



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:52 AM GMT

PDB ID : 1C58
Title : CRYSTAL STRUCTURE OF CYCLOAMYLOSE 26
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Deposited on : 1999-11-04
Resolution : 0.99 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

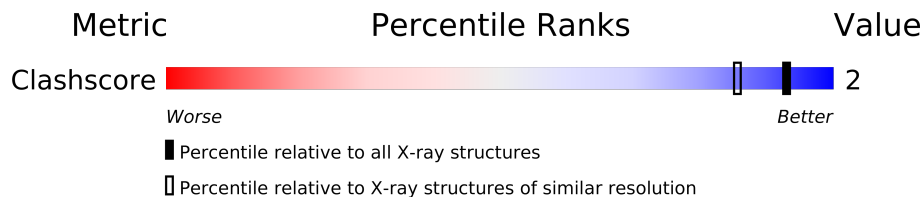
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 0.99 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	79885	1028 (1.10-0.90)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1307 atoms, of which 571 are hydrogens and 0 are deuterium.

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 (26-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
1	A	26	Total	C	H	O	0	9
			582	156	287	139		
1	B	26	Total	C	H	O	0	8
			578	156	284	138		

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	55	Total	O	0	0
			55	55		

3 Residue-property plots

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

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	21.84Å 22.92Å 29.05Å 87.36° 89.51° 61.98°	Depositor
Resolution (Å)	29.02 – 0.99	Depositor
% Data completeness (in resolution range)	96.7 (29.02-0.99)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.082 , 0.100	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1307	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: GLC

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	295	287	0	1	0
1	B	294	284	0	0	0
2	A	92	0	0	2	26
2	B	55	0	0	0	24
All	All	736	571	0	2	26

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:GLC:H2	2:A:292:HOH:O	2.05	0.56

The worst 5 of 26 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	Distance(Å)	Clash(Å)
2:A:344:HOH:O	2:B:222:HOH:O[1_655]	0.77	1.43
2:A:346:HOH:O	2:B:298:HOH:O[1_655]	0.91	1.29
2:A:306:HOH:O	2:B:294:HOH:O[1_545]	0.94	1.26
2:A:288:HOH:O	2:B:305:HOH:O[1_655]	0.99	1.21
2:A:347:HOH:O	2:B:241:HOH:O[1_655]	1.04	1.16

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 69 carbohydrates modelled in this entry, 34 are modelled with single atom - leaving 35 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
1	GLC	A	1	1	10,11,12	0.60	0	11,15,17	1.04	1 (9%)
1	GLC	A	12	1	10,11,12	0.60	0	11,15,17	1.04	1 (9%)
1	GLC	A	13	1	10,11,12	0.57	0	11,15,17	0.79	0
1	GLC	A	14	1	10,11,12	0.78	0	11,15,17	1.25	1 (9%)
1	GLC	A	15	1	10,11,12	0.78	0	11,15,17	0.95	1 (9%)
1	GLC	A	17	1	10,11,12	0.76	0	11,15,17	0.83	0
1	GLC	A	18	1	10,11,12	0.77	0	11,15,17	0.81	0
1	GLC	A	19	1	10,11,12	0.63	0	11,15,17	0.67	0
1	GLC	A	2	1	10,11,12	0.52	0	11,15,17	1.35	1 (9%)
1	GLC	A	20	1	10,11,12	0.52	0	11,15,17	0.80	0
1	GLC	A	21	1	10,11,12	0.62	0	11,15,17	0.61	0
1	GLC	A	25	1	10,11,12	0.64	0	11,15,17	0.81	0
1	GLC	A	26	1	10,11,12	0.65	0	11,15,17	0.96	1 (9%)
1	GLC	A	3	1	10,11,12	0.68	0	11,15,17	0.93	0
1	GLC	A	6	1	10,11,12	0.73	0	11,15,17	0.73	0
1	GLC	A	7	1	10,11,12	0.60	0	11,15,17	0.73	0
1	GLC	A	8	1	10,11,12	0.56	0	11,15,17	0.89	0
1	GLC	B	101	1	10,11,12	0.64	0	11,15,17	0.99	1 (9%)
1	GLC	B	102	1	10,11,12	0.94	1 (10%)	11,15,17	1.39	2 (18%)
1	GLC	B	103	1	10,11,12	0.70	0	11,15,17	0.86	0
1	GLC	B	104	1	10,11,12	0.56	0	11,15,17	0.62	0
1	GLC	B	105	1	10,11,12	0.67	0	11,15,17	0.73	0
1	GLC	B	106	1	10,11,12	0.68	0	11,15,17	0.64	0
1	GLC	B	107	1	10,11,12	0.67	0	11,15,17	0.72	0
1	GLC	B	108	1	10,11,12	0.90	0	11,15,17	1.11	1 (9%)
1	GLC	B	109	1	10,11,12	0.71	0	11,15,17	1.04	1 (9%)
1	GLC	B	110	1	10,11,12	0.72	0	11,15,17	0.91	0
1	GLC	B	114	1	10,11,12	0.62	0	11,15,17	1.19	1 (9%)
1	GLC	B	115	1	10,11,12	0.57	0	11,15,17	1.06	1 (9%)
1	GLC	B	116	1	10,11,12	0.71	0	11,15,17	1.23	1 (9%)
1	GLC	B	118	1	10,11,12	0.55	0	11,15,17	0.68	0
1	GLC	B	120	1	10,11,12	0.59	0	11,15,17	0.84	0
1	GLC	B	121	1	10,11,12	0.71	0	11,15,17	0.79	0
1	GLC	B	122	1	10,11,12	0.60	0	11,15,17	0.90	0
1	GLC	B	123	1	10,11,12	0.81	0	11,15,17	0.93	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
1	GLC	A	1	1	-	0/2/19/22	0/1/1/1
1	GLC	A	12	1	-	0/2/19/22	0/1/1/1
1	GLC	A	13	1	-	0/2/19/22	0/1/1/1
1	GLC	A	14	1	-	0/2/19/22	0/1/1/1
1	GLC	A	15	1	-	0/2/19/22	0/1/1/1
1	GLC	A	17	1	-	0/2/19/22	0/1/1/1
1	GLC	A	18	1	-	0/2/19/22	0/1/1/1
1	GLC	A	19	1	-	0/2/19/22	0/1/1/1
1	GLC	A	2	1	-	0/2/19/22	0/1/1/1
1	GLC	A	20	1	-	0/2/19/22	0/1/1/1
1	GLC	A	21	1	-	0/2/19/22	0/1/1/1
1	GLC	A	25	1	-	0/2/19/22	0/1/1/1
1	GLC	A	26	1	-	0/2/19/22	0/1/1/1
1	GLC	A	3	1	-	0/2/19/22	0/1/1/1
1	GLC	A	6	1	-	0/2/19/22	0/1/1/1
1	GLC	A	7	1	-	0/2/19/22	0/1/1/1
1	GLC	A	8	1	-	0/2/19/22	0/1/1/1
1	GLC	B	101	1	-	0/2/19/22	0/1/1/1
1	GLC	B	102	1	-	0/2/19/22	0/1/1/1
1	GLC	B	103	1	-	0/2/19/22	0/1/1/1
1	GLC	B	104	1	-	0/2/19/22	0/1/1/1
1	GLC	B	105	1	-	0/2/19/22	0/1/1/1
1	GLC	B	106	1	-	0/2/19/22	0/1/1/1
1	GLC	B	107	1	-	0/2/19/22	0/1/1/1
1	GLC	B	108	1	-	0/2/19/22	0/1/1/1
1	GLC	B	109	1	-	0/2/19/22	0/1/1/1
1	GLC	B	110	1	-	0/2/19/22	0/1/1/1
1	GLC	B	114	1	-	0/2/19/22	0/1/1/1
1	GLC	B	115	1	-	0/2/19/22	0/1/1/1
1	GLC	B	116	1	-	0/2/19/22	0/1/1/1
1	GLC	B	118	1	-	0/2/19/22	0/1/1/1
1	GLC	B	120	1	-	0/2/19/22	0/1/1/1
1	GLC	B	121	1	-	0/2/19/22	0/1/1/1
1	GLC	B	122	1	-	0/2/19/22	0/1/1/1
1	GLC	B	123	1	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLC	O2-C2	-2.10	1.39	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2	GLC	O5-C5-C4	-3.48	106.24	110.65
1	A	12	GLC	O5-C5-C6	-2.95	103.88	106.98
1	B	102	GLC	O5-C5-C4	-2.94	106.93	110.65
1	B	115	GLC	O5-C5-C4	-2.86	107.02	110.65
1	B	114	GLC	O5-C5-C4	-2.58	107.38	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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.