Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 10:49 PM JST

PDB ID	:	5YDJ
Title	:	Crystal structure of anopheles gambiae acetylcholinesterase in complex with PMSF
Authors	:	Han, Q.; Guan, H.; Ding, H.; Liao, C.; Robinson, H.; Li, J.
Deposited on	:	2017-09-13
Resolution	:	3.04 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 ⓘ 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:

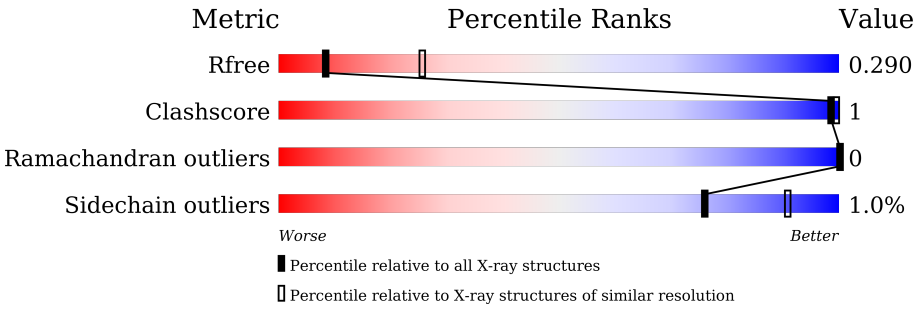
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	737	72% · 27%
1	B	737	71% · 27%
2	C	2	100%
2	D	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8813 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.

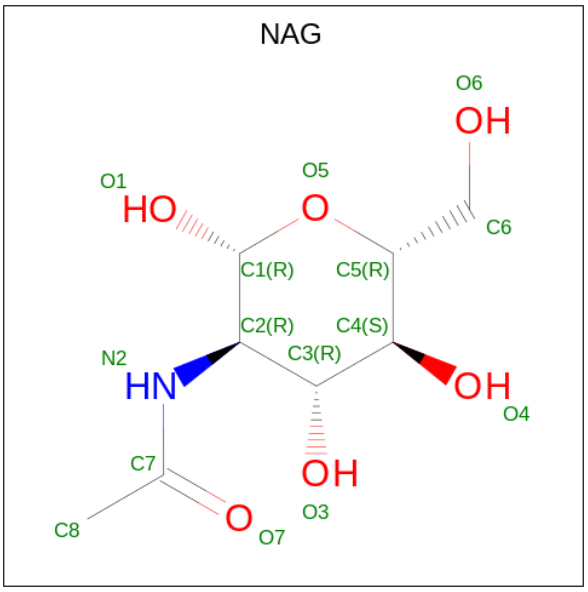
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4267	2718	743	792	14			
1	B	538	Total	C	N	O	S	0	0	0
			4267	2718	743	792	14			

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

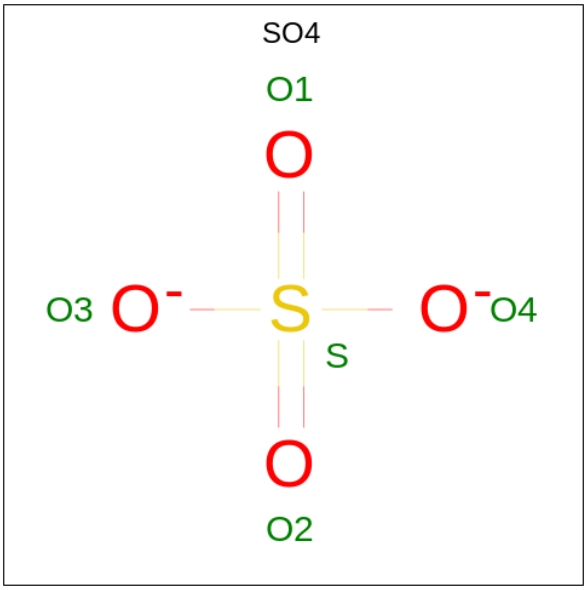
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

- Molecule 5 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Co 1 1	0	0
5	B	1	Total Co 1 1	0	0

- Molecule 6 is water.

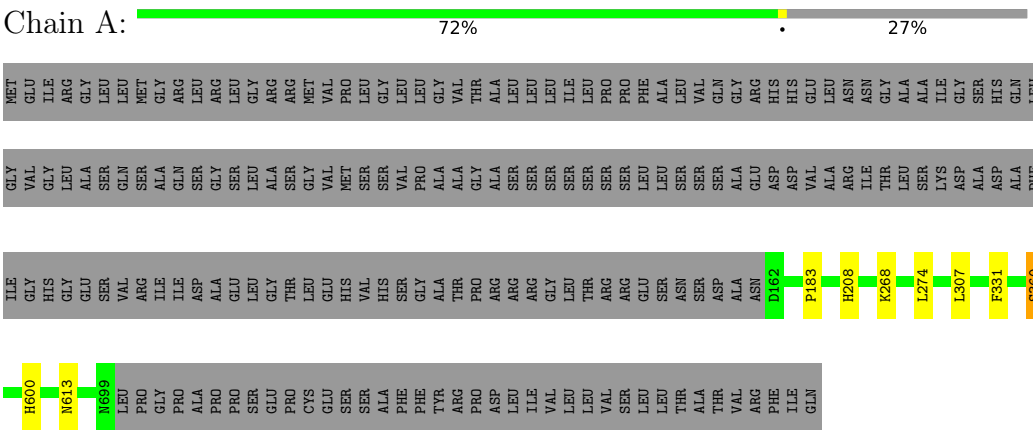
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	25	Total O 25 25	0	0

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.

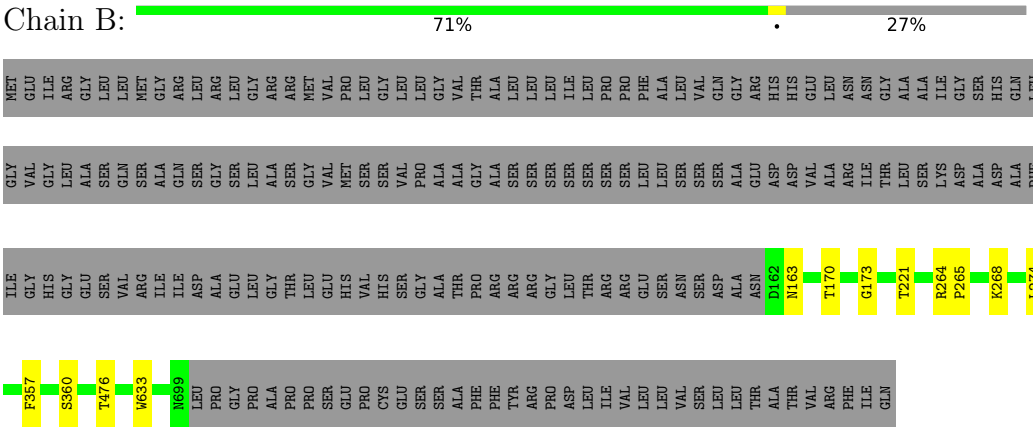
• Molecule 1: Acetylcholinesterase

Chain A:



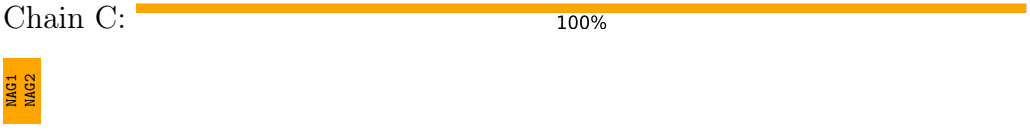
• Molecule 1: Acetylcholinesterase

Chain B:



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

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	147.65Å 147.65Å 224.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.48 – 3.04 61.48 – 3.04	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.48-3.04) 100.0 (61.48-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.251 , 0.286 0.253 , 0.290	Depositor DCC
R_{free} test set	2701 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 24.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.367 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8813	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SEB, CO, SO4

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	0.38	0/4374	0.60	0/5968
1	B	0.38	0/4374	0.59	0/5968
All	All	0.38	0/8748	0.60	0/11936

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

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	4267	0	4111	4	0
1	B	4267	0	4111	4	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	65	0	0	0	0
4	B	80	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	25	0	0	0	0
All	All	8813	0	8298	9	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 1.

All (9) 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:274:LEU:HD21	1:A:307:LEU:HD23	1.88	0.56
1:B:221:THR:O	1:B:221:THR:HG23	2.14	0.48
1:B:264:ARG:HA	1:B:265:PRO:C	2.34	0.48
1:A:360:SEB:HE2	1:A:600:HIS:NE2	2.30	0.46
2:C:1:NAG:H3	2:C:2:NAG:O5	2.17	0.45
1:A:208:HIS:CE1	1:A:331:PHE:CE2	3.06	0.44
1:B:170:THR:N	1:B:173:GLY:O	2.53	0.41
1:B:313:SER:O	1:B:317:LEU:HB2	2.21	0.41
1:A:183:PRO:HB2	1:A:613:ASN:HA	2.02	0.40

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	535/737 (73%)	504 (94%)	31 (6%)	0	100	100
1	B	535/737 (73%)	505 (94%)	30 (6%)	0	100	100
All	All	1070/1474 (73%)	1009 (94%)	61 (6%)	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	454/611 (74%)	451 (99%)	3 (1%)	84 93
1	B	454/611 (74%)	448 (99%)	6 (1%)	69 88
All	All	908/1222 (74%)	899 (99%)	9 (1%)	76 91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LYS
1	A	496	THR
1	A	571	TYR
1	B	163	ASN
1	B	268	LYS
1	B	274	LEU
1	B	357	PHE
1	B	476	THR
1	B	633	TRP

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

Mol	Chain	Res	Type
1	A	520	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	SEB	A	360	1	15,16,17	2.99	1 (6%)	15,21,23	0.92	1 (6%)
1	SEB	B	360	1	15,16,17	2.85	1 (6%)	15,21,23	0.94	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
1	SEB	A	360	1	-	3/9/13/15	0/1/1/1
1	SEB	B	360	1	-	6/9/13/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	SEB	CE-SD	-11.34	1.67	1.78
1	B	360	SEB	CE-SD	-10.79	1.67	1.78

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	SEB	OG-SD-CE	2.51	111.09	104.18
1	A	360	SEB	OG-SD-CE	2.15	110.10	104.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	360	SEB	CZ-CE-SD-OD2
1	A	360	SEB	CZ-CE-SD-OD1
1	A	360	SEB	CZ-CE-SD-OG
1	B	360	SEB	CB-OG-SD-OD2
1	B	360	SEB	SD-CE-CZ-CH2
1	B	360	SEB	SD-CE-CZ-CH1
1	B	360	SEB	CZ-CE-SD-OD2

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Mol	Chain	Res	Type	Atoms
1	B	360	SEB	CZ-CE-SD-OG
1	B	360	SEB	CB-OG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	360	SEB	1	0

5.5 Carbohydrates (i)

4 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	1,2	14,14,15	0.89	0	17,19,21	1.60	3 (17%)
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	2.75	5 (29%)
2	NAG	D	1	1,2	14,14,15	0.44	0	17,19,21	1.03	0
2	NAG	D	2	2	14,14,15	0.36	0	17,19,21	0.94	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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	7.23	121.98	112.19
2	C	2	NAG	O5-C1-C2	5.63	120.18	111.29
2	C	1	NAG	C4-C3-C2	4.78	118.02	111.02
2	C	2	NAG	C1-C2-N2	-4.63	102.58	110.49
2	C	2	NAG	C3-C4-C5	2.46	114.63	110.24
2	C	2	NAG	O5-C5-C4	2.36	116.58	110.83
2	C	1	NAG	C3-C4-C5	2.29	114.33	110.24
2	C	1	NAG	C6-C5-C4	2.05	117.80	113.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7

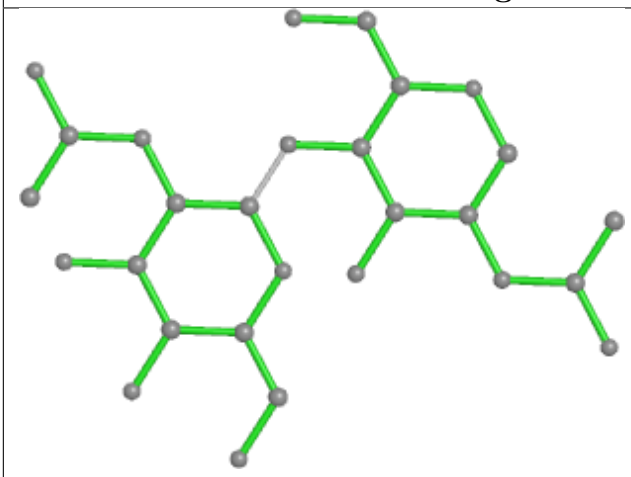
There are no ring outliers.

2 monomers are involved in 1 short contact:

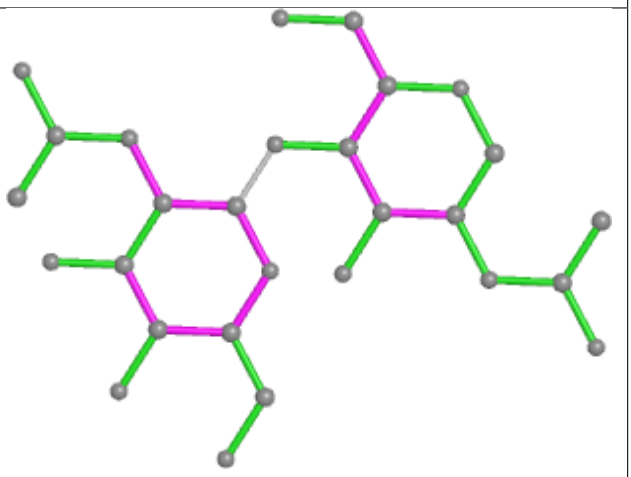
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	C	2	NAG	1	0

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

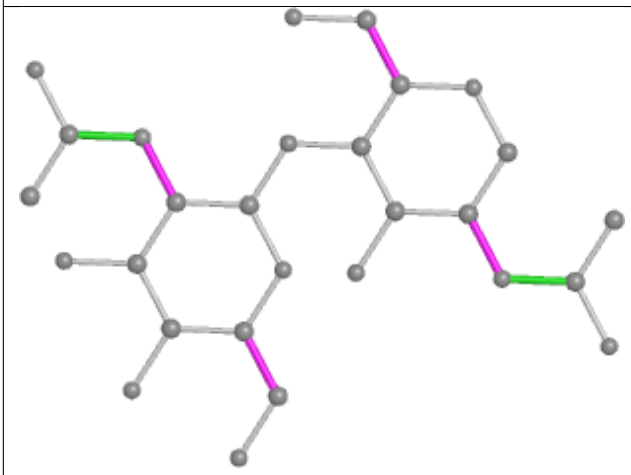
Oligosaccharide Chain C



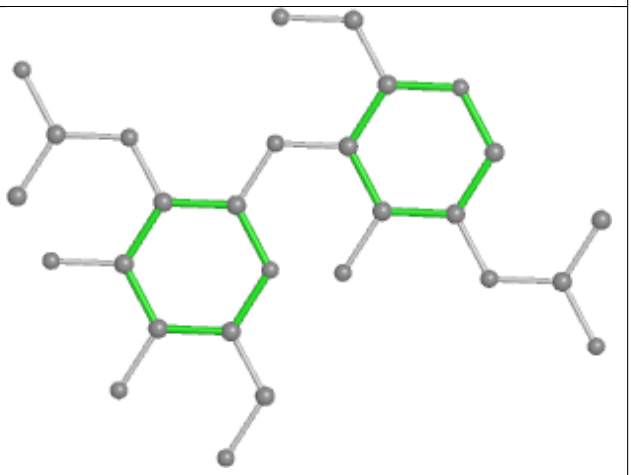
Bond lengths



Bond angles

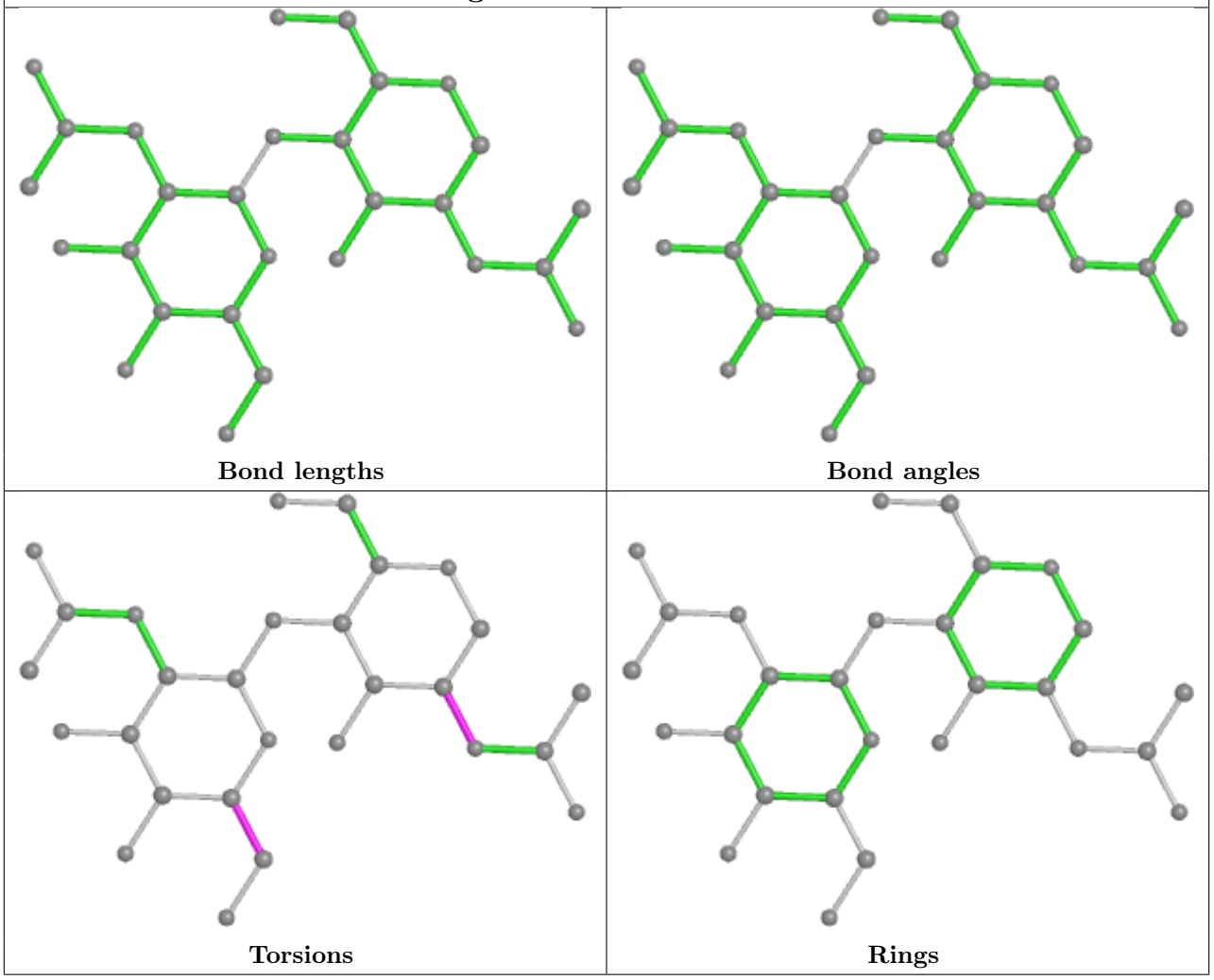


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	801	1	14,14,15	0.37	0	17,19,21	0.80	0
4	SO4	A	806	-	4,4,4	0.33	0	6,6,6	0.04	0
4	SO4	A	810	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	A	804	-	4,4,4	0.34	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	809	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	812	-	4,4,4	0.34	0	6,6,6	0.04	0
4	SO4	A	802	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	811	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	810	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	A	805	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	802	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	B	817	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	803	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	A	809	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	814	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	A	813	-	4,4,4	0.35	0	6,6,6	0.05	0
4	SO4	B	813	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	A	807	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	A	808	-	4,4,4	0.33	0	6,6,6	0.04	0
4	SO4	B	804	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	B	806	-	4,4,4	0.32	0	6,6,6	0.04	0
4	SO4	B	807	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	A	803	-	4,4,4	0.32	0	6,6,6	0.05	0
3	NAG	A	801	1	14,14,15	0.40	0	17,19,21	1.15	2 (11%)
4	SO4	A	811	-	4,4,4	0.34	0	6,6,6	0.04	0
4	SO4	A	814	-	4,4,4	0.31	0	6,6,6	0.05	0
4	SO4	B	808	-	4,4,4	0.31	0	6,6,6	0.06	0
4	SO4	B	816	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	815	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	B	805	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	A	812	-	4,4,4	0.32	0	6,6,6	0.06	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	801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	NAG	C2-N2-C7	2.97	127.14	122.90
3	A	801	NAG	C8-C7-N2	2.37	120.11	116.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	NAG	O5-C5-C6-O6
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	B	801	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

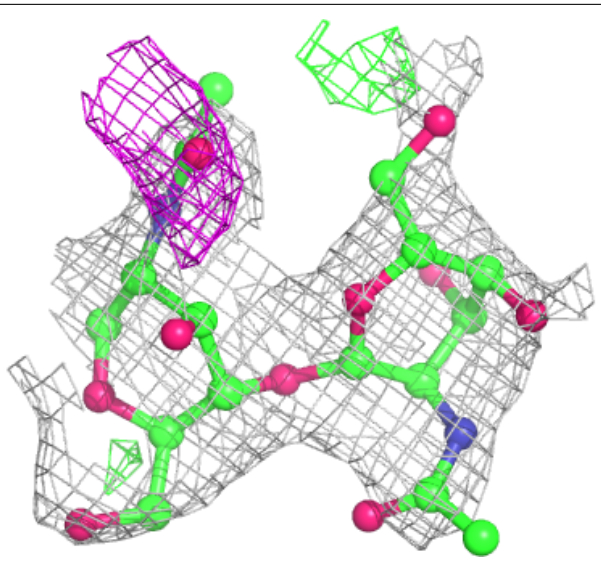
6.3 Carbohydrates

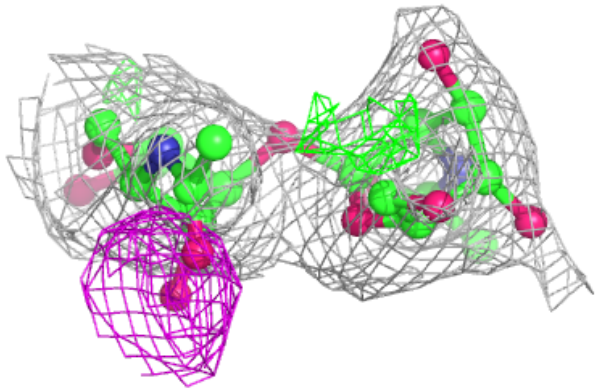
Unable to reproduce the depositors R factor - this section is therefore empty.

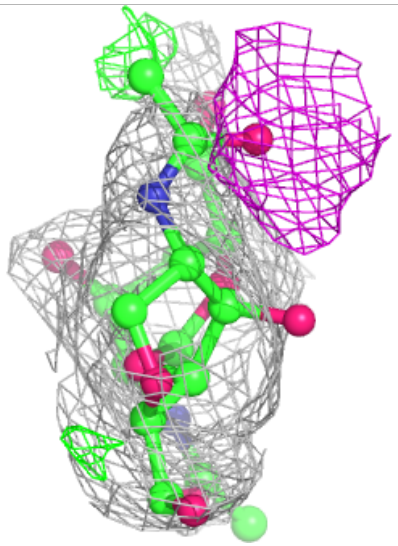
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

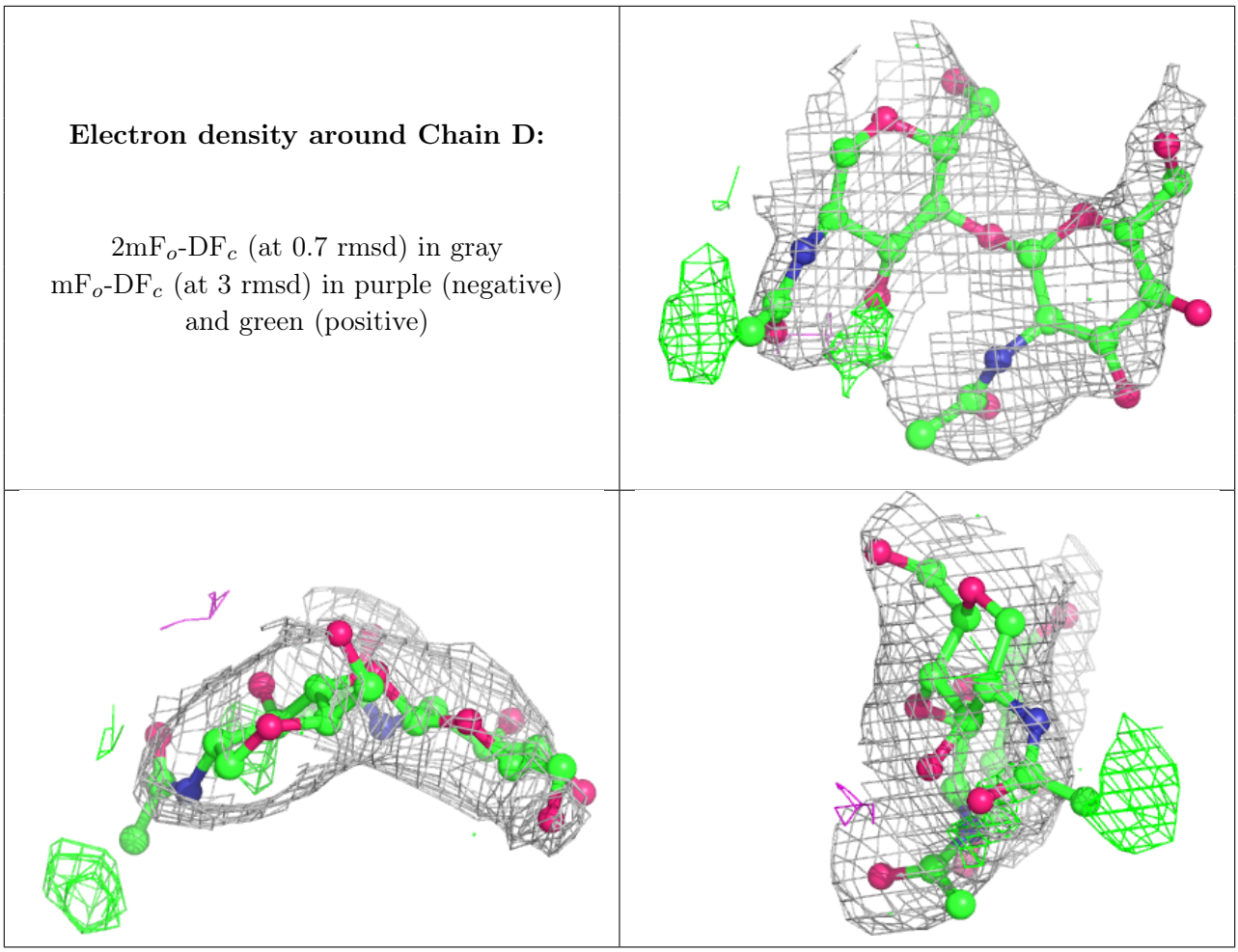






Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.