



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2023 – 06:20 pm GMT

PDB ID : 6EZ2
Title : Human butyrylcholinesterase carbamylated.
Authors : Brazzolotto, X.; de la Mora, E.; Dighe, S.N.; Ross, B.P.
Deposited on : 2017-11-14
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

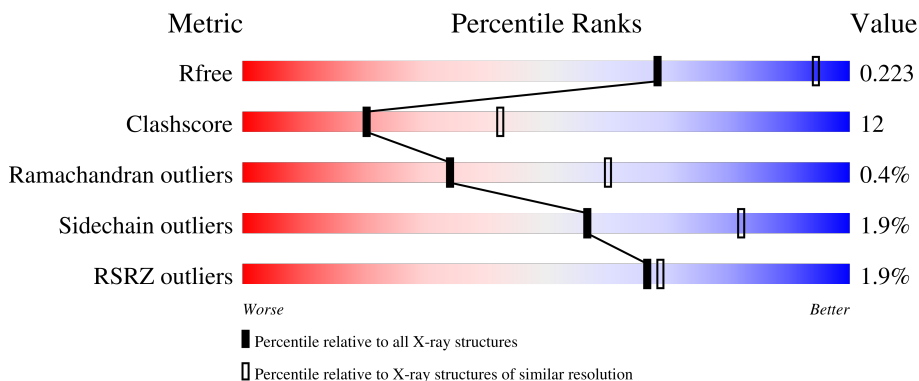
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


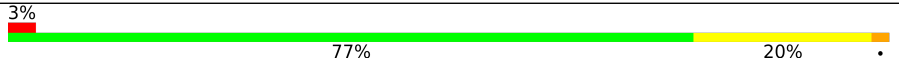

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	 76% 23% .
1	B	527	 3% 77% 20% .
2	C	2	 50% 50%

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
3	NAG	A	606	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8524 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	527	4106	2657	681	753	15	0	1	0
1	B	525	4065	2629	674	747	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	BXT	SER	conflict	UNP P06276
B	198	BXT	SER	conflict	UNP P06276

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

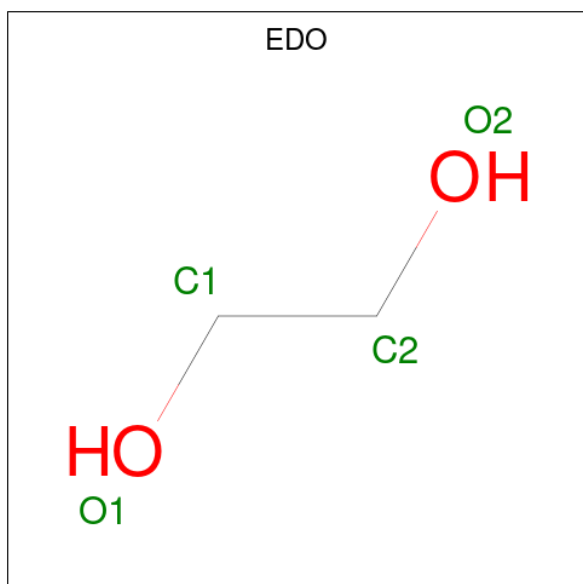


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

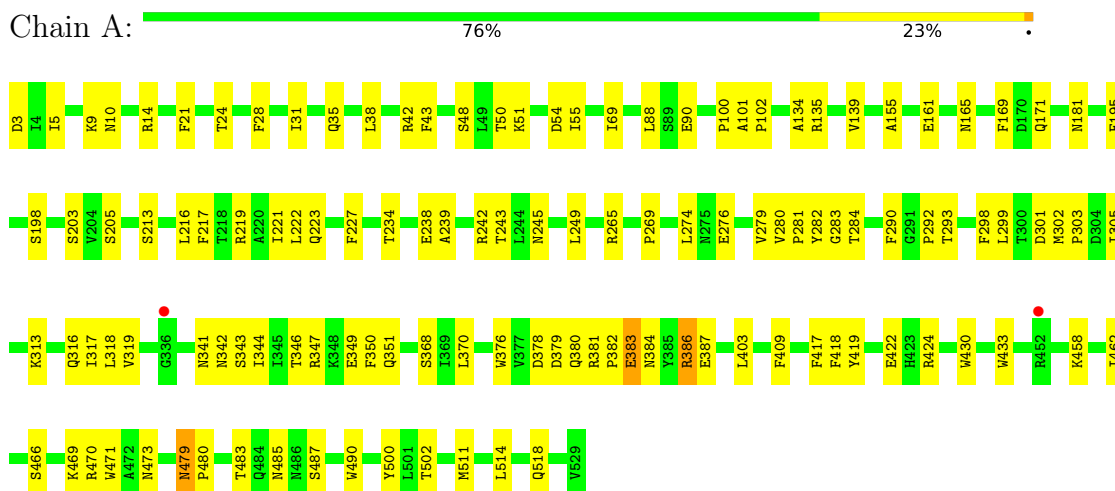
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	59	Total	O	0	0
			59	59		
7	B	63	Total	O	0	0
			63	63		

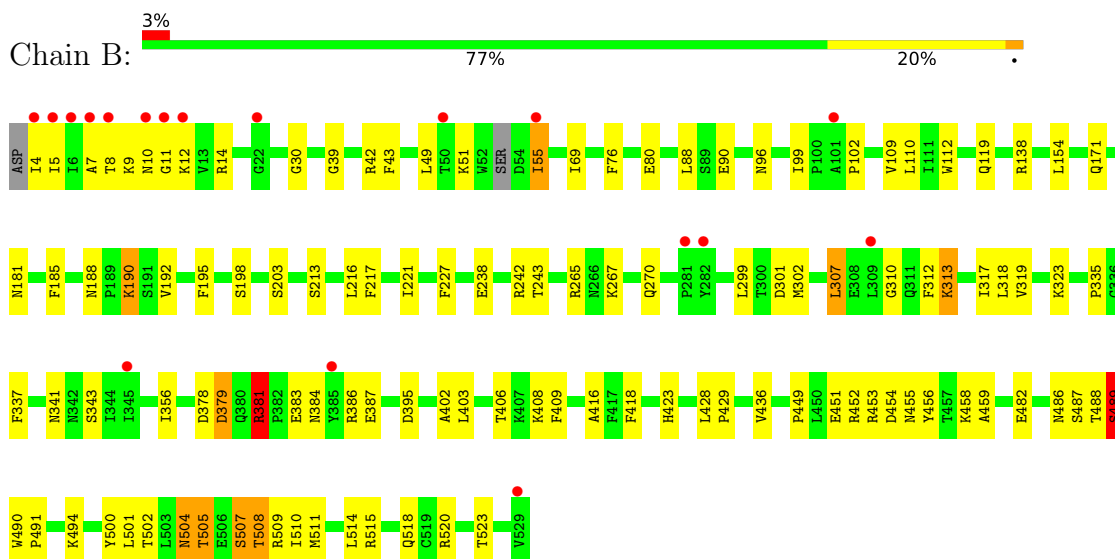
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cholinesterase



- Molecule 1: Cholinesterase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.01Å 79.94Å 231.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.70 46.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.97-2.70) 99.4 (46.88-2.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.186 , 0.223 0.187 , 0.223	Depositor DCC
R_{free} test set	1183 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.300	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8524	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BXT, CL, EDO, GOL, NAG

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	0.39	0/4213	0.58	0/5739
1	B	0.36	0/4167	0.62	7/5680 (0.1%)
All	All	0.37	0/8380	0.60	7/11419 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	SER	N-CA-CB	-10.39	94.92	110.50
1	B	55	ILE	CG1-CB-CG2	-8.59	92.50	111.40
1	B	55	ILE	CA-CB-CG1	6.93	124.17	111.00
1	B	381	ARG	N-CA-C	-6.75	92.77	111.00
1	B	307	LEU	CA-CB-CG	5.49	127.93	115.30

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	4106	0	3879	89	0
1	B	4065	0	3811	114	0
2	C	28	0	25	2	0
3	A	84	0	78	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	98	0	91	3	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	1	0	0	0	0
6	B	8	0	12	1	0
7	A	59	0	0	1	0
7	B	63	0	0	5	0
All	All	8524	0	7912	203	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 12.

The worst 5 of 203 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:NH2	1:B:55:ILE:HD11	1.71	1.06
1:B:482:GLU:OE1	1:B:487:SER:HB2	1.62	0.98
1:B:14:ARG:HH22	1:B:55:ILE:HD11	1.26	0.94
1:B:14:ARG:CZ	1:B:55:ILE:CD1	2.46	0.94
1:B:14:ARG:NH2	1:B:55:ILE:CD1	2.31	0.92

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	525/527 (100%)	501 (95%)	21 (4%)	3 (1%)	25	50
1	B	520/527 (99%)	498 (96%)	21 (4%)	1 (0%)	47	73
All	All	1045/1054 (99%)	999 (96%)	42 (4%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	A	283	GLY
1	A	383	GLU
1	B	486	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	419/451 (93%)	413 (99%)	6 (1%)	67 86
1	B	412/451 (91%)	402 (98%)	10 (2%)	49 77
All	All	831/902 (92%)	815 (98%)	16 (2%)	57 82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	507	SER
1	B	505	THR
1	B	379	ASP
1	B	504	ASN
1	B	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	ASN
1	B	397	ASN
1	B	504	ASN
1	B	384	ASN
1	A	479	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	BXT	B	198	1	9,11,12	2.18	1 (11%)	6,13,15	3.13	3 (50%)
1	BXT	A	198	1	9,11,12	2.18	1 (11%)	6,13,15	3.11	3 (50%)

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
1	BXT	B	198	1	-	4/11/13/15	-
1	BXT	A	198	1	-	4/11/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	BXT	OG-C1	6.13	1.46	1.34
1	B	198	BXT	OG-C1	6.11	1.46	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	BXT	OG-C1-N3	6.49	117.50	111.19
1	A	198	BXT	OG-C1-N3	6.46	117.47	111.19
1	B	198	BXT	OG-C1-O2	-3.08	119.53	124.78
1	A	198	BXT	OG-C1-O2	-3.05	119.59	124.78
1	B	198	BXT	CB-OG-C1	2.59	120.50	115.72

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	BXT	C2-C4-N3-C1
1	A	198	BXT	C-CA-CB-OG
1	B	198	BXT	C2-C4-N3-C1
1	B	198	BXT	C-CA-CB-OG
1	A	198	BXT	C2-C4-N3-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 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	C	1	2,1	14,14,15	1.36	1 (7%)	17,19,21	1.30	2 (11%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.40	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-4.84	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	3.48	116.11	111.02
2	C	1	NAG	C1-O5-C5	-2.04	109.42	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

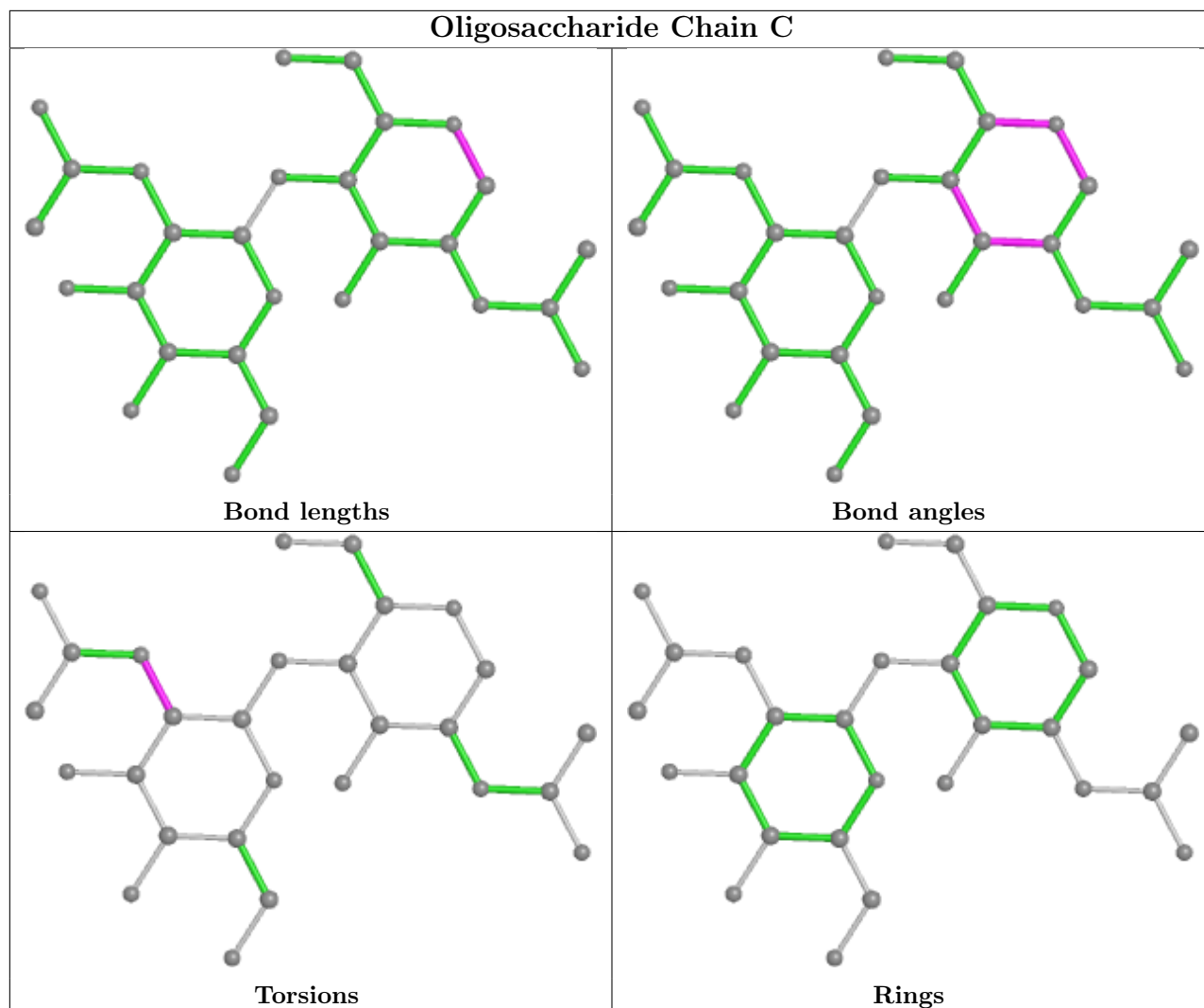
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	1	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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$
3	NAG	B	607	1	14,14,15	0.34	0	17,19,21	0.43	0
4	GOL	A	609	-	5,5,5	0.31	0	5,5,5	1.12	0
3	NAG	B	602	1	14,14,15	0.64	1 (7%)	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	604	1	14,14,15	0.24	0	17,19,21	0.37	0
3	NAG	A	604	1	14,14,15	0.33	0	17,19,21	1.21	1 (5%)
4	GOL	B	610	-	5,5,5	0.33	0	5,5,5	0.44	0
3	NAG	A	601	1	14,14,15	1.06	1 (7%)	17,19,21	1.53	1 (5%)
3	NAG	A	605	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
3	NAG	A	606	1	14,14,15	0.99	1 (7%)	17,19,21	1.24	1 (5%)
3	NAG	B	601	1	14,14,15	0.58	0	17,19,21	0.41	0
3	NAG	A	602	1	14,14,15	0.71	1 (7%)	17,19,21	0.58	0
3	NAG	B	603	1	14,14,15	0.27	0	17,19,21	0.30	0
3	NAG	B	605	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	B	606	1	14,14,15	0.42	0	17,19,21	0.63	0
6	EDO	B	608	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	B	609	-	3,3,3	0.44	0	2,2,2	0.27	0
3	NAG	A	603	1	14,14,15	0.23	0	17,19,21	0.63	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
3	NAG	B	607	1	-	4/6/23/26	0/1/1/1
4	GOL	A	609	-	-	4/4/4/4	-
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	2/6/23/26	0/1/1/1
3	NAG	A	604	1	-	4/6/23/26	0/1/1/1
4	GOL	B	610	-	-	0/4/4/4	-
3	NAG	A	601	1	-	3/6/23/26	0/1/1/1
3	NAG	A	605	1	-	3/6/23/26	0/1/1/1
3	NAG	A	606	1	-	4/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	3/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1	-	1/6/23/26	0/1/1/1
3	NAG	B	606	1	-	2/6/23/26	0/1/1/1
6	EDO	B	608	-	-	0/1/1/1	-
6	EDO	B	609	-	-	0/1/1/1	-
3	NAG	A	603	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAG	O5-C1	3.80	1.49	1.43
3	A	606	NAG	O5-C1	3.43	1.49	1.43
3	A	602	NAG	C1-C2	2.23	1.55	1.52
3	B	602	NAG	C1-C2	2.17	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	C1-O5-C5	5.86	120.14	112.19
3	A	606	NAG	C1-O5-C5	4.68	118.53	112.19
3	A	604	NAG	C1-O5-C5	4.47	118.25	112.19
3	A	605	NAG	C1-O5-C5	3.70	117.20	112.19
3	B	602	NAG	C1-O5-C5	2.50	115.57	112.19

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	GOL	O1-C1-C2-C3
4	A	609	GOL	C1-C2-C3-O3
3	B	604	NAG	O5-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
3	B	606	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAG	1	0
3	B	601	NAG	1	0
3	A	602	NAG	2	0
3	B	603	NAG	1	0
6	B	609	EDO	1	0

5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/527 (99%)	-0.15	2 (0%) 92 93	37, 62, 99, 163	1 (0%)
1	B	524/527 (99%)	0.06	18 (3%) 45 45	40, 69, 115, 192	0
All	All	1050/1054 (99%)	-0.05	20 (1%) 66 69	37, 67, 109, 192	1 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	GLY	6.0
1	B	8	THR	3.8
1	B	12	LYS	3.7
1	B	281	PRO	3.7
1	B	4	ILE	3.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

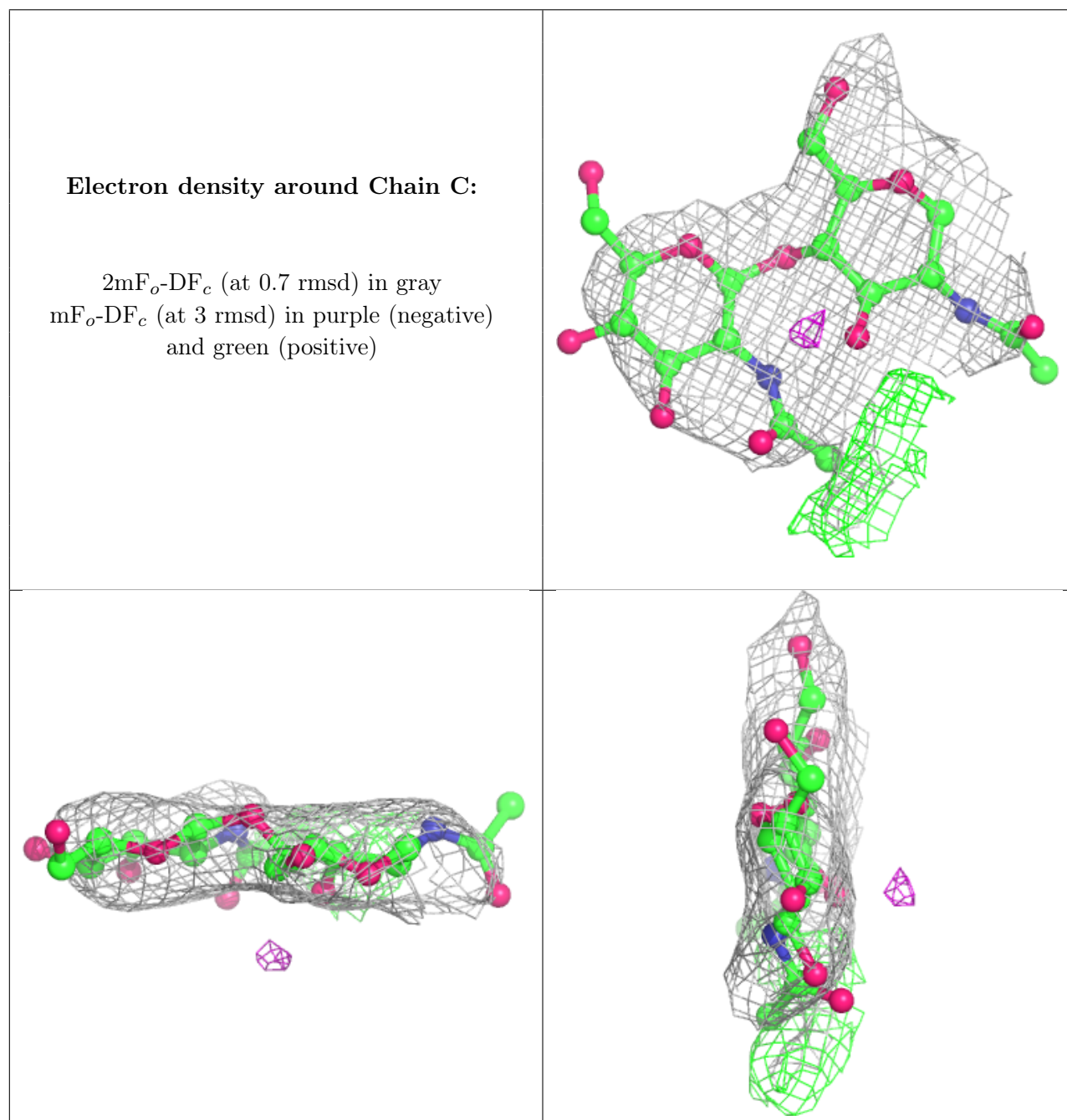
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	BXT	B	198	12/13	0.96	0.25	45,49,53,55	0
1	BXT	A	198	12/13	0.99	0.25	40,52,58,59	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.79	0.28	144,152,160,163	0
2	NAG	C	1	14/15	0.89	0.21	96,107,131,132	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	A	610	1/1	0.46	0.16	108,108,108,108	0
3	NAG	B	602	14/15	0.58	0.25	112,144,159,163	0
3	NAG	A	606	14/15	0.68	0.46	136,163,176,178	0
3	NAG	A	604	14/15	0.71	0.21	119,148,160,164	0
3	NAG	B	601	14/15	0.72	0.29	158,166,173,182	0
3	NAG	A	601	14/15	0.73	0.39	108,147,154,155	0
3	NAG	A	602	14/15	0.74	0.19	103,112,123,127	0
3	NAG	B	604	14/15	0.77	0.29	154,171,178,180	0
3	NAG	A	605	14/15	0.82	0.28	113,126,132,134	0
3	NAG	B	605	14/15	0.84	0.20	113,122,127,128	0
6	EDO	B	608	4/4	0.84	0.28	79,89,89,93	0
3	NAG	B	607	14/15	0.85	0.22	111,126,146,147	0
6	EDO	B	609	4/4	0.86	0.33	85,88,89,95	0
3	NAG	B	606	14/15	0.88	0.22	91,107,120,122	0
3	NAG	B	603	14/15	0.89	0.29	136,149,156,157	0
4	GOL	A	609	6/6	0.91	0.43	63,74,86,95	0
4	GOL	B	610	6/6	0.93	0.25	52,63,73,89	0
3	NAG	A	603	14/15	0.93	0.22	74,89,97,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.