



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:15 PM GMT

PDB ID : 4AQD
Title : Crystal structure of fully glycosylated human butyrylcholinesterase
Authors : Brazzolotto, X.; Wandhammer, M.; Ronco, C.; Trovaslet, M.; Jean, L.; Lockridge, O.; Renard, P.Y.; Nachon, F.
Deposited on : 2012-04-16
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

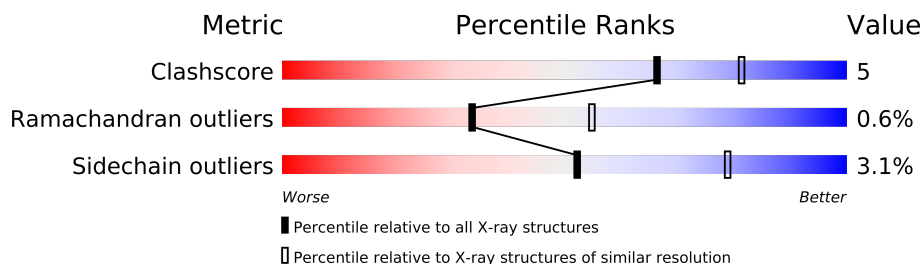
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	531	
1	B	531	

2 Entry composition i

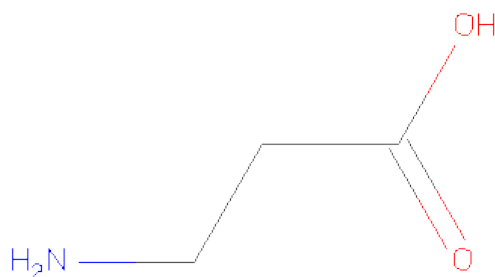
There are 13 unique types of molecules in this entry. The entry contains 9253 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BUTYRYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	12	3	0
			4222	2723	714	770	15			
1	B	526	Total	C	N	O	S	35	0	0
			4191	2704	705	767	15			

- Molecule 2 is BETA-ALANINE (three-letter code: BAL) (formula: $C_3H_7NO_2$).



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

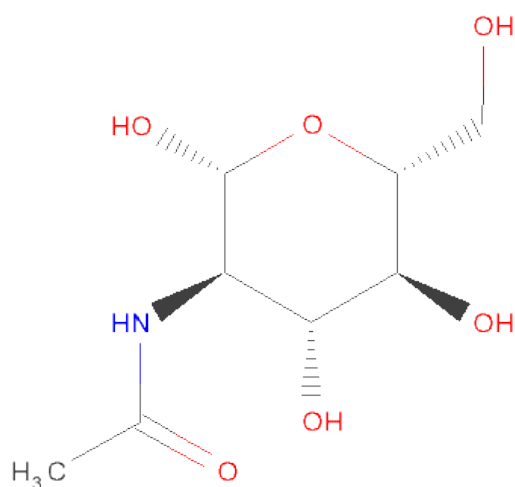
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		
4	A	3	Total	C	N	O	0	0
			38	22	2	14		
4	A	3	Total	C	N	O	0	0
			38	22	2	14		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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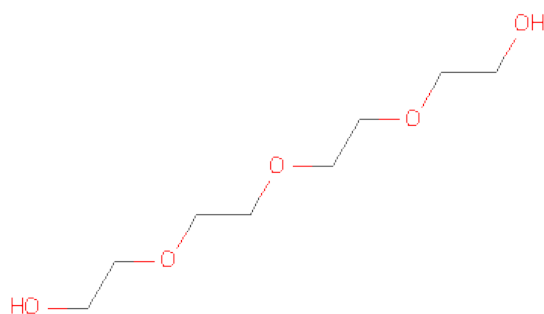
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

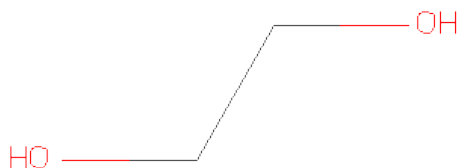
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

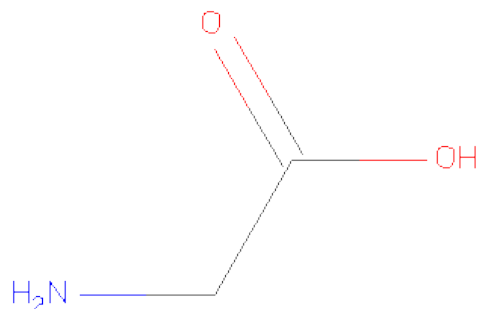
- Molecule 9 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	5	Total	X	0	0
			5	5		
9	A	5	Total	X	0	0
			5	5		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

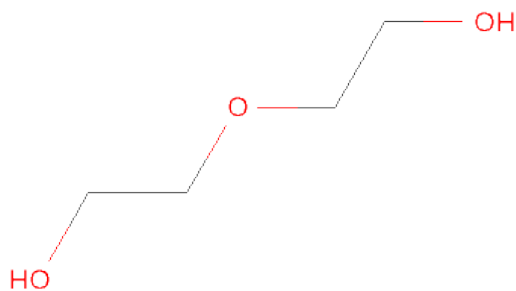
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	4	Total	Cl	0	0
			4	4		
10	A	3	Total	Cl	0	0
			3	3		

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			5	2	1	2		
11	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is water.

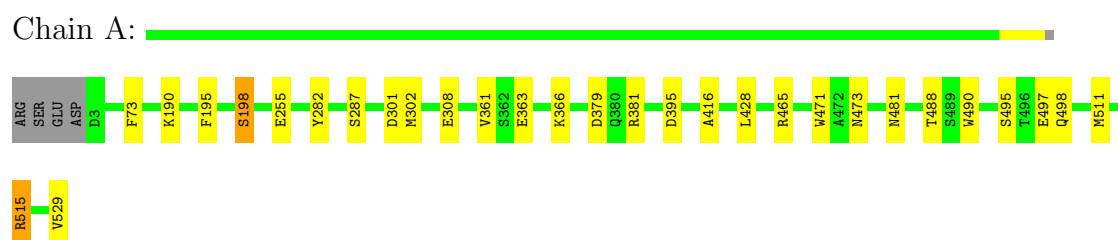
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	160	Total	O	0	0
			160	160		
13	B	118	Total	O	0	0
			118	118		

3 Residue-property plots

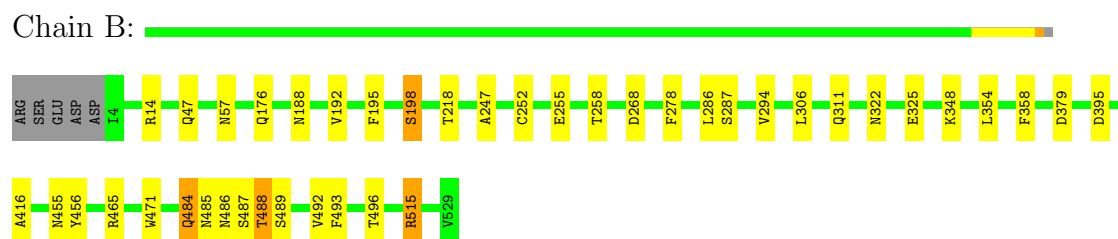
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

• Molecule 1: BUTYRYLCHOLINESTERASE



• Molecule 1: BUTYRYLCHOLINESTERASE



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 79.26Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.50	Depositor
% Data completeness (in resolution range)	99.4 (39.04-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.232	Depositor
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.384	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46097 reflections	Xtriage
Total number of atoms	9253	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, UNX, EDO, PG4, BAL, PEG, FUL, MAN

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	0.41	0/4351	0.57	0/5906
1	B	0.39	0/4310	0.54	0/5852
All	All	0.40	0/8661	0.56	0/11758

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	1	0
4	B	1	0
6	A	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	673	MAN	C1
4	A	681	NAG	C1
4	B	641	NAG	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4222	0	0	16	0
1	B	4191	0	0	18	0
2	A	6	0	6	2	0
2	B	6	0	6	2	0
3	A	56	0	50	0	0
4	A	114	0	102	2	0
4	B	114	0	102	4	0
5	A	14	0	13	2	0
5	B	70	0	64	1	0
6	A	39	0	34	0	0
7	A	26	0	36	0	0
8	A	36	0	54	0	0
8	B	40	0	60	3	0
9	A	5	0	0	4	0
9	B	5	0	0	7	0
10	A	3	0	0	1	0
10	B	4	0	0	0	0
11	A	5	0	2	0	0
11	B	5	0	2	0	0
12	B	14	0	20	0	0
13	A	160	0	0	6	0
13	B	118	0	0	2	0
All	All	9253	0	551	48	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:B:1542:UNX:X	9:B:1544:UNX:X	1.80	1.54
9:B:1543:UNX:X	9:B:1544:UNX:X	2.01	1.39
9:A:1542:UNX:X	9:A:1544:UNX:X	2.04	1.35
9:B:1544:UNX:X	9:B:1545:UNX:X	2.08	1.31
9:B:1543:UNX:X	9:B:1545:UNX:X	2.16	1.23

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	A	528/531 (99%)	506 (96%)	20 (4%)	2 (0%)	43 66
1	B	524/531 (99%)	494 (94%)	26 (5%)	4 (1%)	27 46
All	All	1052/1062 (99%)	1000 (95%)	46 (4%)	6 (1%)	33 55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	GLN
1	B	485	ASN
1	B	488	THR
1	B	489	SER
1	A	255	GLU

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	A	455/456 (100%)	444 (98%)	11 (2%)	61 86
1	B	451/456 (99%)	434 (96%)	17 (4%)	44 71
All	All	906/912 (99%)	878 (97%)	28 (3%)	52 79

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	195	PHE

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Mol	Chain	Res	Type
1	B	258	THR
1	B	492	VAL
1	B	198	SER
1	B	255	GLU

Some 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 chains 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 ⓘ

25 carbohydrates 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	$\# Z > 2$
3	NAG	A	601	1,3	12,14,15	0.70	1 (8%)	15,19,21	0.95	0
3	NAG	A	602	3	12,14,15	0.53	0	15,19,21	0.96	0
4	NAG	A	611	1,4	12,14,15	0.56	0	15,19,21	1.43	1 (6%)
4	NAG	A	612	4	12,14,15	0.47	0	15,19,21	1.36	1 (6%)
4	FUL	A	613	4	9,10,11	0.86	0	10,14,16	0.71	0
3	NAG	A	621	1,3	12,14,15	0.74	0	15,19,21	1.32	3 (20%)
3	NAG	A	622	3	12,14,15	0.82	1 (8%)	15,19,21	1.00	1 (6%)
4	NAG	A	631	1,4	12,14,15	0.64	1 (8%)	15,19,21	0.87	0
4	NAG	A	632	4	12,14,15	0.50	0	15,19,21	1.36	1 (6%)
4	FUL	A	633	4	9,10,11	0.78	0	10,14,16	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	671	1,6	12,14,15	0.51	0	15,19,21	1.36	2 (13%)
6	NAG	A	672	6	12,14,15	0.73	1 (8%)	15,19,21	0.93	0
6	MAN	A	673	6	10,11,12	0.70	0	11,15,17	1.00	1 (9%)
4	NAG	A	681	1,4	12,14,15	0.78	1 (8%)	15,19,21	1.48	3 (20%)
4	NAG	A	682	4	12,14,15	0.64	0	15,19,21	0.88	1 (6%)
4	FUL	A	683	4	9,10,11	0.90	1 (11%)	10,14,16	0.79	0
4	NAG	B	631	1,4	12,14,15	0.56	0	15,19,21	1.34	2 (13%)
4	NAG	B	632	4	12,14,15	0.59	0	15,19,21	1.11	1 (6%)
4	FUL	B	633	4	9,10,11	0.79	0	10,14,16	1.15	1 (10%)
4	NAG	B	641	1,4	12,14,15	0.60	0	15,19,21	0.82	0
4	NAG	B	642	4	12,14,15	0.57	0	15,19,21	0.86	0
4	FUL	B	643	4	9,10,11	0.87	1 (11%)	10,14,16	0.73	0
4	NAG	B	661	1,4	12,14,15	0.51	0	15,19,21	1.55	3 (20%)
4	NAG	B	662	4	12,14,15	0.60	0	15,19,21	1.23	2 (13%)
4	FUL	B	663	4	9,10,11	0.86	1 (11%)	10,14,16	0.80	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
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
4	NAG	A	611	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	612	4	-	0/6/23/26	1/1/1/1
4	FUL	A	613	4	-	0/0/17/20	0/1/1/1
3	NAG	A	621	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	622	3	-	0/6/23/26	0/1/1/1
4	NAG	A	631	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	632	4	-	0/6/23/26	1/1/1/1
4	FUL	A	633	4	-	0/0/17/20	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	672	6	-	0/6/23/26	0/1/1/1
6	MAN	A	673	6	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	A	681	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	682	4	-	0/6/23/26	0/1/1/1
4	FUL	A	683	4	-	0/0/17/20	0/1/1/1
4	NAG	B	631	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	632	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUL	B	633	4	-	0/0/17/20	0/1/1/1
4	NAG	B	641	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	642	4	-	0/6/23/26	0/1/1/1
4	FUL	B	643	4	-	0/0/17/20	0/1/1/1
4	NAG	B	661	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	662	4	-	0/6/23/26	0/1/1/1
4	FUL	B	663	4	-	0/0/17/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	622	NAG	O5-C5	-2.48	1.40	1.45
6	A	672	NAG	O5-C5	-2.27	1.41	1.45
4	A	681	NAG	O5-C5	-2.19	1.41	1.45
4	A	683	FUL	O5-C5	-2.17	1.41	1.45
4	B	643	FUL	O5-C5	-2.08	1.41	1.45

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	632	NAG	O5-C5-C6	4.68	111.89	106.98
4	B	661	NAG	O5-C5-C6	4.40	111.59	106.98
4	A	612	NAG	O5-C5-C6	3.97	111.15	106.98
4	B	631	NAG	O4-C4-C3	-3.54	102.41	110.35
4	A	681	NAG	O5-C5-C6	3.42	110.56	106.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	673	MAN	C1
4	A	681	NAG	C1
4	B	641	NAG	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	612	NAG	C1-C2-C3-C4-C5-O5
4	A	632	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 10 are unknown and 7 are monoatomic - leaving 33 for Mogul analysis.

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	$\# Z > 2$
7	PG4	A	1530	-	12,12,12	0.65	0	11,11,11	1.42	0
7	PG4	A	1531	-	12,12,12	0.66	0	11,11,11	1.39	0
8	EDO	A	1532	-	3,3,3	0.58	0	2,2,2	0.43	0
8	EDO	A	1533	-	3,3,3	0.60	0	2,2,2	0.25	0
8	EDO	A	1534	-	3,3,3	0.61	0	2,2,2	0.31	0
8	EDO	A	1535	-	3,3,3	0.59	0	2,2,2	0.22	0
8	EDO	A	1536	-	3,3,3	0.54	0	2,2,2	0.48	0
8	EDO	A	1537	-	3,3,3	0.60	0	2,2,2	0.33	0
8	EDO	A	1538	-	3,3,3	0.56	0	2,2,2	0.30	0
8	EDO	A	1539	-	3,3,3	0.59	0	2,2,2	0.19	0
8	EDO	A	1540	-	3,3,3	0.65	0	2,2,2	0.10	0
11	GLY	A	1643	-	4,4,4	0.93	0	4,4,4	1.27	1 (25%)
2	BAL	A	550	-	5,5,5	0.63	0	5,5,5	2.12	3 (60%)
5	NAG	A	651	1	12,14,15	0.63	0	15,19,21	0.71	1 (6%)
12	PEG	B	1530	-	6,6,6	0.59	0	5,5,5	1.33	0
12	PEG	B	1531	-	6,6,6	0.68	0	5,5,5	1.15	0
8	EDO	B	1532	-	3,3,3	0.59	0	2,2,2	0.33	0
8	EDO	B	1533	-	3,3,3	0.57	0	2,2,2	0.29	0
8	EDO	B	1534	-	3,3,3	0.53	0	2,2,2	0.63	0
8	EDO	B	1535	-	3,3,3	0.60	0	2,2,2	0.23	0
8	EDO	B	1536	-	3,3,3	0.55	0	2,2,2	0.44	0
8	EDO	B	1537	-	3,3,3	0.53	0	2,2,2	0.59	0
8	EDO	B	1538	-	3,3,3	0.55	0	2,2,2	0.31	0
8	EDO	B	1539	-	3,3,3	0.54	0	2,2,2	0.35	0
8	EDO	B	1540	-	3,3,3	0.57	0	2,2,2	0.36	0
8	EDO	B	1541	-	3,3,3	0.51	0	2,2,2	0.49	0
11	GLY	B	1642	-	4,4,4	0.98	0	4,4,4	1.27	1 (25%)
2	BAL	B	550	-	5,5,5	0.89	0	5,5,5	2.04	3 (60%)
5	NAG	B	601	1	12,14,15	0.70	0	15,19,21	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	611	1	12,14,15	0.59	0	15,19,21	0.89	1 (6%)
5	NAG	B	621	1	12,14,15	0.58	0	15,19,21	1.27	2 (13%)
5	NAG	B	651	1	12,14,15	0.60	0	15,19,21	1.09	2 (13%)
5	NAG	B	671	1	12,14,15	0.66	0	15,19,21	1.19	1 (6%)

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
7	PG4	A	1530	-	-	0/10/10/10	0/0/0/0
7	PG4	A	1531	-	-	0/10/10/10	0/0/0/0
8	EDO	A	1532	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1533	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1534	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1535	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1536	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1537	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1538	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1539	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1540	-	-	0/1/1/1	0/0/0/0
11	GLY	A	1643	-	-	0/2/2/2	0/0/0/0
2	BAL	A	550	-	-	0/3/3/3	0/0/0/0
5	NAG	A	651	1	1/1/5/7	1/6/23/26	0/1/1/1
12	PEG	B	1530	-	-	0/4/4/4	0/0/0/0
12	PEG	B	1531	-	-	0/4/4/4	0/0/0/0
8	EDO	B	1532	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1533	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1534	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1535	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1536	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1537	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1538	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1539	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1540	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1541	-	-	0/1/1/1	0/0/0/0
11	GLY	B	1642	-	-	0/2/2/2	0/0/0/0
2	BAL	B	550	-	-	0/3/3/3	0/0/0/0
5	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	611	1	-	0/6/23/26	0/1/1/1
5	NAG	B	621	1	1/1/5/7	1/6/23/26	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	651	1	-	0/6/23/26	0/1/1/1
5	NAG	B	671	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	671	NAG	O5-C5-C6	3.54	110.70	106.98
5	B	601	NAG	O5-C5-C6	3.22	110.36	106.98
2	B	550	BAL	O-C-CA	-2.89	113.10	123.03
5	B	651	NAG	O5-C5-C6	2.80	109.92	106.98
2	A	550	BAL	OXT-C-O	-2.76	116.28	123.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	651	NAG	C1
5	B	671	NAG	C1
5	B	621	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	621	NAG	C1-C2-N2-C7
5	A	651	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	621	NAG	C1-C2-C3-C4-C5-O5

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.