



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 11:54 AM EDT

PDB ID : 3SQ6  
Title : Crystal Structures of the Ligand Binding Domain of a Pentameric Alpha7 Nicotinic Receptor Chimera with its Agonist Epibatidine  
Authors : Li, S.-X.; Huang, S.; Bren, N.; Noridomi, K.; Dellisanti, C.; Sine, S.; Chen, L.  
Deposited on : 2011-07-05  
Resolution : 2.80 Å(reported)

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

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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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

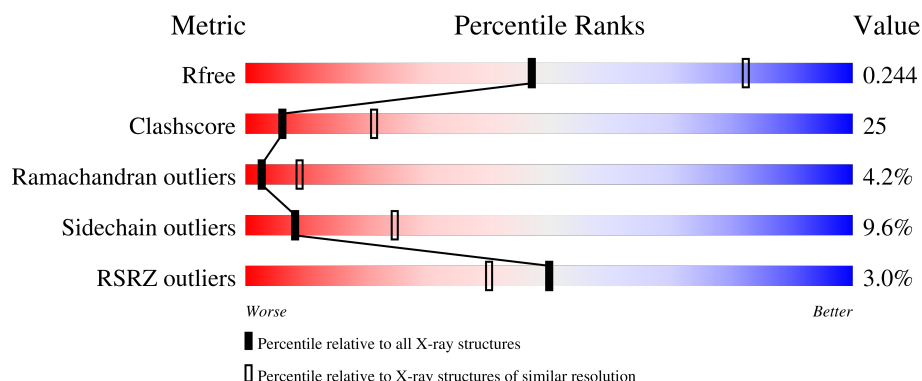
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>60%</span> <span>32%</span> <span>• •</span> </div> </div>
1	B	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>57%</span> <span>34%</span> <span>6% •</span> </div> </div>
1	C	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>58%</span> <span>32%</span> <span>5% •</span> </div> </div>
1	D	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>58%</span> <span>34%</span> <span>7% •</span> </div> </div>
1	E	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>58%</span> <span>30%</span> <span>9% ••</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	204	
1	G	204	
1	H	204	
1	I	204	
1	J	204	
2	K	2	

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
2	NAG	K	1	-	-	X	-
4	NAG	A	801	-	-	-	X
4	NAG	B	801	-	-	-	X
4	NAG	C	801	-	-	-	X
4	NAG	D	801	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16938 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 Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein.

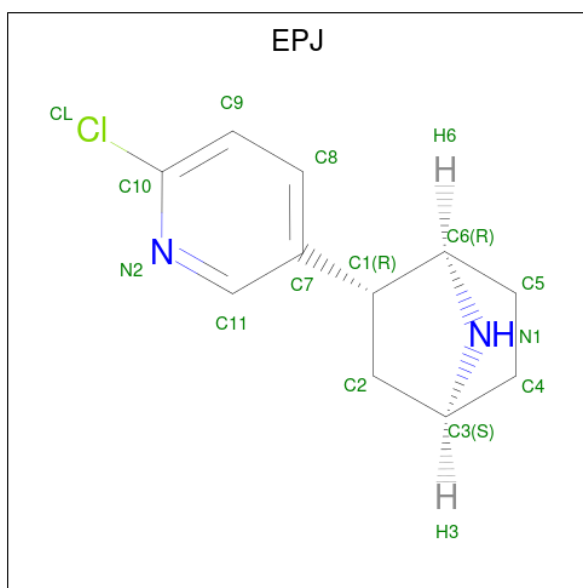
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1667	1069	278	313	7			
1	B	204	Total	C	N	O	S	0	0	0
			1667	1069	278	313	7			
1	C	203	Total	C	N	O	S	0	0	0
			1658	1064	277	310	7			
1	D	204	Total	C	N	O	S	0	0	0
			1667	1069	278	313	7			
1	E	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	F	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	G	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	H	203	Total	C	N	O	S	0	0	0
			1658	1064	277	310	7			
1	I	204	Total	C	N	O	S	0	0	0
			1667	1069	278	313	7			
1	J	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			

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



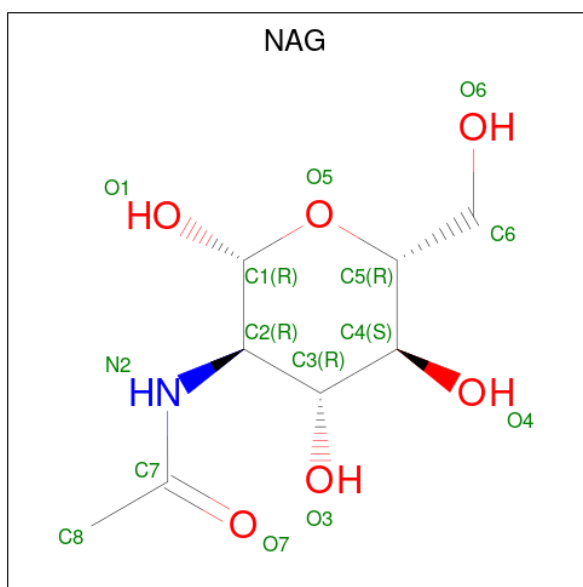
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is EPIBATIDINE (three-letter code: EPJ) (formula:  $C_{11}H_{13}ClN_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	B	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	C	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	D	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	E	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	F	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	G	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	H	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	I	1	Total	C	Cl	N	0	0
			14	11	1	2		
3	J	1	Total	C	Cl	N	0	0
			14	11	1	2		

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

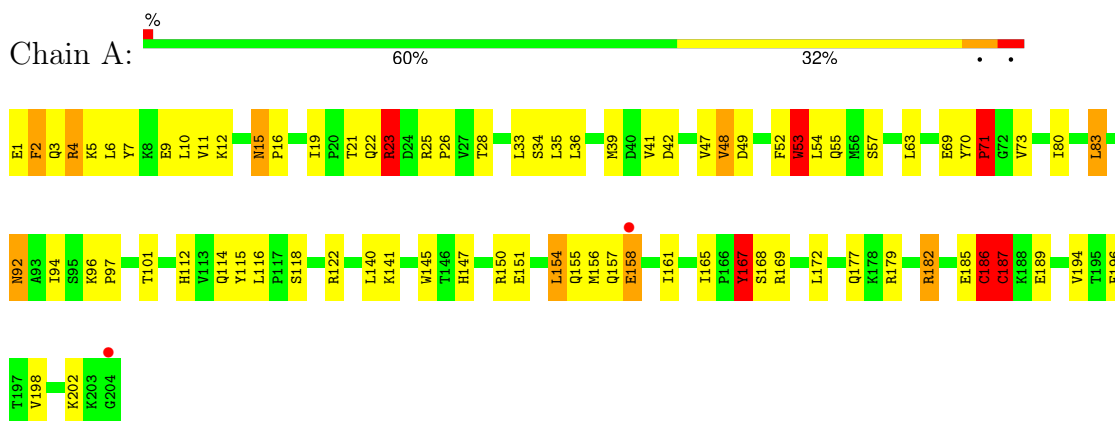
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	2	Total 2	O 2	0	0
5	E	3	Total 3	O 3	0	0
5	F	3	Total 3	O 3	0	0
5	H	2	Total 2	O 2	0	0
5	I	2	Total 2	O 2	0	0
5	J	1	Total 1	O 1	0	0

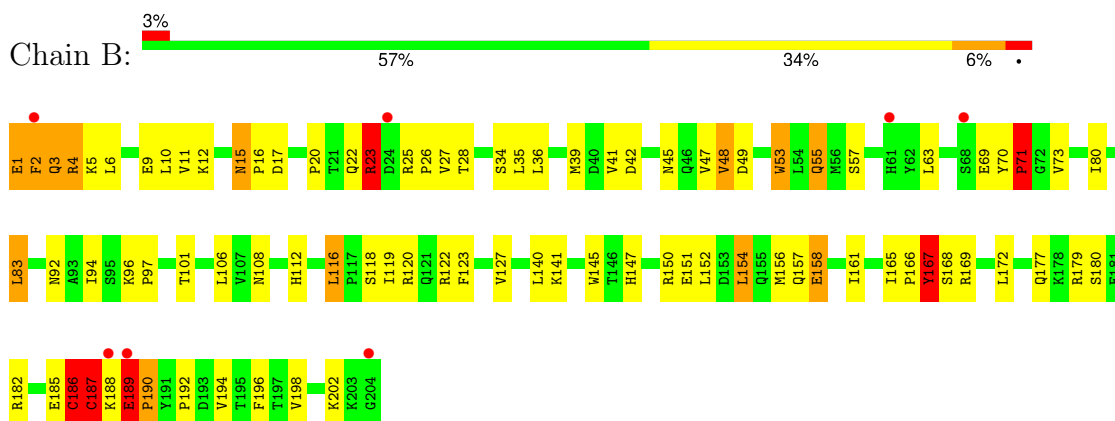
### 3 Residue-property plots

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.

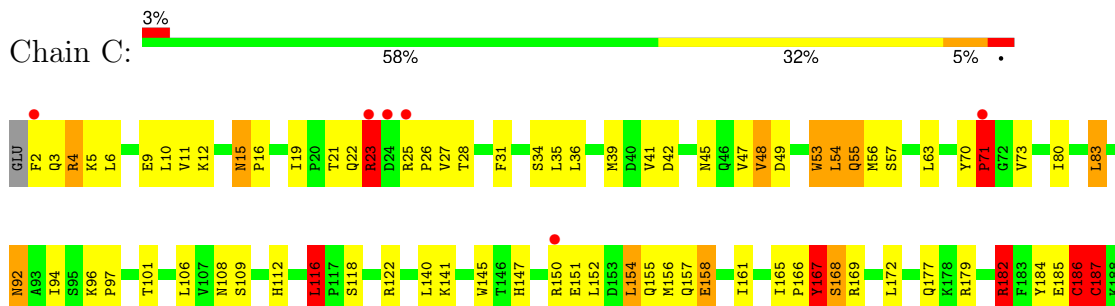
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



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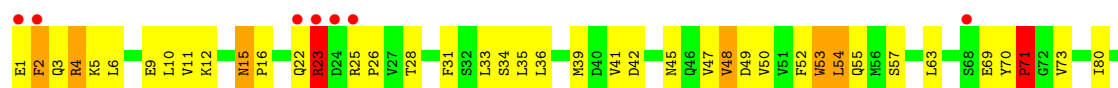
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



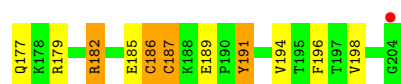
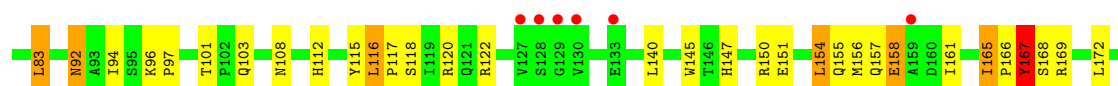
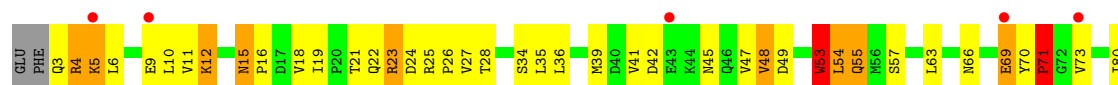




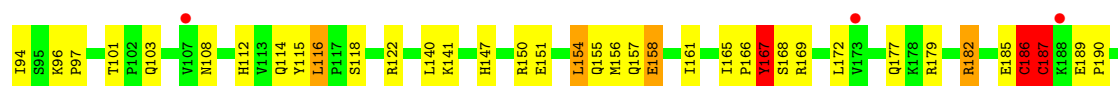
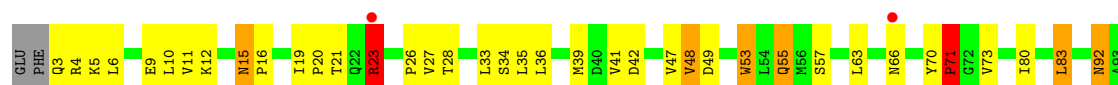
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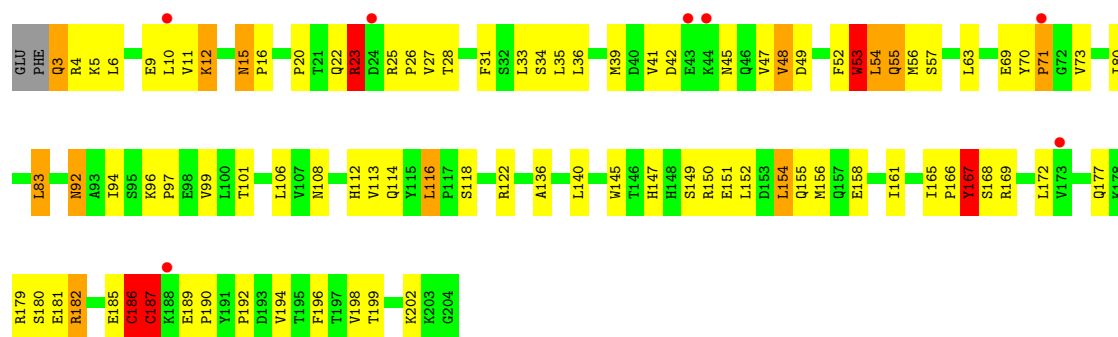


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein

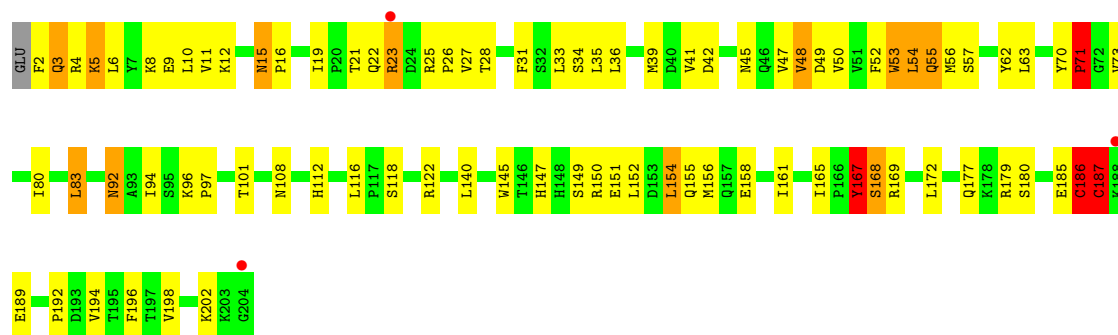


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein

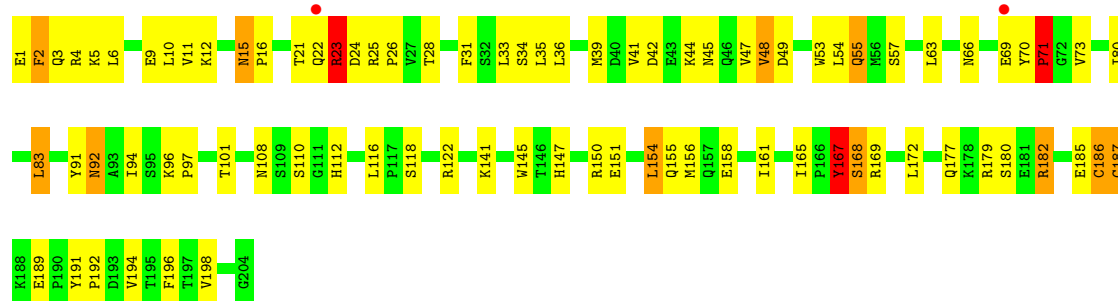




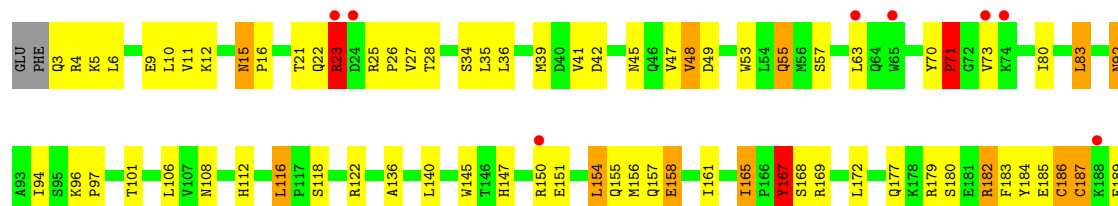
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



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- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.24Å 141.07Å 130.21Å 90.00° 99.65° 90.00°	Depositor
Resolution (Å)	47.47 – 2.80 47.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.4 (47.47-2.80) 86.3 (47.47-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.81Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.234 , 0.260 0.220 , 0.244	Depositor DCC
$R_{free}$ test set	6245 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPJ, 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	0.46	0/1712	0.74	3/2328 (0.1%)
1	B	0.50	0/1712	0.74	3/2328 (0.1%)
1	C	0.47	0/1703	0.73	3/2316 (0.1%)
1	D	0.47	0/1712	0.72	1/2328 (0.0%)
1	E	0.48	0/1691	0.72	2/2300 (0.1%)
1	F	0.47	0/1691	0.74	2/2300 (0.1%)
1	G	0.49	0/1691	0.75	4/2300 (0.2%)
1	H	0.48	0/1703	0.74	2/2316 (0.1%)
1	I	0.48	0/1712	0.72	1/2328 (0.0%)
1	J	0.47	0/1691	0.72	1/2300 (0.0%)
All	All	0.48	0/17018	0.73	22/23144 (0.1%)

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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
1	I	0	1
1	J	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	LEU	CA-CB-CG	6.41	130.03	115.30
1	B	186	CYS	CA-CB-SG	6.20	125.17	114.00
1	F	186	CYS	CA-CB-SG	6.16	125.08	114.00
1	A	53	TRP	CA-CB-CG	6.07	125.23	113.70
1	G	186	CYS	CA-CB-SG	5.83	124.50	114.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	B	182	ARG	Sidechain
1	C	182	ARG	Sidechain
1	D	182	ARG	Sidechain
1	E	182	ARG	Sidechain

## 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	1667	0	1628	91	0
1	B	1667	0	1628	85	0
1	C	1658	0	1618	87	0
1	D	1667	0	1629	90	0
1	E	1647	0	1611	128	0
1	F	1647	0	1610	75	0
1	G	1647	0	1611	84	0
1	H	1658	0	1618	106	0
1	I	1667	0	1628	88	0
1	J	1647	0	1612	80	0
2	K	28	0	25	9	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
3	C	14	0	13	0	0
3	D	14	0	13	4	0
3	E	14	0	13	2	0
3	F	14	0	13	2	0
3	G	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	14	0	13	0	0
3	I	14	0	13	4	0
3	J	14	0	13	1	0
4	A	28	0	26	0	0
4	B	28	0	26	1	0
4	C	28	0	26	3	0
4	D	14	0	13	0	0
4	E	14	0	13	1	0
4	F	14	0	13	2	0
4	G	14	0	13	1	0
4	H	28	0	26	4	0
4	I	14	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	1	0
5	H	2	0	0	0	0
5	I	2	0	0	1	0
5	J	1	0	0	0	0
All	All	16938	0	16517	825	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 25.

The worst 5 of 825 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:E:5:LYS:HG2	1:H:5:LYS:HG2	1.26	1.15
1:E:5:LYS:CG	1:H:5:LYS:HG2	1.78	1.14
1:A:182:ARG:HB3	1:A:182:ARG:NH1	1.64	1.12
1:E:23:ARG:HD2	1:E:23:ARG:N	1.61	1.11
1:J:182:ARG:HH11	1:J:182:ARG:HB3	1.17	1.07

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	202/204 (99%)	182 (90%)	12 (6%)	8 (4%)	3	9
1	B	202/204 (99%)	178 (88%)	12 (6%)	12 (6%)	1	4
1	C	201/204 (98%)	179 (89%)	14 (7%)	8 (4%)	3	9
1	D	202/204 (99%)	181 (90%)	11 (5%)	10 (5%)	2	6
1	E	200/204 (98%)	179 (90%)	14 (7%)	7 (4%)	3	12
1	F	200/204 (98%)	181 (90%)	12 (6%)	7 (4%)	3	12
1	G	200/204 (98%)	181 (90%)	11 (6%)	8 (4%)	3	9
1	H	201/204 (98%)	181 (90%)	12 (6%)	8 (4%)	3	9
1	I	202/204 (99%)	178 (88%)	15 (7%)	9 (4%)	2	8
1	J	200/204 (98%)	179 (90%)	14 (7%)	7 (4%)	3	12
All	All	2010/2040 (98%)	1799 (90%)	127 (6%)	84 (4%)	3	9

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	71	PRO
1	A	186	CYS
1	A	187	CYS
1	B	3	GLN

### 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	190/190 (100%)	171 (90%)	19 (10%)	7	22
1	B	190/190 (100%)	171 (90%)	19 (10%)	7	22
1	C	189/190 (100%)	169 (89%)	20 (11%)	6	20
1	D	190/190 (100%)	173 (91%)	17 (9%)	9	28
1	E	188/190 (99%)	170 (90%)	18 (10%)	8	24
1	F	188/190 (99%)	170 (90%)	18 (10%)	8	24
1	G	188/190 (99%)	168 (89%)	20 (11%)	6	20
1	H	189/190 (100%)	170 (90%)	19 (10%)	7	22
1	I	190/190 (100%)	175 (92%)	15 (8%)	12	34
1	J	188/190 (99%)	172 (92%)	16 (8%)	10	31
All	All	1890/1900 (100%)	1709 (90%)	181 (10%)	8	24

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	28	THR
1	H	116	LEU
1	G	54	LEU
1	G	187	CYS
1	I	2	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	147	HIS
1	H	15	ASN
1	J	177	GLN
1	F	177	GLN
1	G	55	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

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	K	1	1,2	14,14,15	1.29	1 (7%)	17,19,21	0.90	0
2	NAG	K	2	2	14,14,15	0.87	0	17,19,21	0.82	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
2	NAG	K	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	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	K	1	NAG	C1-C2	3.91	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6

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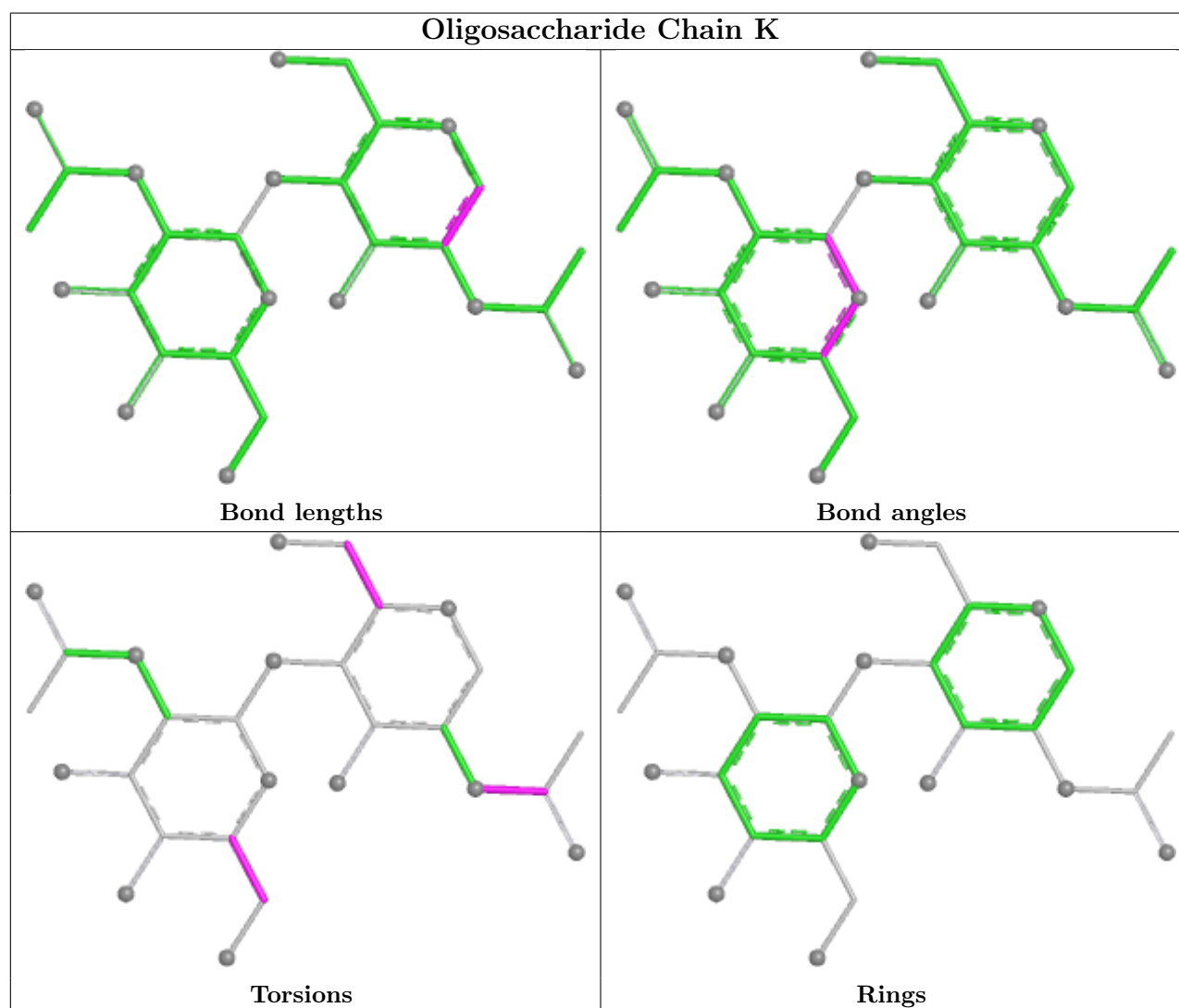
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	9	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](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	H	801	1	14,14,15	1.00	1 (7%)	17,19,21	1.10	2 (11%)
4	NAG	B	901	1	14,14,15	1.21	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	F	801	1	14,14,15	0.95	1 (7%)	17,19,21	0.90	1 (5%)
3	EPJ	C	300	-	16,16,16	2.44	7 (43%)	19,23,23	2.41	9 (47%)
3	EPJ	F	300	-	16,16,16	2.02	5 (31%)	19,23,23	2.47	6 (31%)
4	NAG	D	801	1	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
4	NAG	I	801	1	14,14,15	0.93	1 (7%)	17,19,21	0.99	1 (5%)
3	EPJ	E	300	-	16,16,16	1.88	5 (31%)	19,23,23	2.69	8 (42%)
4	NAG	B	801	1	14,14,15	0.92	1 (7%)	17,19,21	0.65	0
3	EPJ	H	300	-	16,16,16	2.25	6 (37%)	19,23,23	2.46	8 (42%)
3	EPJ	I	300	-	16,16,16	2.17	6 (37%)	19,23,23	2.57	8 (42%)
3	EPJ	G	300	-	16,16,16	2.09	5 (31%)	19,23,23	2.54	6 (31%)
4	NAG	G	901	1	14,14,15	0.96	1 (7%)	17,19,21	0.67	0
4	NAG	C	901	1	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	EPJ	D	300	-	16,16,16	2.07	5 (31%)	19,23,23	2.61	8 (42%)
3	EPJ	A	300	-	16,16,16	2.25	7 (43%)	19,23,23	2.53	8 (42%)
4	NAG	E	801	1	14,14,15	0.90	1 (7%)	17,19,21	0.68	0
4	NAG	C	801	1	14,14,15	0.81	1 (7%)	17,19,21	0.64	0
4	NAG	H	901	1	14,14,15	0.95	1 (7%)	17,19,21	0.86	1 (5%)
3	EPJ	J	300	-	16,16,16	1.93	4 (25%)	19,23,23	2.62	7 (36%)
4	NAG	A	801	1	14,14,15	0.89	1 (7%)	17,19,21	0.77	0
4	NAG	A	901	1	14,14,15	1.06	1 (7%)	17,19,21	0.87	0
3	EPJ	B	300	-	16,16,16	2.02	6 (37%)	19,23,23	2.89	8 (42%)

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	H	801	1	-	6/6/23/26	0/1/1/1
4	NAG	B	901	1	-	4/6/23/26	0/1/1/1
4	NAG	F	801	1	-	5/6/23/26	0/1/1/1
3	EPJ	C	300	-	-	2/4/21/21	0/4/3/3
3	EPJ	F	300	-	-	2/4/21/21	0/4/3/3
4	NAG	D	801	1	-	6/6/23/26	0/1/1/1
4	NAG	I	801	1	-	3/6/23/26	0/1/1/1
3	EPJ	E	300	-	-	2/4/21/21	0/4/3/3
4	NAG	B	801	1	-	6/6/23/26	0/1/1/1
3	EPJ	H	300	-	-	2/4/21/21	0/4/3/3
3	EPJ	I	300	-	-	3/4/21/21	0/4/3/3
3	EPJ	G	300	-	-	4/4/21/21	0/4/3/3
4	NAG	G	901	1	-	3/6/23/26	0/1/1/1
4	NAG	C	901	1	-	4/6/23/26	0/1/1/1
3	EPJ	D	300	-	-	2/4/21/21	0/4/3/3
3	EPJ	A	300	-	-	2/4/21/21	0/4/3/3
4	NAG	E	801	1	-	5/6/23/26	0/1/1/1
4	NAG	C	801	1	-	5/6/23/26	0/1/1/1
4	NAG	H	901	1	-	3/6/23/26	0/1/1/1
3	EPJ	J	300	-	-	2/4/21/21	0/4/3/3
4	NAG	A	801	1	-	5/6/23/26	0/1/1/1
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	EPJ	B	300	-	-	2/4/21/21	0/4/3/3

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	300	EPJ	C5-C6	5.45	1.63	1.53
3	C	300	EPJ	C5-C6	5.31	1.63	1.53
3	F	300	EPJ	C5-C6	5.29	1.63	1.53
3	A	300	EPJ	C5-C6	5.21	1.62	1.53
3	I	300	EPJ	C5-C6	5.13	1.62	1.53

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	300	EPJ	C11-N2-C10	6.27	123.86	116.33
3	B	300	EPJ	C4-C3-C2	-6.09	103.60	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	300	EPJ	C5-C6-C1	-5.99	103.49	109.74
3	B	300	EPJ	C11-N2-C10	5.96	123.49	116.33
3	E	300	EPJ	C11-N2-C10	5.85	123.35	116.33

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	901	NAG	C8-C7-N2-C2
4	A	901	NAG	O7-C7-N2-C2
4	B	801	NAG	C1-C2-N2-C7

There are no ring outliers.

17 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	801	NAG	2	0
4	F	801	NAG	2	0
3	F	300	EPJ	2	0
4	I	801	NAG	1	0
3	E	300	EPJ	2	0
4	B	801	NAG	1	0
3	I	300	EPJ	4	0
3	G	300	EPJ	1	0
4	G	901	NAG	1	0
4	C	901	NAG	2	0
3	D	300	EPJ	4	0
3	A	300	EPJ	1	0
4	E	801	NAG	1	0
4	C	801	NAG	1	0
4	H	901	NAG	2	0
3	J	300	EPJ	1	0
3	B	300	EPJ	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	204/204 (100%)	0.22	2 (0%) 82 77	31, 58, 87, 102	0
1	B	204/204 (100%)	0.32	7 (3%) 45 35	29, 59, 88, 110	0
1	C	203/204 (99%)	0.29	6 (2%) 50 40	32, 60, 90, 110	0
1	D	204/204 (100%)	0.29	7 (3%) 45 35	35, 59, 91, 116	0
1	E	202/204 (99%)	0.38	12 (5%) 22 14	37, 57, 89, 97	0
1	F	202/204 (99%)	0.31	6 (2%) 50 40	39, 60, 88, 98	0
1	G	202/204 (99%)	0.33	7 (3%) 44 34	39, 60, 87, 104	0
1	H	203/204 (99%)	0.20	3 (1%) 73 68	33, 59, 90, 118	0
1	I	204/204 (100%)	0.12	2 (0%) 82 77	37, 58, 89, 102	0
1	J	202/204 (99%)	0.38	9 (4%) 33 23	40, 60, 91, 110	0
All	All	2030/2040 (99%)	0.28	61 (3%) 50 40	29, 59, 90, 118	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	LYS	5.5
1	C	24	ASP	4.5
1	E	73	VAL	4.4
1	J	204	GLY	4.2
1	B	2	PHE	3.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

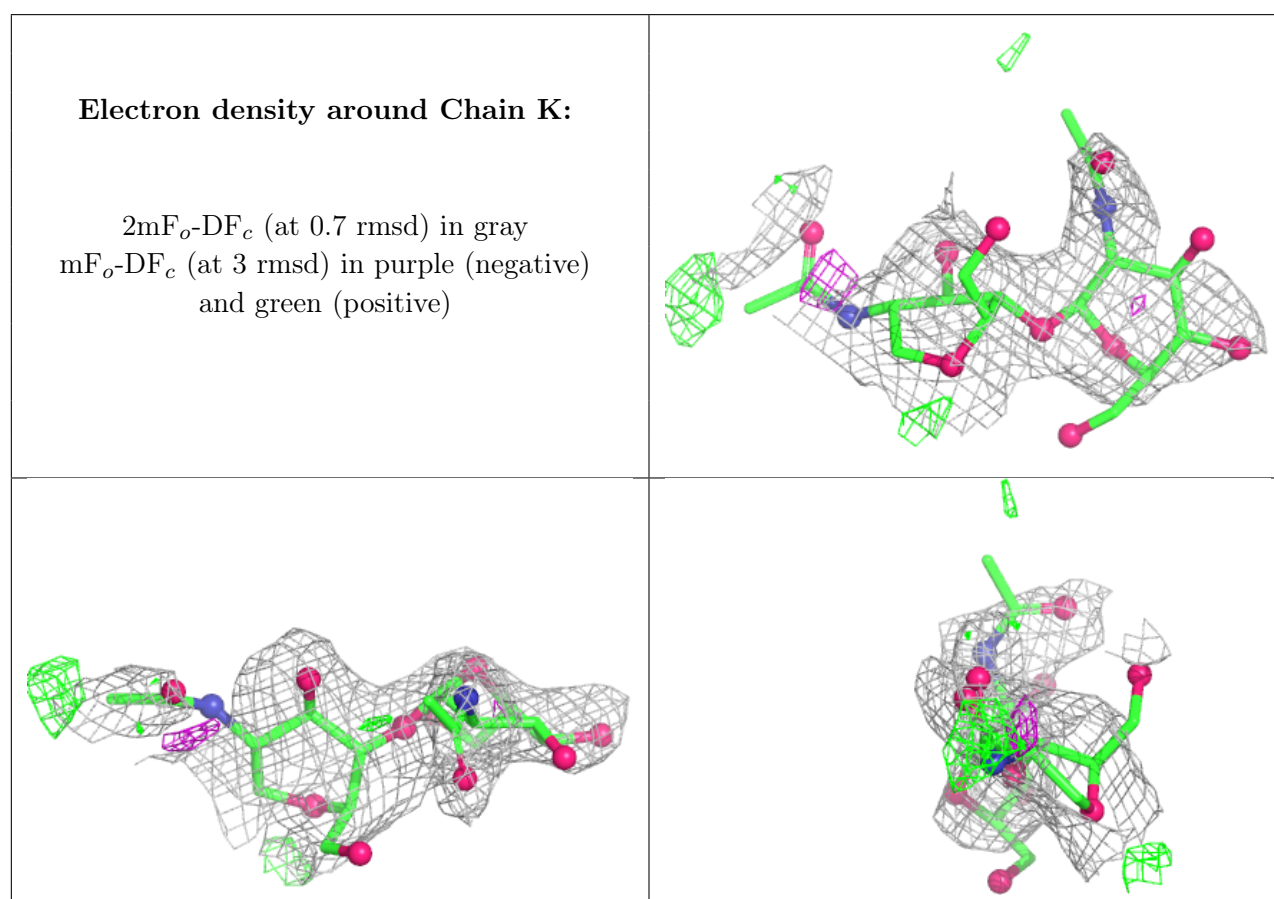


### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	K	1	14/15	0.73	0.36	99,105,110,112	0
2	NAG	K	2	14/15	0.82	0.53	104,112,114,118	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	801	14/15	0.64	0.56	121,127,128,128	0
4	NAG	B	901	14/15	0.64	0.35	78,90,97,100	0
4	NAG	H	801	14/15	0.68	0.18	91,105,108,109	0
4	NAG	E	801	14/15	0.70	0.20	95,104,109,109	0
4	NAG	C	901	14/15	0.70	0.28	86,88,92,94	0
4	NAG	I	801	14/15	0.71	0.30	92,107,111,112	0
4	NAG	A	901	14/15	0.73	0.31	91,93,98,98	0
4	NAG	B	801	14/15	0.73	0.41	103,111,114,115	0
4	NAG	D	801	14/15	0.73	0.46	101,122,126,129	0
4	NAG	F	801	14/15	0.75	0.39	110,115,118,119	0
4	NAG	G	901	14/15	0.76	0.39	73,85,93,99	0
4	NAG	C	801	14/15	0.79	0.56	113,119,125,127	0
4	NAG	H	901	14/15	0.81	0.26	71,79,81,81	0
3	EPJ	A	300	14/14	0.85	0.28	21,39,43,46	0
3	EPJ	F	300	14/14	0.86	0.29	31,43,48,48	0
3	EPJ	G	300	14/14	0.87	0.25	9,34,41,43	0
3	EPJ	E	300	14/14	0.88	0.32	32,43,48,48	0
3	EPJ	B	300	14/14	0.88	0.27	23,38,43,46	0
3	EPJ	D	300	14/14	0.89	0.25	30,49,52,53	0
3	EPJ	I	300	14/14	0.90	0.35	30,47,50,51	0
3	EPJ	H	300	14/14	0.90	0.23	21,34,48,50	0
3	EPJ	J	300	14/14	0.91	0.33	37,42,50,50	0
3	EPJ	C	300	14/14	0.93	0.20	33,47,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.