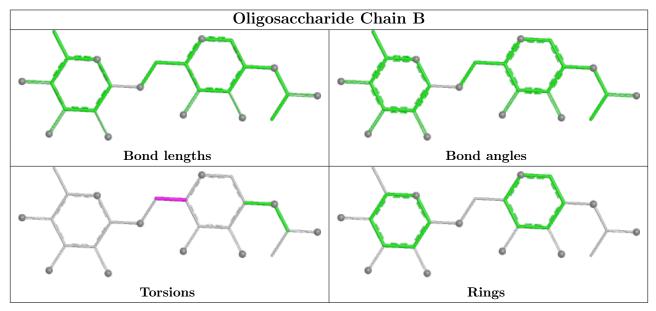
There are no ring outliers.

1 monomer is involved in 2 short contacts:

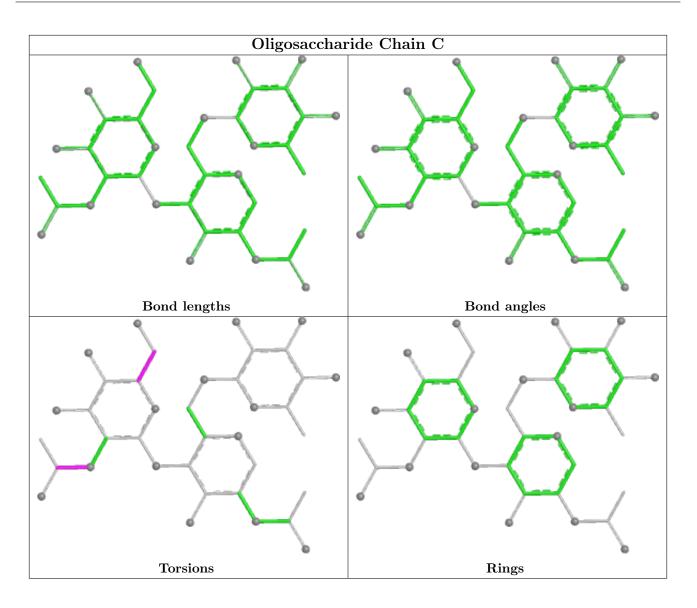


Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	2	NAG	2	0

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

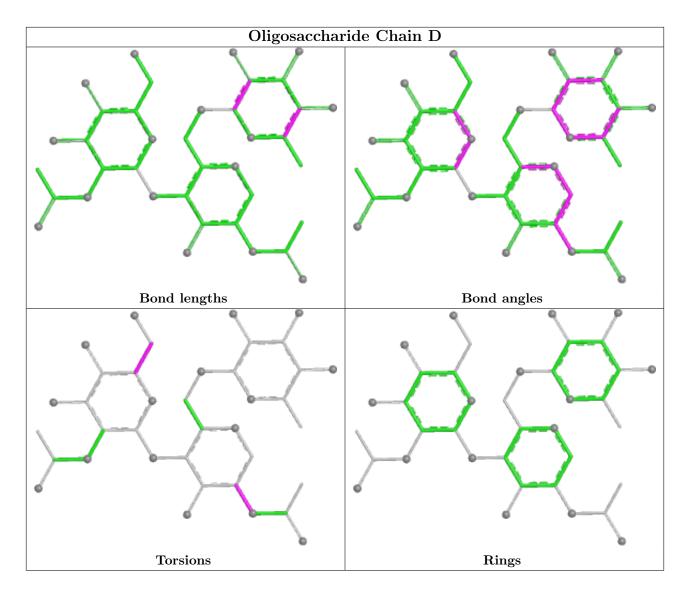












5.6 Ligand geometry (i)

10 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	True	Chain	Dec	T in le	Link Bond lengths				ond ang	les
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	NAG	А	601	1	14,14,15	0.71	0	17,19,21	0.62	0
6	SO4	А	605	-	4,4,4	0.19	0	6,6,6	0.22	0
6	SO4	А	607	-	4,4,4	0.17	0	6,6,6	0.07	0



Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	GOL	А	608	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.95	0
8	S78	А	610	-	$35,\!37,\!37$	1.97	7 (20%)	$45,\!51,\!51$	1.71	7 (15%)
7	GOL	А	609	-	$5,\!5,\!5$	1.37	1 (20%)	$5,\!5,\!5$	0.75	0
5	MES	А	604	-	12,12,12	2.04	1 (8%)	14,16,16	2.46	6 (42%)
4	NAG	А	602	1	14,14,15	0.71	1 (7%)	17,19,21	0.55	0
6	SO4	А	606	-	4,4,4	0.17	0	$6,\!6,\!6$	0.07	0
4	NAG	А	603	1	14,14,15	0.56	0	17,19,21	0.72	1 (5%)

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
4	NAG	А	601	1	-	2/6/23/26	0/1/1/1
7	GOL	А	608	-	-	2/4/4/4	-
8	S78	А	610	-	-	11/21/31/31	0/4/4/4
7	GOL	А	609	-	-	4/4/4/4	-
5	MES	А	604	-	-	3/6/14/14	0/1/1/1
4	NAG	А	602	1	-	0/6/23/26	0/1/1/1
4	NAG	А	603	1	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	604	MES	C8-S	-6.74	1.67	1.77
8	А	610	S78	C34-C12	-6.20	1.44	1.52
8	А	610	S78	C13-N14	4.60	1.54	1.47
8	А	610	S78	C34-N08	4.10	1.51	1.46
8	А	610	S78	C10-C11	2.84	1.60	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
8	А	610	S78	C34-N08-C06	-5.67	103.95	121.93
5	А	604	MES	C5-N4-C3	5.08	120.26	108.83
8	А	610	S78	O05-C06-N08	4.42	116.82	111.01
8	А	610	S78	O07-C06-N08	-4.31	117.11	124.32
8	А	610	S78	C10-C09-N08	-3.27	104.20	110.66



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
5	А	604	MES	C8-C7-N4-C3
5	А	604	MES	N4-C7-C8-S
7	А	609	GOL	O1-C1-C2-C3
8	А	610	S78	C34-C12-C13-N14
8	А	610	S78	O05-C06-N08-C34

5 of 22 torsion outliers are listed below:

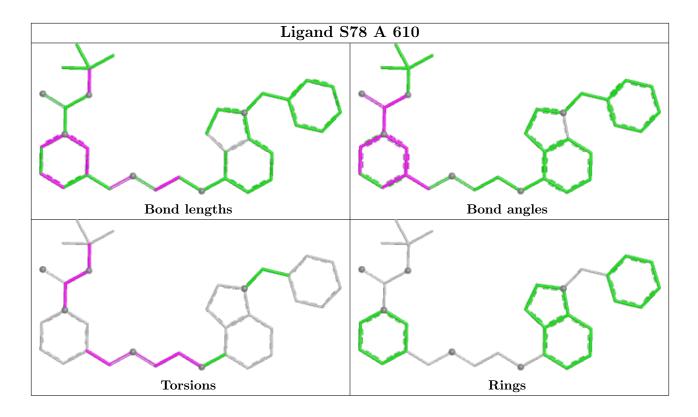
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	604	MES	2	0
4	А	602	NAG	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.

