wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:55 PM GMT

PDB ID	:	1HYA
Title	:	HYALURONIC ACID, STRUCTURE OF A FULLY EXTENDED 3-FOLD HELICAL SODIUM SALT AND COMPARISON WITH THE LESS EXTENDED 4-FOLD HELICAL FORMS
Authors	:	Arnott, S.
Deposited on	:	1977-11-20
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

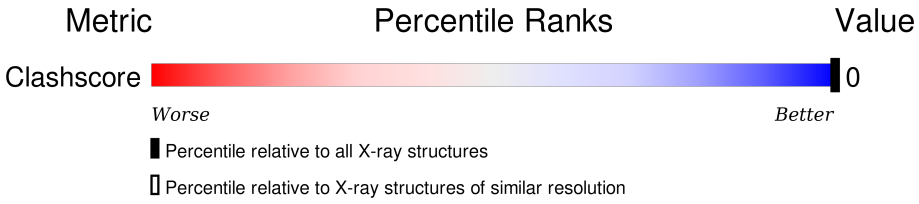
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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	102246	1912 (3.00-3.00)

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
1	GCU	A	1	-	-	X	-
1	NAG	A	2	-	-	X	-
1	GCU	A	3	X	-	X	-
1	NAG	A	4	-	-	X	-
1	GCU	A	5	X	-	X	-
1	NAG	A	6	-	-	X	-
2	NA	A	771	-	-	X	-
2	NA	A	772	-	-	X	-
2	NA	A	773	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 141 atoms, of which 48 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 polysaccharide(D) called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
1	A	6	126	42	48	3	33	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	3	3	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	12	12	12	0	0

3 Residue-property plots

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	11.70Å 11.70Å 28.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	LALS	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	141	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GCU, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	GCU	C1
1	A	5	GCU	C1

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	78	48	55	0	391
2	A	3	0	0	0	3
3	A	12	0	0	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	93	48	55	0	400

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 0.

There are no clashes within the asymmetric unit.

The worst 5 of 400 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:NAG:O4	1:A:6:NAG:O4[2_654]	0.00	2.20
1:A:4:NAG:C2	1:A:6:NAG:C2[2_654]	0.00	2.20
1:A:4:NAG:O5	1:A:6:NAG:O5[2_654]	0.00	2.20
3:A:993:HOH:O	3:A:1001:HOH:O[3_664]	0.00	2.20
1:A:1:GCU:O6A	1:A:3:GCU:O6A[2_654]	0.00	2.20

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

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

6 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	$\#\|Z\| > 2$
1	GCU	A	1	1	9,12,13	0.22	0	13,17,19	0.57	0
1	NAG	A	2	1	14,14,15	0.46	0	15,19,21	0.98	1 (6%)
1	GCU	A	3	1	9,12,13	0.21	0	13,17,19	0.58	0
1	NAG	A	4	1	14,14,15	0.46	0	15,19,21	0.98	1 (6%)
1	GCU	A	5	1	9,12,13	0.20	0	13,17,19	0.58	0
1	NAG	A	6	1	14,14,15	0.46	0	15,19,21	0.99	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	GCU	A	1	1	-	0/0/21/24	0/1/1/1
1	NAG	A	2	1	-	0/6/23/26	0/1/1/1
1	GCU	A	3	1	1/1/6/6	0/0/21/24	0/1/1/1
1	NAG	A	4	1	-	0/6/23/26	0/1/1/1
1	GCU	A	5	1	1/1/6/6	0/0/21/24	0/1/1/1
1	NAG	A	6	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	NAG	C2-N2-C7	-3.22	118.90	123.04
1	A	4	NAG	C2-N2-C7	-3.22	118.91	123.04
1	A	2	NAG	C2-N2-C7	-3.20	118.93	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	GCU	C1
1	A	5	GCU	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	GCU	0	107
1	A	2	NAG	0	154
1	A	3	GCU	0	106
1	A	4	NAG	0	154
1	A	5	GCU	0	106
1	A	6	NAG	0	155

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.