



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:43 AM JST

PDB ID : 8YG6
EMDB ID : EMD-39237
Title : The pre-fusion structure of baculovirus fusion protein GP64
Authors : Du, D.; Guo, J.; Li, S.
Deposited on : 2024-02-26
Resolution : 2.77 Å (reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

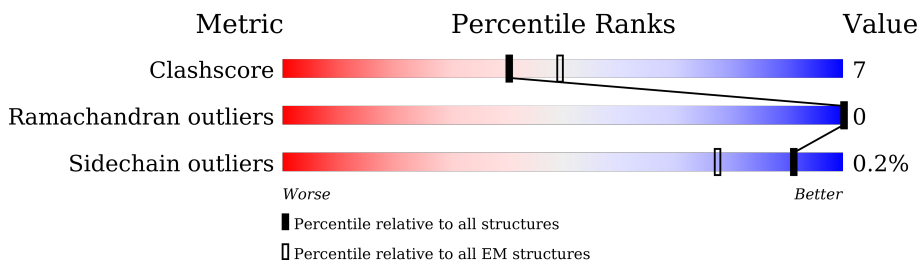
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	465	84% (green), 15% (yellow)
1	B	465	85% (green), 15% (yellow)
1	C	465	84% (green), 16% (yellow)
2	D	3	67% (green), 33% (yellow)
2	E	3	33% (green), 67% (yellow)
2	F	3	100% (green)

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11442 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Major envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	465	3730	2319	650	732	29	0	0
1	B	465	3730	2319	650	732	29	0	0
1	C	465	3730	2319	650	732	29	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	3	42	24	3	15	0	0
2	E	3	42	24	3	15	0	0
2	F	3	42	24	3	15	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

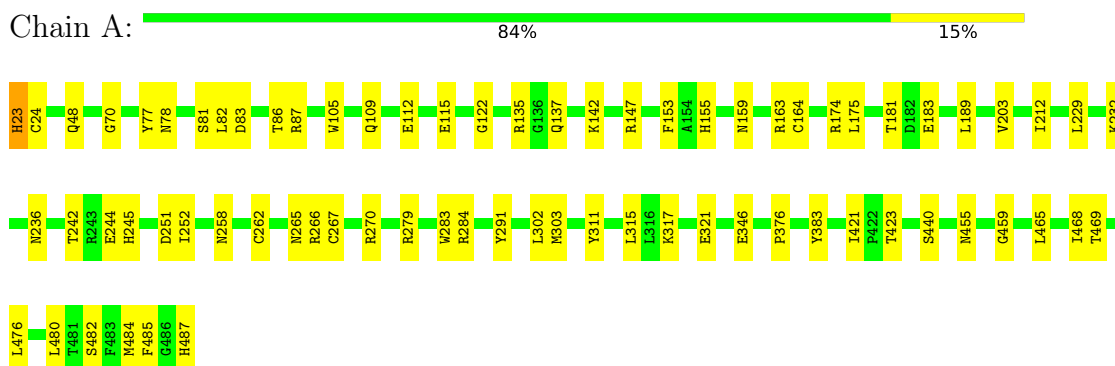


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0

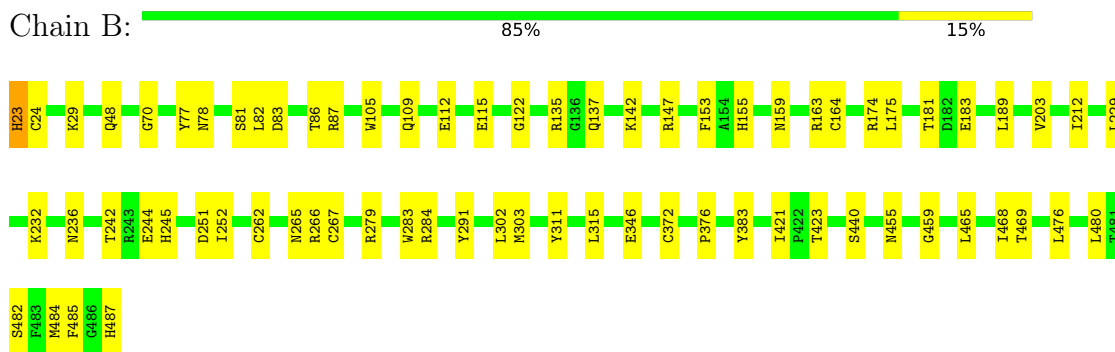
3 Residue-property plots [i](#)

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. 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. 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.

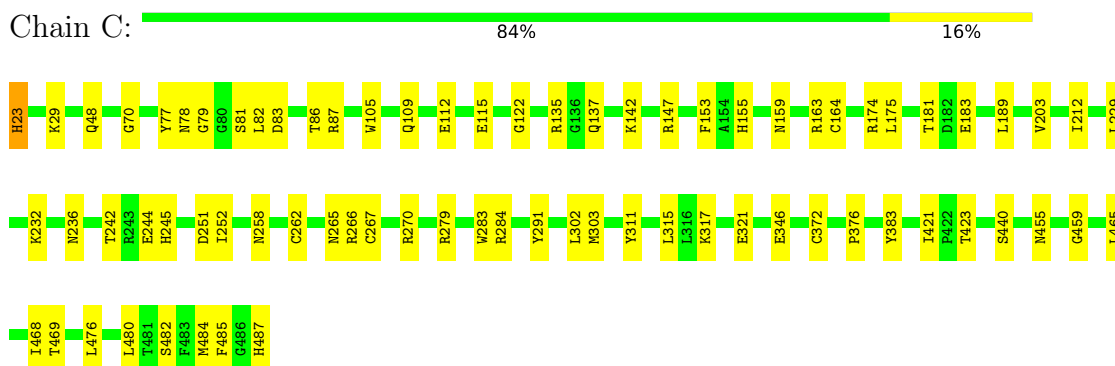
- Molecule 1: Major envelope glycoprotein



- Molecule 1: Major envelope glycoprotein



- Molecule 1: Major envelope glycoprotein




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

Chain D:  67% 33%

NAG1
NAG2
NAG3

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

Chain E:  33% 67%

NAG1
NAG2
NAG3

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

Chain F:  100%

NAG1
NAG2
NAG3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26747	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.02	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.26	0/3804	0.50	0/5145
1	B	0.26	0/3804	0.50	0/5145
1	C	0.26	0/3804	0.50	0/5145
All	All	0.26	0/11412	0.50	0/15435

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	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	ARG	Sidechain
1	A	87	ARG	Sidechain
1	B	284	ARG	Sidechain
1	B	87	ARG	Sidechain
1	C	284	ARG	Sidechain
1	C	87	ARG	Sidechain

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	3730	0	3593	58	0
1	B	3730	0	3593	59	0
1	C	3730	0	3593	62	0
2	D	42	0	37	1	0
2	E	42	0	37	2	0
2	F	42	0	37	0	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
3	C	42	0	39	0	0
All	All	11442	0	11007	153	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 7.

All (153) 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:236:ASN:ND2	1:B:48:GLN:OE1	2.15	0.79
1:A:302:LEU:HD23	1:B:283:TRP:CH2	2.18	0.79
1:B:236:ASN:ND2	1:C:48:GLN:OE1	2.17	0.78
1:A:283:TRP:CH2	1:C:302:LEU:HD23	2.19	0.77
1:B:302:LEU:HD23	1:C:283:TRP:CH2	2.19	0.77
1:A:48:GLN:OE1	1:C:236:ASN:ND2	2.17	0.76
1:A:23:HIS:O	1:A:23:HIS:CD2	2.46	0.69
1:C:23:HIS:CD2	1:C:23:HIS:O	2.46	0.68
1:B:23:HIS:O	1:B:23:HIS:CD2	2.46	0.68
1:A:440:SER:OG	1:C:346:GLU:OE2	2.15	0.64
1:A:346:GLU:OE2	1:B:440:SER:OG	2.16	0.63
1:B:346:GLU:OE2	1:C:440:SER:OG	2.16	0.62
1:C:482:SER:HA	1:C:485:PHE:CE1	2.40	0.57
1:B:262:CYS:HB3	1:B:267:CYS:HA	1.88	0.56
1:A:262:CYS:HB3	1:A:267:CYS:HA	1.88	0.56
1:A:482:SER:HA	1:A:485:PHE:CE1	2.40	0.56
1:B:482:SER:HA	1:B:485:PHE:CE1	2.40	0.56
1:B:142:LYS:H	1:B:164:CYS:HB3	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:CYS:HB3	1:C:267:CYS:HA	1.88	0.55
1:A:142:LYS:H	1:A:164:CYS:HB3	1.70	0.55
1:C:142:LYS:H	1:C:164:CYS:HB3	1.70	0.55
1:C:484:MET:O	1:C:487:HIS:ND1	2.33	0.54
1:B:484:MET:O	1:B:487:HIS:ND1	2.33	0.54
1:B:115:GLU:OE1	1:B:137:GLN:NE2	2.42	0.53
1:A:23:HIS:O	1:A:23:HIS:HD2	1.91	0.53
1:A:251:ASP:OD1	1:A:252:ILE:N	2.42	0.53
1:A:115:GLU:OE1	1:A:137:GLN:NE2	2.41	0.53
1:C:251:ASP:OD1	1:C:252:ILE:N	2.42	0.53
1:C:23:HIS:O	1:C:23:HIS:HD2	1.91	0.53
1:A:83:ASP:O	1:A:86:THR:HG22	2.09	0.53
1:A:244:GLU:O	1:A:245:HIS:HD2	1.92	0.53
1:C:115:GLU:OE1	1:C:137:GLN:NE2	2.42	0.53
1:B:244:GLU:O	1:B:245:HIS:HD2	1.92	0.52
1:C:376:PRO:O	1:C:383:TYR:OH	2.28	0.52
1:B:83:ASP:O	1:B:86:THR:HG22	2.09	0.52
1:C:83:ASP:O	1:C:86:THR:HG22	2.09	0.52
1:B:251:ASP:OD1	1:B:252:ILE:N	2.42	0.52
1:B:105:TRP:O	1:B:109:GLN:N	2.41	0.51
1:C:262:CYS:CB	1:C:267:CYS:HA	2.41	0.51
2:D:3:NAG:O7	2:D:3:NAG:O4	2.21	0.51
1:A:376:PRO:O	1:A:383:TYR:OH	2.28	0.51
1:B:78:ASN:OD1	1:B:153:PHE:HA	2.11	0.51
1:C:78:ASN:OD1	1:C:153:PHE:HA	2.11	0.51
1:A:78:ASN:OD1	1:A:153:PHE:HA	2.11	0.51
1:B:376:PRO:O	1:B:383:TYR:OH	2.28	0.51
1:B:23:HIS:O	1:B:23:HIS:HD2	1.91	0.51
1:B:262:CYS:CB	1:B:267:CYS:HA	2.41	0.51
1:A:262:CYS:CB	1:A:267:CYS:HA	2.41	0.51
1:C:244:GLU:O	1:C:245:HIS:HD2	1.92	0.51
1:C:105:TRP:O	1:C:109:GLN:N	2.41	0.50
1:B:262:CYS:HB2	1:B:266:ARG:O	2.12	0.50
1:A:421:ILE:HG22	1:A:423:THR:HG23	1.93	0.50
1:A:465:LEU:HD23	1:A:465:LEU:H	1.77	0.50
1:C:465:LEU:H	1:C:465:LEU:HD23	1.77	0.50
1:B:421:ILE:HG22	1:B:423:THR:HG23	1.93	0.50
1:B:465:LEU:HD23	1:B:465:LEU:H	1.77	0.50
1:A:105:TRP:O	1:A:109:GLN:N	2.41	0.49
1:C:262:CYS:HB2	1:C:266:ARG:O	2.12	0.49
1:C:421:ILE:HG22	1:C:423:THR:HG23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:CYS:HB2	1:A:266:ARG:O	2.12	0.49
1:C:78:ASN:CG	1:C:153:PHE:HA	2.33	0.49
1:B:78:ASN:CG	1:B:153:PHE:HA	2.33	0.48
1:A:78:ASN:CG	1:A:153:PHE:HA	2.33	0.48
1:A:484:MET:O	1:A:487:HIS:ND1	2.33	0.48
1:C:203:VAL:HG22	1:C:212:ILE:HD11	1.96	0.48
1:B:468:ILE:HG22	1:B:469:THR:H	1.78	0.47
1:C:468:ILE:HG22	1:C:469:THR:H	1.78	0.47
1:A:203:VAL:HG22	1:A:212:ILE:HD11	1.96	0.47
1:B:203:VAL:HG22	1:B:212:ILE:HD11	1.96	0.47
1:C:122:GLY:O	1:C:155:HIS:HB3	2.14	0.47
1:A:468:ILE:HG22	1:A:469:THR:H	1.78	0.47
1:C:258:ASN:ND2	1:C:270:ARG:O	2.41	0.47
1:B:122:GLY:O	1:B:155:HIS:HB3	2.14	0.46
2:E:3:NAG:O7	2:E:3:NAG:O4	2.21	0.46
1:A:283:TRP:CZ3	1:C:302:LEU:HD23	2.51	0.46
1:A:302:LEU:HD23	1:B:283:TRP:CZ3	2.49	0.46
1:A:122:GLY:O	1:A:155:HIS:HB3	2.14	0.46
1:B:302:LEU:HD23	1:C:283:TRP:CZ3	2.51	0.45
1:C:181:THR:HG22	1:C:183:GLU:HG2	1.98	0.45
1:A:244:GLU:O	1:A:245:HIS:CD2	2.70	0.45
1:B:175:LEU:HB3	1:B:265:ASN:HA	1.99	0.45
1:B:244:GLU:O	1:B:245:HIS:CD2	2.70	0.45
1:A:175:LEU:HB3	1:A:265:ASN:HA	1.99	0.45
1:C:244:GLU:O	1:C:245:HIS:CD2	2.70	0.45
1:A:181:THR:HG22	1:A:183:GLU:HG2	1.98	0.44
1:A:455:ASN:ND2	1:B:459:GLY:O	2.50	0.44
1:B:181:THR:HG22	1:B:183:GLU:HG2	1.98	0.44
1:A:476:LEU:O	1:A:480:LEU:HG	2.18	0.44
1:C:175:LEU:HB3	1:C:265:ASN:HA	1.99	0.44
1:C:476:LEU:O	1:C:480:LEU:HG	2.18	0.44
1:A:311:TYR:HE2	1:C:279:ARG:CZ	2.30	0.44
1:A:229:LEU:HD13	1:B:315:LEU:HD23	2.00	0.44
1:B:229:LEU:HD13	1:C:315:LEU:HD23	2.00	0.44
1:B:279:ARG:CZ	1:C:311:TYR:HE2	2.31	0.44
1:A:279:ARG:CZ	1:B:311:TYR:HE2	2.31	0.43
1:A:258:ASN:ND2	1:A:270:ARG:O	2.41	0.43
1:A:265:ASN:N	1:A:265:ASN:OD1	2.51	0.43
1:B:265:ASN:N	1:B:265:ASN:OD1	2.51	0.43
1:B:476:LEU:O	1:B:480:LEU:HG	2.18	0.43
1:C:70:GLY:H	1:C:163:ARG:HB3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:CYS:HB2	1:C:372:CYS:HB3	1.14	0.43
1:A:24:CYS:HB2	1:B:372:CYS:HB3	1.14	0.43
1:B:70:GLY:H	1:B:163:ARG:HB3	1.84	0.43
2:E:2:NAG:H4	2:E:3:NAG:H2	1.76	0.43
1:A:291:TYR:HE1	1:B:303:MET:CE	2.32	0.42
1:A:315:LEU:HD23	1:C:229:LEU:HD13	2.00	0.42
1:B:455:ASN:ND2	1:C:459:GLY:O	2.52	0.42
1:A:70:GLY:H	1:A:163:ARG:HB3	1.84	0.42
1:A:78:ASN:O	1:A:86:THR:HB	2.20	0.42
1:A:112:GLU:OE1	1:A:135:ARG:HD3	2.19	0.42
1:B:147:ARG:HG3	1:B:159:ASN:HD22	1.85	0.42
1:C:174:ARG:HB2	1:C:189:LEU:HD11	2.02	0.42
1:C:265:ASN:N	1:C:265:ASN:OD1	2.51	0.42
1:C:147:ARG:HG3	1:C:159:ASN:HD22	1.85	0.42
1:A:303:MET:CE	1:C:291:TYR:HE1	2.32	0.42
1:B:291:TYR:HE1	1:C:303:MET:CE	2.33	0.42
1:A:77:TYR:O	1:A:86:THR:HA	2.20	0.42
1:A:147:ARG:HG3	1:A:159:ASN:HD22	1.85	0.42
1:B:112:GLU:OE1	1:B:135:ARG:HD3	2.19	0.42
1:C:112:GLU:OE1	1:C:135:ARG:HD3	2.19	0.42
1:C:78:ASN:HA	1:C:86:THR:OG1	2.20	0.42
1:B:291:TYR:HE1	1:C:303:MET:HE3	1.85	0.42
1:B:468:ILE:HG22	1:B:469:THR:N	2.35	0.42
1:C:78:ASN:O	1:C:86:THR:HB	2.20	0.42
1:C:232:LYS:HG2	1:C:242:THR:HG22	2.01	0.42
1:B:232:LYS:HG2	1:B:242:THR:HG22	2.01	0.41
1:A:232:LYS:HG2	1:A:242:THR:HG22	2.01	0.41
1:C:77:TYR:O	1:C:86:THR:HA	2.20	0.41
1:C:142:LYS:N	1:C:164:CYS:HB3	2.35	0.41
1:A:174:ARG:HB2	1:A:189:LEU:HD11	2.02	0.41
1:A:459:GLY:O	1:C:455:ASN:ND2	2.53	0.41
1:B:77:TYR:O	1:B:86:THR:HA	2.20	0.41
1:B:480:LEU:O	1:B:484:MET:HG2	2.21	0.41
1:C:81:SER:O	1:C:82:LEU:C	2.59	0.41
1:A:480:LEU:O	1:A:484:MET:HG2	2.21	0.41
1:B:78:ASN:O	1:B:86:THR:HB	2.20	0.41
1:A:468:ILE:HG22	1:A:469:THR:N	2.35	0.41
1:B:174:ARG:HB2	1:B:189:LEU:HD11	2.02	0.41
1:C:468:ILE:HG22	1:C:469:THR:N	2.35	0.41
1:A:303:MET:HE3	1:C:291:TYR:HE1	1.85	0.41
1:C:29:LYS:H	1:C:29:LYS:HG2	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LEU:O	1:C:484:MET:HG2	2.21	0.41
1:A:81:SER:O	1:A:82:LEU:C	2.59	0.41
1:C:232:LYS:HA	1:C:242:THR:HG22	2.03	0.41
1:A:291:TYR:HE1	1:B:303:MET:HE3	1.85	0.40
1:B:29:LYS:H	1:B:29:LYS:HG2	1.71	0.40
1:B:78:ASN:HA	1:B:86:THR:OG1	2.20	0.40
1:C:78:ASN:O	1:C:79:GLY:C	2.60	0.40
1:A:78:ASN:HA	1:A:86:THR:OG1	2.20	0.40
1:A:317:LYS:O	1:A:321:GLU:OE1	2.40	0.40
1:B:78:ASN:OD1	1:B:78:ASN:N	2.55	0.40
1:B:81:SER:O	1:B:82:LEU:C	2.59	0.40
1:C:317:LYS:O	1:C:321:GLU:OE1	2.40	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 PDB entries followed by that with respect to all EM entries.

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	463/465 (100%)	431 (93%)	32 (7%)	0	100	100
1	B	463/465 (100%)	431 (93%)	32 (7%)	0	100	100
1	C	463/465 (100%)	431 (93%)	32 (7%)	0	100	100
All	All	1389/1395 (100%)	1293 (93%)	96 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 PDB entries followed by that with respect to all EM entries.

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	421/421 (100%)	420 (100%)	1 (0%)	92	97
1	B	421/421 (100%)	420 (100%)	1 (0%)	92	97
1	C	421/421 (100%)	420 (100%)	1 (0%)	92	97
All	All	1263/1263 (100%)	1260 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	B	23	HIS
1	C	23	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	27	GLN
1	A	85	ASN
1	B	23	HIS
1	B	27	GLN
1	B	85	ASN
1	B	245	HIS
1	B	285	HIS
1	B	286	ASN
1	C	23	HIS
1	C	27	GLN
1	C	85	ASN
1	C	245	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

9 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	D	1	1,2	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	0.34	0
2	NAG	D	3	2	14,14,15	0.45	0	17,19,21	0.76	0
2	NAG	E	1	1,2	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.33	0
2	NAG	E	3	2	14,14,15	0.46	0	17,19,21	0.76	0
2	NAG	F	1	1,2	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	F	2	2	14,14,15	0.38	0	17,19,21	0.34	0
2	NAG	F	3	2	14,14,15	0.46	0	17,19,21	0.76	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	3	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	3	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	3	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

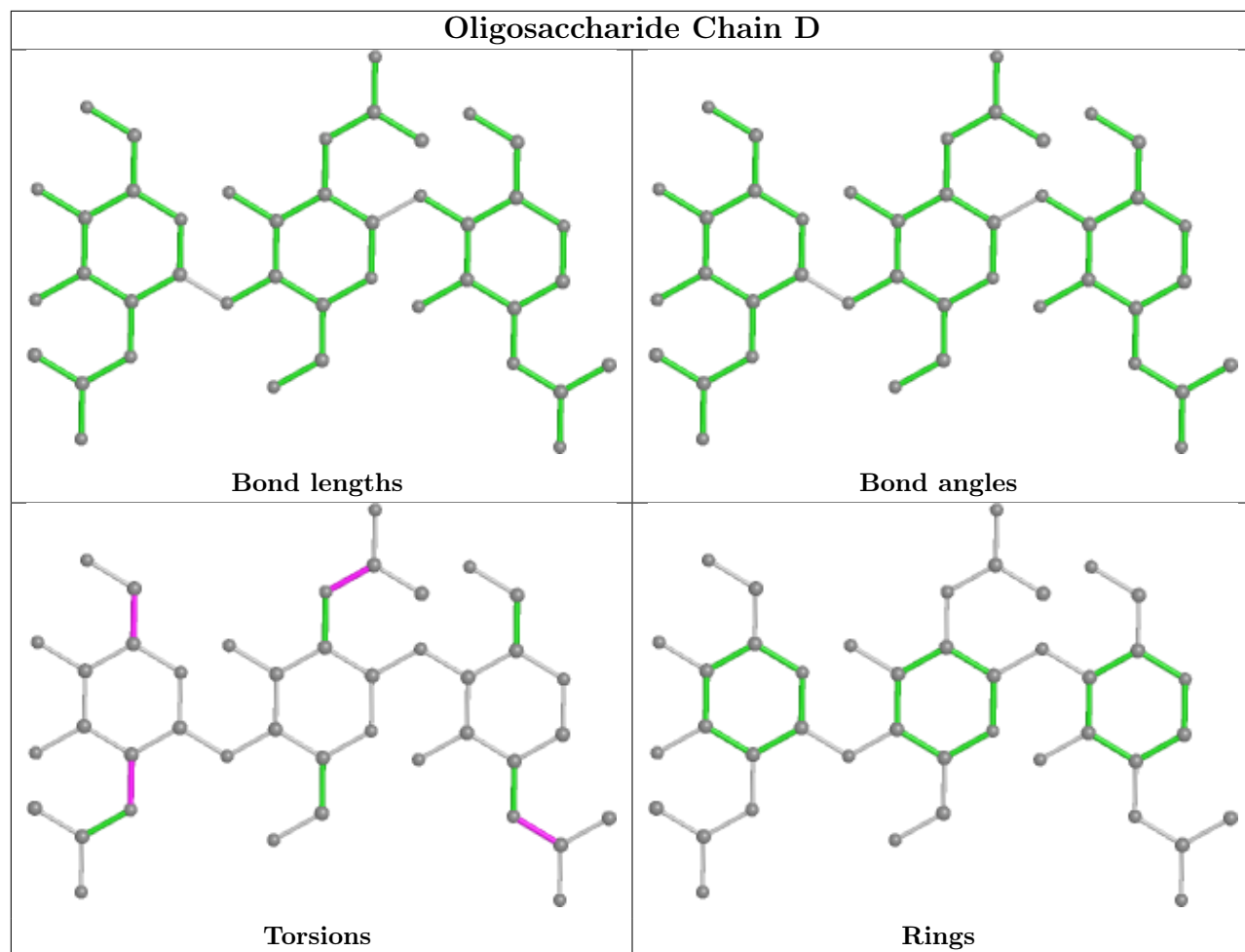
Mol	Chain	Res	Type	Atoms
2	D	3	NAG	O5-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
2	F	3	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	3	NAG	C4-C5-C6-O6
2	E	3	NAG	C4-C5-C6-O6
2	F	3	NAG	C4-C5-C6-O6
2	D	3	NAG	C3-C2-N2-C7
2	E	3	NAG	C3-C2-N2-C7
2	F	3	NAG	C3-C2-N2-C7
2	D	3	NAG	C1-C2-N2-C7
2	E	3	NAG	C1-C2-N2-C7
2	F	3	NAG	C1-C2-N2-C7

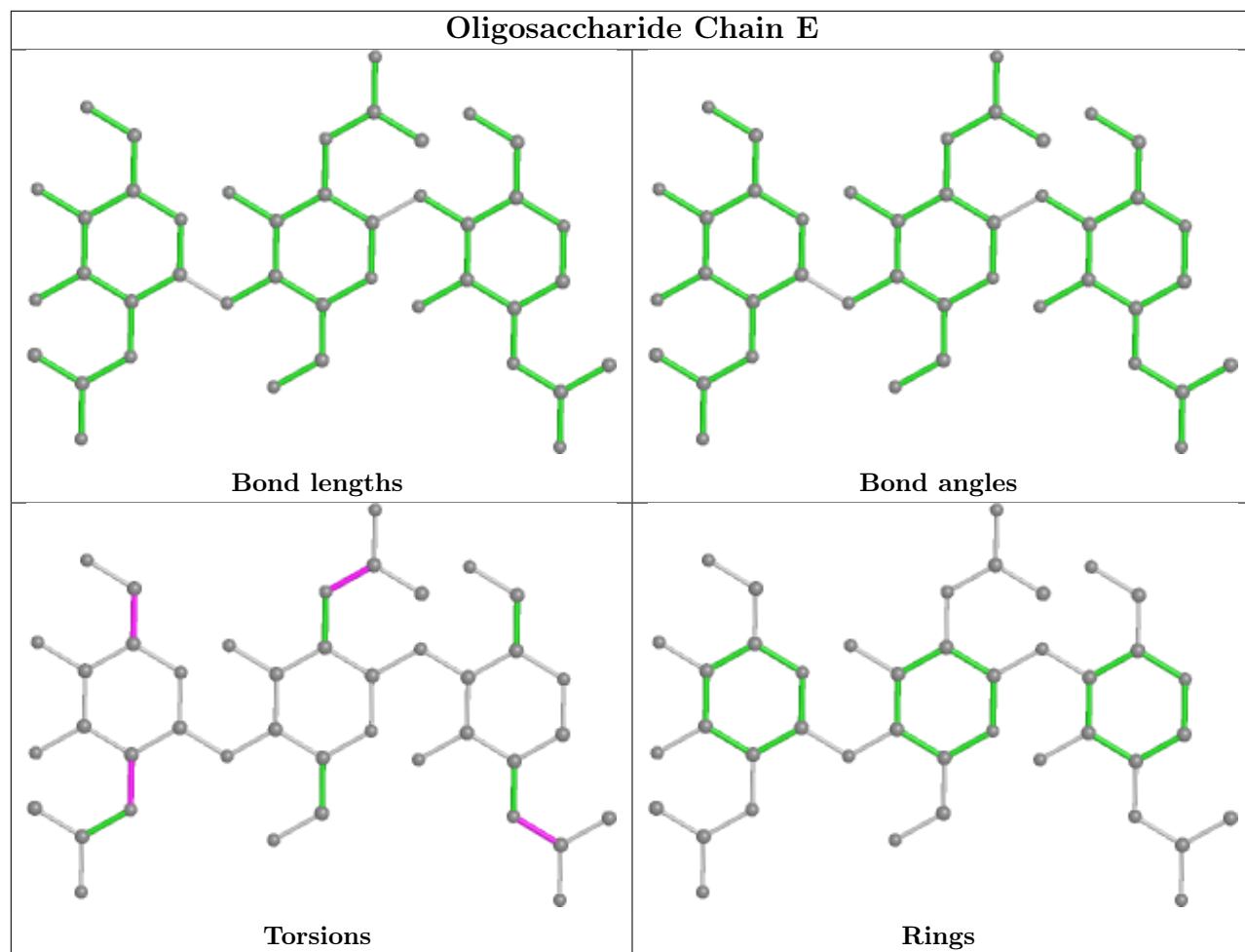
There are no ring outliers.

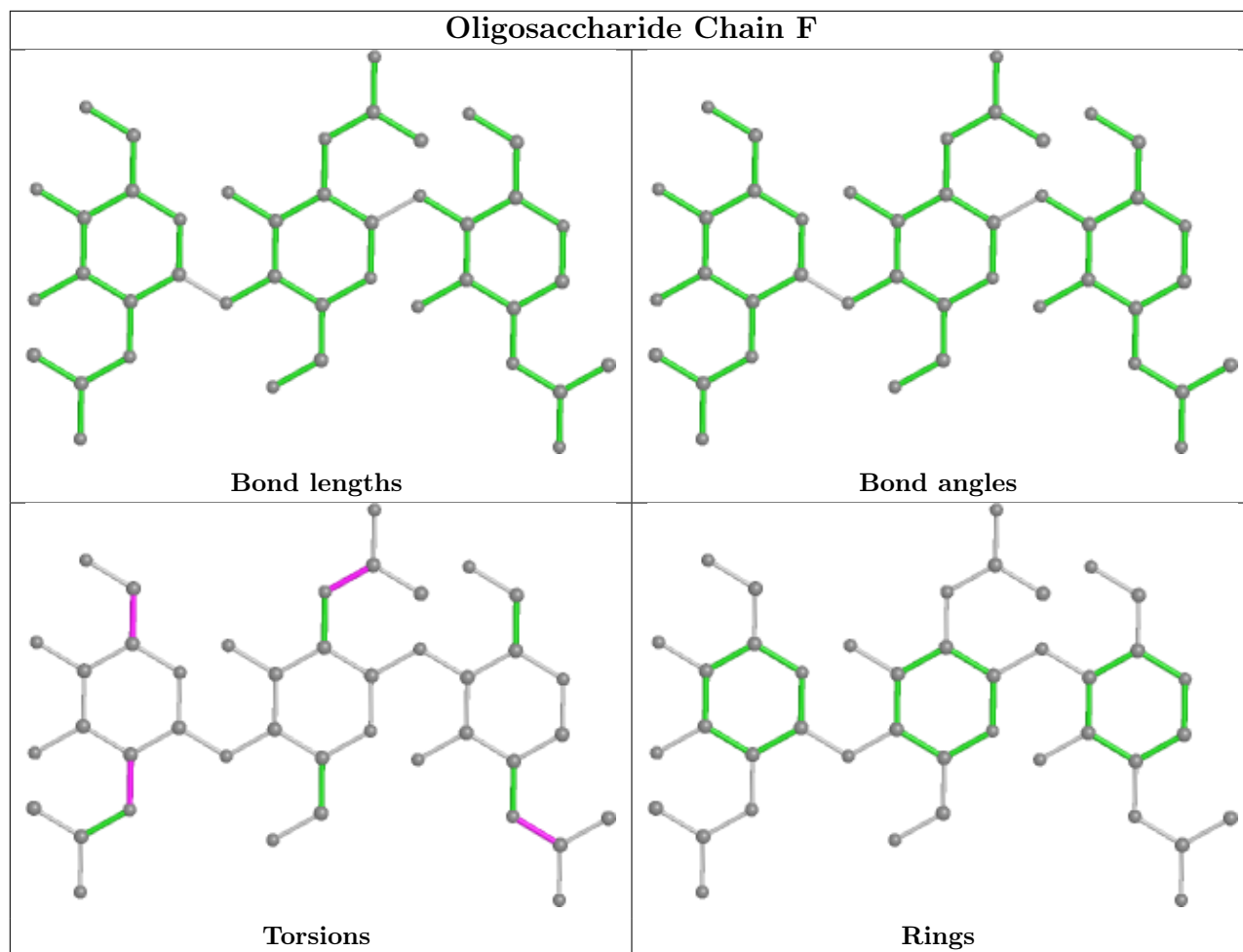
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	E	3	NAG	2	0
2	D	3	NAG	1	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](#)

9 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	503	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	B	501	1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	A	501	1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	B	502	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	C	502	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	C	501	1	14,14,15	0.27	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	503	1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	B	503	1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	A	502	1	14,14,15	0.23	0	17,19,21	0.45	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	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	4/6/23/26	0/1/1/1
3	NAG	A	501	1	-	4/6/23/26	0/1/1/1
3	NAG	B	502	1	-	4/6/23/26	0/1/1/1
3	NAG	C	502	1	-	4/6/23/26	0/1/1/1
3	NAG	C	501	1	-	4/6/23/26	0/1/1/1
3	NAG	C	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	503	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	NAG	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6
3	C	503	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	B	501	NAG	C4-C5-C6-O6
3	C	501	NAG	C4-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6
3	C	502	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	503	NAG	C4-C5-C6-O6
3	C	503	NAG	C4-C5-C6-O6
3	A	501	NAG	C8-C7-N2-C2
3	A	501	NAG	O7-C7-N2-C2
3	A	502	NAG	C8-C7-N2-C2
3	A	502	NAG	O7-C7-N2-C2
3	B	501	NAG	C8-C7-N2-C2
3	B	501	NAG	O7-C7-N2-C2
3	B	502	NAG	C8-C7-N2-C2
3	B	502	NAG	O7-C7-N2-C2
3	C	501	NAG	C8-C7-N2-C2
3	C	501	NAG	O7-C7-N2-C2
3	C	502	NAG	C8-C7-N2-C2
3	C	502	NAG	O7-C7-N2-C2
3	A	502	NAG	C4-C5-C6-O6
3	B	502	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6

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.