



Full wwPDB Geometry-Only Validation Report ⓘ

Aug 7, 2020 – 09:04 AM BST

PDB ID : 1JA7
Title : BINDING OF N-ACETYLGLUCOSAMINE TO CHICKEN EGG
LYSOZYME: A POWDER DIFFRACTION STUDY
Authors : Von Dreele, R.B.
Deposited on : 2001-05-29
Resolution : 2.98 Å(reported)

This is a Full wwPDB Geometry-Only 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 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)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

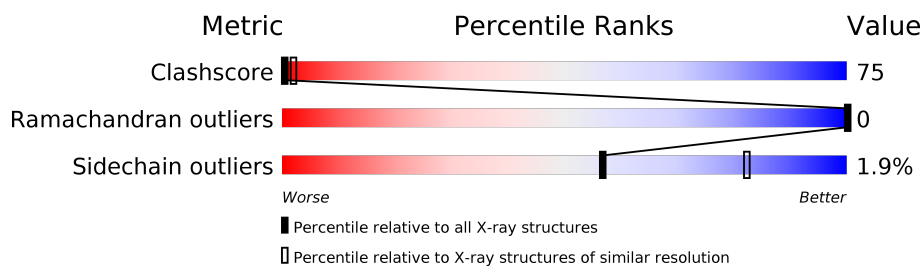
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

POWDER DIFFRACTION

The reported resolution of this entry is 2.98 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	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	129	

2 Entry composition [i](#)

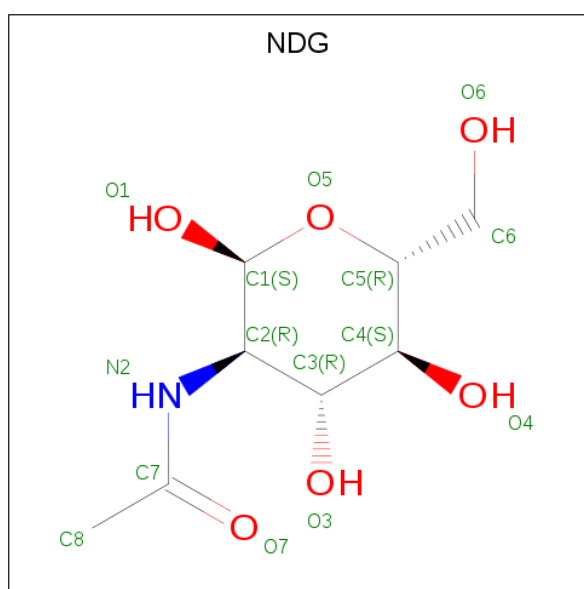
There are 2 unique types of molecules in this entry. The entry contains 1016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1001	613	193	185	10	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy- α -D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0

Note EDS was not executed.

Chain A: 35% 60% 5%

Node	Category
K1	Green
V2	Green
F3	Green
G4	Green
R5	Green
G6	Green
E7	Green
L8	Green
A9	Green
A10	Green
A11	Green
M12	Green
K13	Green
R14	Green
H15	Green
G16	Green
L17	Green
D18	Green
M19	Green
Y20	Green
R21	Green
G22	Green
Y23	Green
S24	Green
L25	Green
G26	Green
M27	Green
W28	Green
V29	Green
K33	Green
F34	Green
E35	Green
S36	Green
R37	Green
F38	Green
K39	Green
A42	Green
T43	Green
R44	Yellow
R45	Yellow
K46	Yellow
Q121	Yellow
A122	Yellow
H123	Yellow
I124	Yellow
G49	Yellow
S50	Yellow
D52	Yellow
F53	Yellow
G54	Yellow
I55	Yellow
L56	Yellow
Q57	Yellow
L58	Yellow
D66	Yellow
G67	Yellow
R68	Yellow
T69	Yellow
P70	Yellow
G71	Yellow
S72	Yellow
R73	Yellow
L78	Yellow
P79	Yellow
A82	Yellow
L83	Yellow
L84	Yellow
I88	Yellow
S91	Yellow
V92	Yellow
N93	Yellow
K96	Yellow
K97	Yellow
I98	Yellow
V99	Yellow
M103	Yellow
G104	Yellow
M105	Yellow
M106	Yellow
V109	Yellow
A110	Yellow
W111	Yellow
R114	Yellow
C115	Yellow
T118	Yellow
D119	Yellow
V120	Yellow
Q121	Yellow
A122	Yellow
H123	Yellow
I124	Yellow
R125	Yellow
L128	Yellow
L129	Yellow

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDG

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	0.53	0/1021	0.84	0/1379

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	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	128	ARG	Sidechain
1	A	14	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	5	ARG	Sidechain
1	A	61	ARG	Sidechain
1	A	73	ARG	Sidechain

4.2 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	1001	0	959	150	0
2	A	15	0	12	2	0
All	All	1016	0	971	150	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 75.

All (150) 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:3:PHE:HB2	1:A:8:LEU:HD12	1.17	1.13
1:A:61:ARG:HA	1:A:69:THR:HG21	1.34	1.10
1:A:36:SER:HB2	1:A:55:ILE:HA	1.35	1.06
1:A:103:ASN:HB3	1:A:106:ASN:HB2	1.38	1.03
1:A:69:THR:HG22	1:A:72:SER:HB2	1.36	1.03
1:A:92:VAL:HG12	1:A:96:LYS:HG3	1.37	1.02
1:A:79:PRO:HG2	1:A:82:ALA:HB2	1.44	0.99
1:A:78:ILE:HG23	1:A:79:PRO:HD2	1.53	0.90
1:A:96:LYS:CB	1:A:96:LYS:NZ	2.36	0.88
1:A:3:PHE:CB	1:A:8:LEU:HD12	2.01	0.88
1:A:3:PHE:HB3	1:A:8:LEU:HB2	1.56	0.87
1:A:26:GLY:HA2	1:A:124:ILE:HG21	1.58	0.85
1:A:36:SER:CB	1:A:55:ILE:HA	2.06	0.84
1:A:96:LYS:HB3	1:A:96:LYS:HZ3	1.42	0.84
1:A:3:PHE:HB2	1:A:8:LEU:CD1	2.04	0.84
1:A:36:SER:HB2	1:A:55:ILE:HD12	1.62	0.82
1:A:33:LYS:HD3	1:A:38:PHE:CE2	2.15	0.81
1:A:1:LYS:HD3	1:A:3:PHE:CZ	2.16	0.81
1:A:59:ASN:OD1	1:A:61:ARG:HB3	1.81	0.81
1:A:96:LYS:HB2	1:A:96:LYS:HZ2	1.46	0.80
1:A:83:LEU:HD22	1:A:91:SER:CB	2.11	0.79
1:A:121:GLN:HA	1:A:124:ILE:HG12	1.64	0.79
1:A:73:ARG:HH11	1:A:73:ARG:HG3	1.48	0.78
1:A:103:ASN:HA	1:A:106:ASN:HD22	1.49	0.78
1:A:8:LEU:HD23	1:A:8:LEU:O	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:CG2	1:A:72:SER:HB2	2.11	0.78
1:A:36:SER:CB	1:A:55:ILE:HD12	2.14	0.77
1:A:88:ILE:CD1	1:A:88:ILE:C	2.51	0.77
1:A:115:CYS:HA	1:A:118:THR:HG21	1.65	0.76
1:A:46:ASN:HB2	1:A:48:ASP:OD1	1.86	0.75
1:A:73:ARG:HH11	1:A:73:ARG:CG	2.00	0.75
1:A:35:GLU:OE1	1:A:57:GLN:HG3	1.88	0.73
1:A:88:ILE:HD13	1:A:88:ILE:C	2.09	0.73
1:A:96:LYS:HB3	1:A:96:LYS:NZ	1.98	0.73
1:A:1:LYS:HG2	1:A:2:VAL:H	1.53	0.71
1:A:59:ASN:ND2	2:A:201:NDG:H6C1	2.05	0.70
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.27	0.70
1:A:50:SER:HB2	1:A:59:ASN:HB2	1.73	0.69
1:A:19:ASN:ND2	1:A:24:SER:HA	2.08	0.68
1:A:1:LYS:HD3	1:A:3:PHE:CE1	2.27	0.68
1:A:50:SER:HB3	1:A:61:ARG:NH2	2.10	0.66
1:A:1:LYS:HG2	1:A:2:VAL:N	2.11	0.65
1:A:39:ASN:N	1:A:55:ILE:HD13	2.11	0.65
1:A:54:GLY:HA2	1:A:84:LEU:HD23	1.77	0.65
1:A:43:THR:HG22	1:A:84:LEU:HD21	1.77	0.65
1:A:103:ASN:CA	1:A:106:ASN:HD22	2.08	0.64
1:A:99:VAL:HA	1:A:104:GLY:HA2	1.79	0.63
1:A:3:PHE:CB	1:A:8:LEU:HB2	2.26	0.63
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.14	0.63
1:A:19:ASN:HD22	1:A:24:SER:HA	1.64	0.62
1:A:34:PHE:CD1	1:A:114:ARG:HD3	2.35	0.62
1:A:50:SER:CB	1:A:59:ASN:HB2	2.30	0.62
1:A:52:ASP:HA	1:A:58:ILE:O	2.00	0.62
1:A:54:GLY:H	1:A:84:LEU:HD21	1.65	0.62
1:A:121:GLN:HG2	1:A:125:ARG:HH22	1.65	0.62
1:A:83:LEU:CD2	1:A:91:SER:HA	2.30	0.62
1:A:11:ALA:O	1:A:14:ARG:HB3	2.01	0.61
1:A:61:ARG:CA	1:A:69:THR:HG21	2.23	0.61
1:A:68:ARG:C	1:A:70:PRO:HD3	2.21	0.61
1:A:59:ASN:HD21	2:A:201:NDG:H6C1	1.65	0.60
1:A:19:ASN:HA	1:A:23:TYR:O	2.01	0.60
1:A:7:GLU:HA	1:A:7:GLU:OE1	2.02	0.60
1:A:36:SER:HB2	1:A:55:ILE:CA	2.23	0.60
1:A:96:LYS:HB2	1:A:96:LYS:NZ	2.06	0.60
1:A:24:SER:HB3	1:A:27:ASN:HD22	1.67	0.60
1:A:122:ALA:HA	1:A:125:ARG:NH1	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:HD1	1:A:114:ARG:HH11	1.50	0.59
1:A:24:SER:HB3	1:A:27:ASN:ND2	2.17	0.59
1:A:79:PRO:CG	1:A:82:ALA:HB2	2.28	0.59
1:A:92:VAL:HG12	1:A:92:VAL:O	2.02	0.58
1:A:9:ALA:HB1	1:A:29:VAL:HG21	1.85	0.58
1:A:26:GLY:HA2	1:A:124:ILE:CG2	2.31	0.58
1:A:83:LEU:HD22	1:A:91:SER:HB3	1.84	0.58
1:A:92:VAL:CG1	1:A:96:LYS:HG3	2.25	0.58
1:A:16:GLY:O	1:A:20:TYR:HB2	2.03	0.57
1:A:69:THR:O	1:A:69:THR:HG22	2.04	0.57
1:A:45:ARG:HE	1:A:49:GLY:HA2	1.70	0.55
1:A:3:PHE:HB3	1:A:8:LEU:CB	2.34	0.55
1:A:34:PHE:HD1	1:A:114:ARG:NH1	2.04	0.55
1:A:51:THR:HB	1:A:53:TYR:CE1	2.42	0.55
1:A:23:TYR:CD1	1:A:105:MET:HE1	2.43	0.54
1:A:46:ASN:HD21	1:A:52:ASP:CG	2.11	0.54
1:A:78:ILE:CG2	1:A:82:ALA:HB3	2.37	0.54
1:A:60:SER:HB2	1:A:66:ASP:OD1	2.07	0.54
1:A:61:ARG:HA	1:A:69:THR:CG2	2.23	0.54
1:A:88:ILE:HD13	1:A:88:ILE:O	2.07	0.54
1:A:1:LYS:HE2	1:A:3:PHE:CE2	2.43	0.54
1:A:54:GLY:HA2	1:A:84:LEU:CD2	2.39	0.53
1:A:23:TYR:HB2	1:A:28:TRP:HZ2	1.72	0.53
1:A:39:ASN:H	1:A:55:ILE:HD13	1.74	0.52
1:A:9:ALA:HB1	1:A:29:VAL:CG2	2.40	0.52
1:A:59:ASN:H	1:A:59:ASN:ND2	2.07	0.51
1:A:121:GLN:CG	1:A:125:ARG:HH22	2.24	0.50
1:A:121:GLN:H	1:A:121:GLN:CD	2.14	0.50
1:A:78:ILE:CG2	1:A:79:PRO:HD2	2.35	0.50
1:A:46:ASN:HB3	1:A:48:ASP:OD2	2.12	0.50
1:A:14:ARG:CZ	1:A:15:HIS:HE1	2.26	0.49
1:A:83:LEU:HD22	1:A:91:SER:CA	2.42	0.49
1:A:1:LYS:CG	1:A:2:VAL:H	2.24	0.48
1:A:50:SER:CB	1:A:61:ARG:HB2	2.43	0.48
1:A:39:ASN:H	1:A:55:ILE:CD1	2.27	0.48
1:A:128:ARG:O	1:A:129:LEU:HD23	2.14	0.48
1:A:93:ASN:HA	1:A:96:LYS:HD3	1.95	0.48
1:A:59:ASN:H	1:A:59:ASN:HD22	1.61	0.47
1:A:111:TRP:CD1	1:A:115:CYS:CB	2.95	0.47
1:A:114:ARG:O	1:A:118:THR:HG21	2.14	0.47
1:A:23:TYR:CG	1:A:105:MET:HE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HA	1:A:51:THR:HA	1.96	0.47
1:A:12:MET:SD	1:A:28:TRP:HB3	2.55	0.47
1:A:121:GLN:O	1:A:125:ARG:HB2	2.15	0.46
1:A:43:THR:HG22	1:A:84:LEU:CD2	2.45	0.46
1:A:13:LYS:HE3	1:A:18:ASP:OD2	2.16	0.46
1:A:103:ASN:HA	1:A:106:ASN:ND2	2.25	0.45
1:A:121:GLN:HA	1:A:124:ILE:CG1	2.42	0.45
1:A:12:MET:HB3	1:A:17:LEU:HD12	1.97	0.45
1:A:50:SER:OG	1:A:59:ASN:HB2	2.16	0.45
1:A:62:TRP:HZ3	1:A:73:ARG:CZ	2.29	0.45
1:A:3:PHE:CD2	1:A:8:LEU:HA	2.51	0.45
1:A:3:PHE:CG	1:A:8:LEU:HD12	2.50	0.45
1:A:12:MET:CB	1:A:17:LEU:HD12	2.47	0.45
1:A:12:MET:SD	1:A:17:LEU:HD13	2.58	0.44
1:A:23:TYR:HB2	1:A:28:TRP:CZ2	2.51	0.44
1:A:83:LEU:HD22	1:A:91:SER:OG	2.16	0.44
1:A:36:SER:HB3	1:A:42:ALA:HB3	1.99	0.44
1:A:115:CYS:CA	1:A:118:THR:HG21	2.43	0.43
1:A:119:ASP:CG	1:A:122:ALA:HB2	2.38	0.43
1:A:50:SER:HB2	1:A:61:ARG:HB2	2.01	0.43
1:A:54:GLY:N	1:A:84:LEU:HD21	2.30	0.43
1:A:23:TYR:CD2	1:A:105:MET:HE3	2.54	0.43
1:A:119:ASP:O	1:A:122:ALA:HB3	2.19	0.43
1:A:83:LEU:HD22	1:A:91:SER:HA	1.99	0.43
1:A:39:ASN:O	1:A:55:ILE:HD13	2.18	0.43
1:A:111:TRP:HD1	1:A:115:CYS:HB2	1.80	0.42
1:A:115:CYS:C	1:A:118:THR:HG23	2.39	0.42
1:A:35:GLU:HB3	1:A:57:GLN:HG3	2.01	0.42
1:A:56:LEU:O	1:A:57:GLN:HB2	2.20	0.41
1:A:23:TYR:CG	1:A:105:MET:CE	3.03	0.41
1:A:35:GLU:HB3	1:A:57:GLN:CG	2.51	0.41
1:A:36:SER:CA	1:A:55:ILE:HD12	2.50	0.41
1:A:88:ILE:HD12	1:A:88:ILE:C	2.35	0.41
1:A:73:ARG:NH1	1:A:73:ARG:CG	2.68	0.41
1:A:88:ILE:HD12	1:A:88:ILE:H	1.86	0.41
1:A:26:GLY:CA	1:A:124:ILE:HD13	2.51	0.41
1:A:92:VAL:HG12	1:A:96:LYS:CG	2.27	0.41
1:A:92:VAL:O	1:A:92:VAL:CG1	2.67	0.41
1:A:98:ILE:O	1:A:98:ILE:HG22	2.21	0.41
1:A:109:VAL:HG13	1:A:110:ALA:N	2.36	0.41
1:A:9:ALA:CB	1:A:29:VAL:HG21	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:HB2	1:A:66:ASP:CG	2.41	0.41
1:A:45:ARG:HG2	1:A:46:ASN:N	2.36	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	127/129 (98%)	119 (94%)	8 (6%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	105/105 (100%)	103 (98%)	2 (2%)	57	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	88	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	19	ASN
1	A	27	ASN
1	A	46	ASN
1	A	57	GLN
1	A	93	ASN
1	A	103	ASN
1	A	106	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

1 ligand is 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	NDG	A	201	-	15,15,15	1.77	2 (13%)	21,21,21	1.65	6 (28%)

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	NDG	A	201	-	-	2/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NDG	C1-C2	4.35	1.58	1.52
2	A	201	NDG	C2-N2	2.81	1.50	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	NDG	C1-O5-C5	-4.22	105.70	113.66
2	A	201	NDG	O3-C3-C2	2.29	114.29	109.66
2	A	201	NDG	C1-C2-C3	2.19	113.54	110.54
2	A	201	NDG	C3-C4-C5	2.18	114.12	110.24
2	A	201	NDG	O5-C5-C4	-2.14	105.81	109.69
2	A	201	NDG	O4-C4-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	NDG	C1-C2-N2-C7
2	A	201	NDG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	NDG	2	0

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.