



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 07:23 am GMT

PDB ID : 2HA3
Title : Crystal structure of mouse acetylcholinesterase complexed with choline
Authors : Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.
Deposited on : 2006-06-12
Resolution : 2.25 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28986

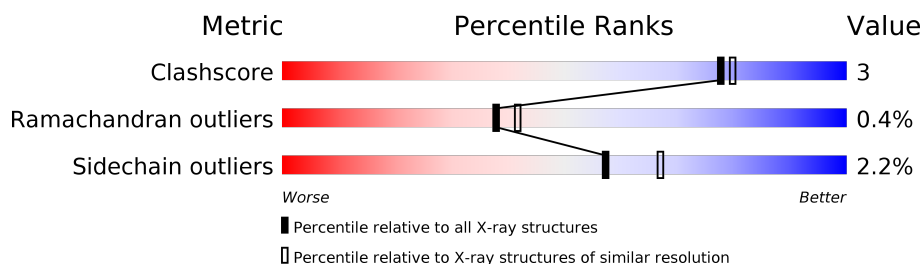
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	543	 91% 8% ..
1	B	543	 90% 8% ..

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	B	601	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9213 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.

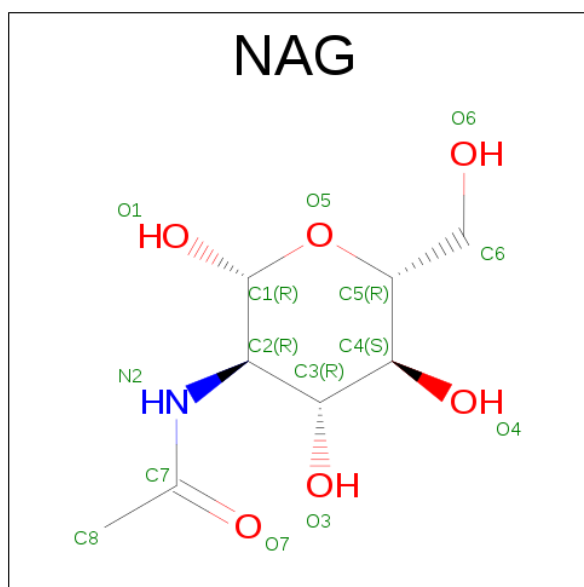
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4196	2692	728	762	14			
1	B	534	Total	C	N	O	S	0	2	0
			4176	2681	720	761	14			

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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



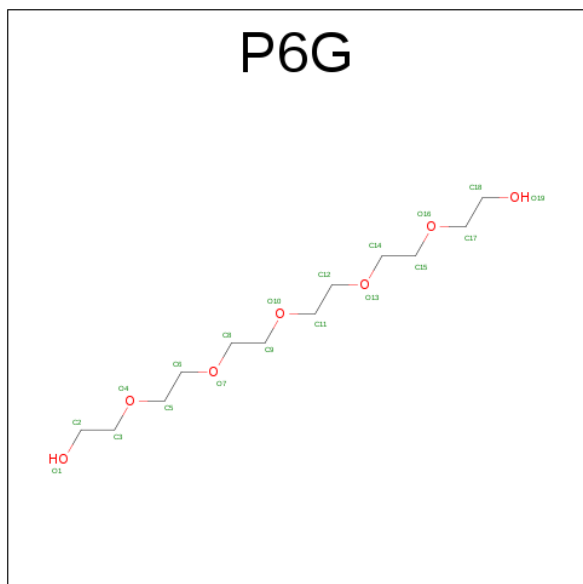
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

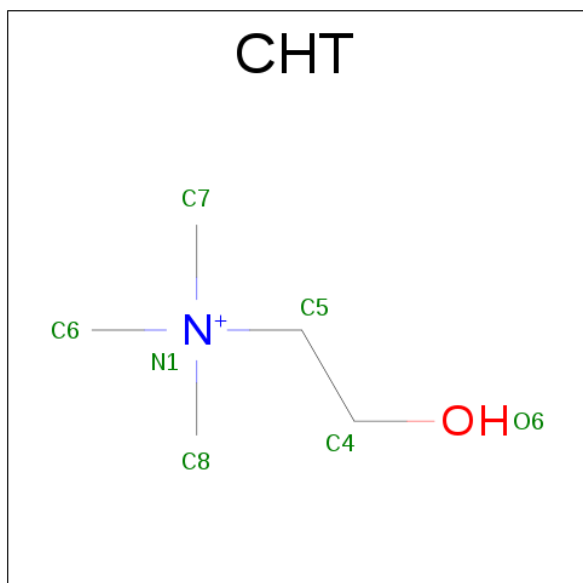
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	5	1	1		
5	A	1	Total	C	N	O	0	0
			7	5	1	1		
5	B	1	Total	C	N	O	0	0
			7	5	1	1		
5	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 6 is water.

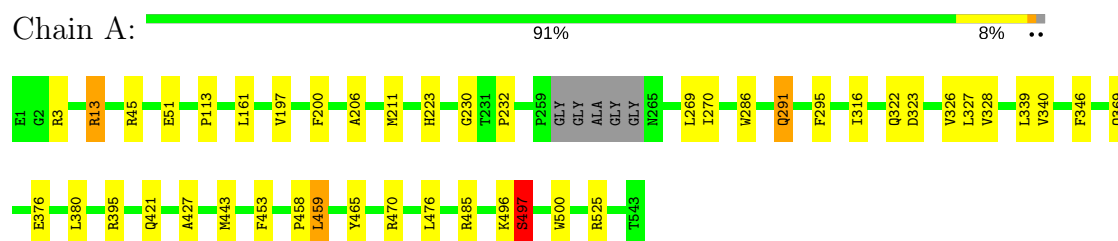
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	396	Total	O	0	0
			396	396		
6	B	346	Total	O	0	0
			346	346		

3 Residue-property plots

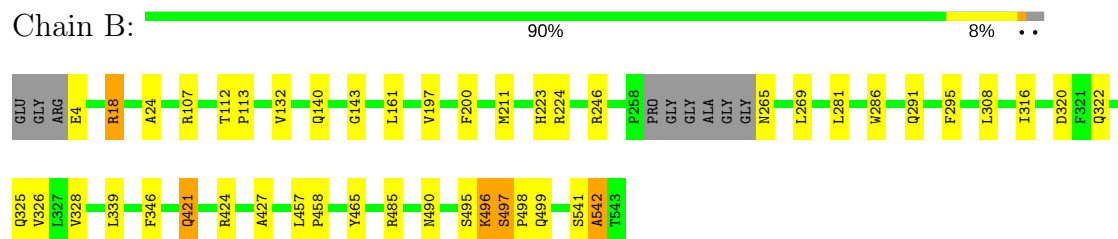
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS failed to run properly.

• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.39Å 111.87Å 227.15Å 89.97° 90.02° 90.04°	Depositor
Resolution (Å)	30.00 – 2.25	Depositor
% Data completeness (in resolution range)	96.0 (30.00-2.25)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.199	Depositor
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.686	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: CHT, NAG, P6G, FUC

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	0.50	0/4321	0.64	1/5906 (0.0%)
1	B	0.47	0/4308	0.63	1/5888 (0.0%)
All	All	0.49	0/8629	0.63	2/11794 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	18	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	4196	0	4079	27	0
1	B	4176	0	4059	30	0
2	A	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	19	0	26	0	0
5	A	14	0	28	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	28	3	0
6	A	396	0	0	1	0
6	B	346	0	0	2	0
All	All	9213	0	8268	57	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 3.

All (57) 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:291:GLN:NE2	1:A:369:GLN:HE21	1.85	0.75
1:A:291:GLN:NE2	1:A:369:GLN:NE2	2.35	0.74
1:A:291:GLN:HE22	1:A:369:GLN:NE2	1.89	0.70
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.73	0.69
1:B:286:TRP:CH2	5:B:962:CHT:H83	2.32	0.64
1:B:497:SER:CB	1:B:498:PRO:C	2.69	0.61
1:A:291:GLN:HE22	1:A:369:GLN:HE21	1.48	0.58
1:B:490:ASN:O	6:B:1124:HOH:O	2.17	0.58
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.86	0.57
1:B:316:ILE:O	1:B:421:GLN:NE2	2.37	0.56
1:B:197:VAL:H	1:B:223:HIS:HD2	1.55	0.55
1:B:328:VAL:O	1:B:427:ALA:HA	2.06	0.55
1:A:496:LYS:HA	1:A:497:SER:C	2.27	0.55
1:B:497:SER:HB2	1:B:498:PRO:C	2.28	0.54
1:A:13:ARG:NH2	6:A:984:HOH:O	2.42	0.52
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.92	0.50
1:A:197:VAL:H	1:A:223:HIS:HD2	1.58	0.50
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.94	0.50
1:B:541:SER:O	1:B:542:ALA:HB2	2.12	0.50
1:B:286:TRP:CH2	5:B:962:CHT:C8	2.94	0.50
1:B:497:SER:HB3	1:B:498:PRO:C	2.32	0.50
1:A:197:VAL:H	1:A:223:HIS:CD2	2.30	0.49
1:B:112:THR:HG21	1:B:143:GLY:O	2.13	0.48
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.96	0.48
1:B:320:ASP:OD1	1:B:322:GLN:HG3	2.14	0.48
1:A:316:ILE:O	1:A:421:GLN:NE2	2.36	0.48
1:B:4:GLU:OE1	1:B:18:ARG:HD3	2.14	0.47
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.96	0.47
1:B:265:ASN:ND2	6:B:1308:HOH:O	2.48	0.46
1:B:286:TRP:CZ3	5:B:962:CHT:H81	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.51	0.46
1:B:197:VAL:H	1:B:223:HIS:CD2	2.33	0.45
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.99	0.45
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.52	0.44
1:A:286:TRP:CH2	5:A:952:CHT:H62	2.52	0.44
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.53	0.44
1:B:495:SER:O	1:B:496:LYS:O	2.36	0.44
1:A:328:VAL:O	1:A:427:ALA:HA	2.18	0.44
1:B:495:SER:OG	1:B:496:LYS:N	2.50	0.44
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.99	0.43
1:A:496:LYS:N	1:A:497:SER:O	2.51	0.43
1:A:161:LEU:HD12	1:A:270:ILE:CG1	2.49	0.43
1:A:496:LYS:CA	1:A:497:SER:C	2.87	0.42
1:B:24:ALA:HB3	1:B:140:GLN:HG3	2.02	0.42
1:A:211:MET:HG3	1:A:232:PRO:HB3	2.01	0.42
1:A:340:VAL:HG11	1:A:443:MET:CE	2.50	0.42
1:B:497:SER:HB2	1:B:498:PRO:CA	2.49	0.42
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.55	0.41
1:A:45:ARG:HD3	1:A:51:GLU:OE1	2.19	0.41
1:A:206:ALA:HB3	1:A:230:GLY:HA3	2.03	0.41
1:A:376:GLU:O	1:A:380:LEU:HG	2.21	0.41
1:A:459:LEU:HD22	1:A:470:ARG:HG2	2.02	0.41
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.01	0.41
1:B:497:SER:HB2	1:B:499:GLN:N	2.36	0.40
1:B:457:LEU:N	1:B:458:PRO:CD	2.84	0.40
1:B:161:LEU:CD1	1:B:269:LEU:HD22	2.49	0.40
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.57	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	534/543 (98%)	516 (97%)	17 (3%)	1 (0%)	51	60
1	B	532/543 (98%)	515 (97%)	14 (3%)	3 (1%)	28	29
All	All	1066/1086 (98%)	1031 (97%)	31 (3%)	4 (0%)	38	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	LYS
1	B	497	SER
1	B	542	ALA
1	A	497	SER

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	441/443 (100%)	431 (98%)	10 (2%)	56	65
1	B	441/443 (100%)	432 (98%)	9 (2%)	60	70
All	All	882/886 (100%)	863 (98%)	19 (2%)	57	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	13	ARG
1	A	200	PHE
1	A	291	GLN
1	A	295	PHE
1	A	322	GLN
1	A	323	ASP
1	A	459	LEU
1	A	497	SER
1	A	525	ARG
1	B	107	ARG
1	B	132	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	200	PHE
1	B	246	ARG
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	421	GLN
1	B	424	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	287	HIS
1	A	291	GLN
1	A	322	GLN
1	A	509	GLN
1	B	223	HIS
1	B	291	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 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
2	NAG	A	544	1,2	14,14,15	0.60	0	15,19,21	1.41	1 (6%)
2	FUC	A	545	2	9,10,11	0.78	0	13,14,16	1.77	4 (30%)

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	A	544	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	545	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	545	FUC	O5-C1-C2	-2.09	107.52	110.79
2	A	545	FUC	C1-C2-C3	2.45	112.75	109.65
2	A	545	FUC	C2-C3-C4	2.87	115.87	110.88
2	A	545	FUC	C3-C4-C5	4.08	116.10	109.68
2	A	544	NAG	C1-O5-C5	4.11	117.83	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

7 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
3	NAG	A	701	1	14,14,15	0.47	0	15,19,21	1.63	3 (20%)
4	P6G	A	901	-	18,18,18	2.21	6 (33%)	17,17,17	1.32	2 (11%)
5	CHT	A	951	-	6,6,6	0.92	0	8,8,8	0.45	0
5	CHT	A	952	-	6,6,6	0.83	0	8,8,8	0.34	0
3	NAG	B	601	1	14,14,15	0.82	1 (7%)	15,19,21	1.32	2 (13%)
5	CHT	B	961	-	6,6,6	0.87	0	8,8,8	0.43	0
5	CHT	B	962	-	6,6,6	0.76	0	8,8,8	0.31	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	701	1	-	0/6/23/26	0/1/1/1
4	P6G	A	901	-	-	0/16/16/16	0/0/0/0
5	CHT	A	951	-	-	0/4/4/4	0/0/0/0
5	CHT	A	952	-	-	0/4/4/4	0/0/0/0
3	NAG	B	601	1	1/1/5/7	1/6/23/26	0/1/1/1
5	CHT	B	961	-	-	0/4/4/4	0/0/0/0
5	CHT	B	962	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	C1-C2	2.39	1.55	1.52
4	A	901	P6G	O7-C6	2.69	1.53	1.42
4	A	901	P6G	O19-C18	3.37	1.59	1.42
4	A	901	P6G	O4-C3	3.54	1.57	1.42
4	A	901	P6G	O16-C15	3.65	1.57	1.42
4	A	901	P6G	O13-C12	3.85	1.58	1.42
4	A	901	P6G	O10-C9	4.46	1.61	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	C4-C3-C2	-2.14	107.89	111.02
4	A	901	P6G	O13-C12-C11	2.13	120.19	110.41
3	A	701	NAG	O5-C1-C2	2.53	114.99	111.47
3	B	601	NAG	C1-C2-N2	2.53	114.81	110.49
3	B	601	NAG	C2-N2-C7	2.88	127.14	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	P6G	O1-C2-C3	3.32	130.94	111.89
3	A	701	NAG	C1-O5-C5	4.44	118.29	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	952	CHT	1	0
5	B	962	CHT	3	0

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.