



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:38 AM UTC

PDB ID : 2Y38 / pdb_00002y38
Title : LAMININ ALPHA5 CHAIN N-TERMINAL FRAGMENT
Authors : Hussain, S.A.; Carafoli, F.; Hohenester, E.
Deposited on : 2010-12-19
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

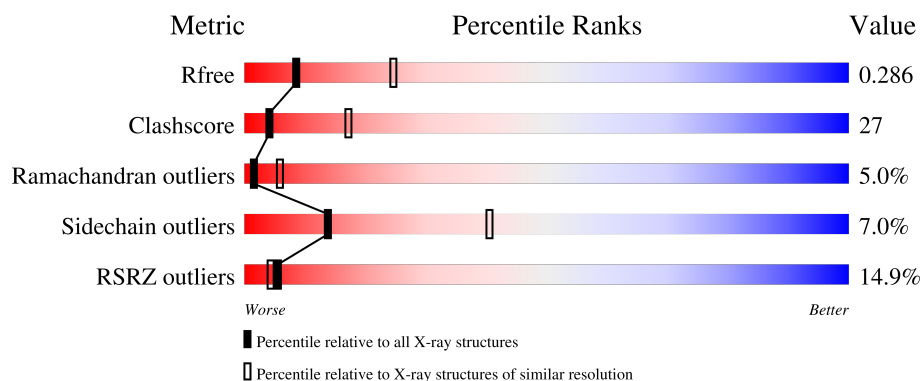
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	403	
2	B	2	

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
4	PO4	A	2004	-	-	X	-
4	PO4	A	2005	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2712 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 LAMININ SUBUNIT ALPHA-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2640	1646	469	503	22	0	0	1

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	-	cloning artifact	UNP Q61001
A	41	PRO	-	cloning artifact	UNP Q61001
A	42	LEU	-	cloning artifact	UNP Q61001
A	43	ALA	-	cloning artifact	UNP Q61001
A	100	ALA	ASN	engineered mutation	UNP Q61001
A	383	GLU	ASN	engineered mutation	UNP Q61001
A	434	ALA	-	expression tag	UNP Q61001
A	435	ALA	-	expression tag	UNP Q61001
A	436	ALA	-	expression tag	UNP Q61001
A	437	HIS	-	expression tag	UNP Q61001
A	438	HIS	-	expression tag	UNP Q61001
A	439	HIS	-	expression tag	UNP Q61001
A	440	HIS	-	expression tag	UNP Q61001
A	441	HIS	-	expression tag	UNP Q61001
A	442	HIS	-	expression tag	UNP Q61001

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



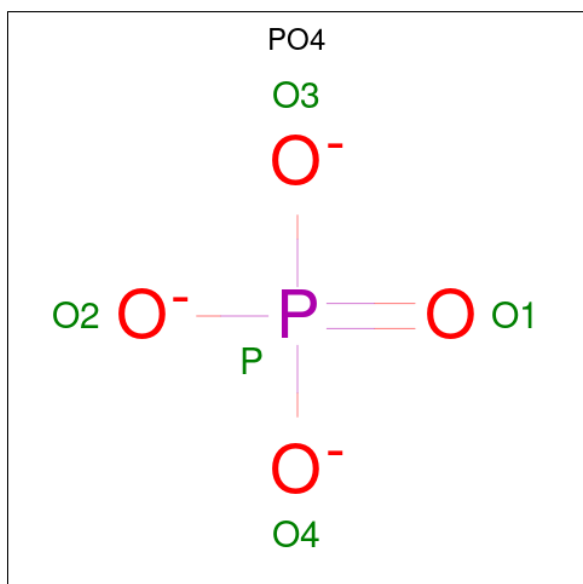
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O				
2	B	2	28	16	2	10		0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

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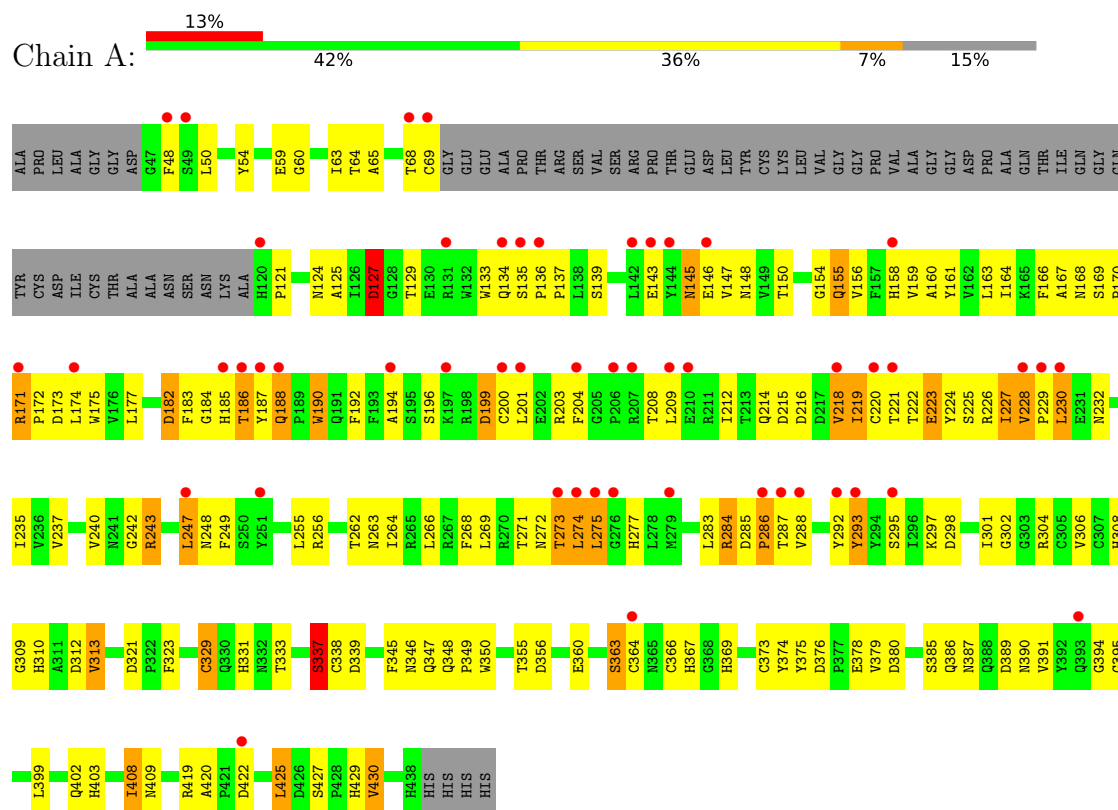
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

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 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.

• Molecule 1: LAMININ SUBUNIT ALPHA-5



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	116.40Å 116.40Å 112.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.90 25.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-2.90) 99.7 (25.00-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.254 , 0.292 0.247 , 0.286	Depositor DCC
R_{free} test set	935 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2712	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: NAG, PO4

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	0.51	0/2714	1.03	12/3707 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	N-CA-C	-8.95	95.89	109.94
1	A	145	ASN	N-CA-C	-8.04	101.55	113.61
1	A	337	SER	N-CA-C	-7.32	95.20	110.80
1	A	188	GLN	CA-C-N	-6.34	114.09	120.31
1	A	188	GLN	C-N-CA	-6.34	114.09	120.31
1	A	321	ASP	CA-C-N	6.19	127.58	119.84
1	A	321	ASP	C-N-CA	6.19	127.58	119.84
1	A	329	CYS	N-CA-C	5.37	118.02	110.23
1	A	240	VAL	N-CA-C	5.33	116.40	111.81
1	A	127	ASP	N-CA-C	-5.17	103.21	110.35
1	A	430	VAL	CB-CA-C	-5.12	105.32	111.88
1	A	190	TRP	N-CA-C	-5.08	107.15	113.55

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	2640	0	2419	141	0
2	B	28	0	25	3	0
3	A	14	0	13	1	0
4	A	30	0	0	5	0
All	All	2712	0	2457	142	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 27.

All (142) 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:386:GLN:H	1:A:409:ASN:HD21	1.03	1.00
1:A:155:GLN:HE21	1:A:155:GLN:H	1.00	0.99
1:A:201:LEU:HD12	1:A:201:LEU:H	1.34	0.91
1:A:264:ILE:HD12	1:A:301:ILE:HD13	1.58	0.85
1:A:347:GLN:HG2	1:A:364:CYS:HA	1.59	0.84
1:A:155:GLN:HE21	1:A:155:GLN:N	1.77	0.83
1:A:171:ARG:HG2	1:A:235:ILE:HD11	1.62	0.81
1:A:155:GLN:H	1:A:155:GLN:NE2	1.78	0.80
1:A:173:ASP:HB2	1:A:272:ASN:HA	1.62	0.79
1:A:230:LEU:HD12	1:A:230:LEU:H	1.48	0.78
1:A:196:SER:OG	1:A:199:ASP:HB2	1.85	0.76
1:A:386:GLN:N	1:A:409:ASN:HD21	1.83	0.75
1:A:386:GLN:H	1:A:409:ASN:ND2	1.84	0.74
1:A:262:THR:HG22	1:A:263:ASN:ND2	2.03	0.74
1:A:427:SER:O	1:A:430:VAL:HG23	1.88	0.74
1:A:121:PRO:HD2	1:A:124:ASN:HD21	1.53	0.73
1:A:48:PHE:CD1	1:A:355:THR:HA	2.24	0.73
1:A:201:LEU:HD12	1:A:201:LEU:N	2.05	0.72
1:A:389:ASP:O	1:A:390:ASN:HB2	1.90	0.71
1:A:420:ALA:HB1	1:A:422:ASP:OD1	1.90	0.71
1:A:376:ASP:CG	1:A:379:VAL:HG23	2.16	0.70
1:A:192:PHE:HB3	1:A:204:PHE:CE2	2.26	0.70
1:A:201:LEU:H	1:A:201:LEU:CD1	2.05	0.70
1:A:48:PHE:HD1	1:A:355:THR:HA	1.56	0.70
1:A:183:PHE:HA	1:A:262:THR:HG21	1.73	0.70
1:A:249:PHE:CZ	1:A:256:ARG:HG3	2.28	0.69
1:A:256:ARG:HG2	4:A:2005:PO4:O1	1.92	0.68
1:A:171:ARG:NH1	1:A:171:ARG:HB2	2.09	0.68
1:A:48:PHE:CE1	1:A:355:THR:HG23	2.29	0.67
1:A:137:PRO:HG3	1:A:293:TYR:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:C	1:A:163:LEU:HD23	2.19	0.67
1:A:283:LEU:O	1:A:284:ARG:HB2	1.93	0.67
1:A:227:ILE:HB	1:A:272:ASN:OD1	1.96	0.66
1:A:419:ARG:HH11	1:A:419:ARG:HG2	1.62	0.64
1:A:170:PRO:HB3	1:A:230:LEU:HA	1.80	0.63
1:A:174:LEU:HD23	1:A:194:ALA:HA	1.79	0.63
1:A:185:HIS:O	1:A:187:TYR:HD1	1.80	0.62
1:A:312:ASP:OD1	1:A:313:VAL:HG12	2.01	0.61
1:A:306:VAL:HA	4:A:2004:PO4:O3	2.00	0.61
1:A:285:ASP:OD1	1:A:287:THR:HB	2.01	0.60
1:A:148:ASN:ND2	2:B:1:NAG:H82	2.16	0.60
1:A:60:GLY:HA3	1:A:323:PHE:CE1	2.38	0.59
1:A:171:ARG:HB2	1:A:171:ARG:HH11	1.67	0.59
1:A:221:THR:HG22	1:A:222:THR:N	2.18	0.59
1:A:346:ASN:HB2	1:A:373:CYS:SG	2.43	0.58
1:A:380:ASP:HB2	1:A:395:GLY:HA3	1.85	0.58
1:A:218:VAL:HG13	1:A:219:ILE:N	2.17	0.58
1:A:227:ILE:O	1:A:228:VAL:C	2.46	0.58
1:A:219:ILE:HG23	1:A:220:CYS:N	2.19	0.57
1:A:273:THR:HG23	1:A:292:TYR:CE2	2.38	0.57
1:A:274:LEU:O	1:A:275:LEU:HB2	2.05	0.56
1:A:68:THR:HG23	1:A:133:TRP:CD1	2.40	0.56
1:A:134:GLN:CD	1:A:168:ASN:HD21	2.14	0.56
1:A:63:ILE:HA	1:A:150:THR:O	2.04	0.56
1:A:277:HIS:HB3	1:A:288:VAL:CG1	2.36	0.56
1:A:166:PHE:O	1:A:232:ASN:HA	2.06	0.55
1:A:339:ASP:HA	1:A:350:TRP:CZ2	2.41	0.55
1:A:380:ASP:HA	1:A:394:GLY:O	2.06	0.55
1:A:277:HIS:HB3	1:A:288:VAL:HG11	1.89	0.55
1:A:121:PRO:HD2	1:A:124:ASN:ND2	2.21	0.54
1:A:284:ARG:NH1	1:A:284:ARG:HG3	2.23	0.54
1:A:200:CYS:HB2	1:A:201:LEU:HD12	1.88	0.54
1:A:218:VAL:O	1:A:219:ILE:HG13	2.08	0.53
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.74	0.53
1:A:169:SER:HB3	1:A:295:SER:HB2	1.91	0.53
1:A:187:TYR:O	1:A:188:GLN:HG3	2.09	0.53
1:A:427:SER:C	1:A:429:HIS:H	2.16	0.53
1:A:219:ILE:CG2	1:A:220:CYS:N	2.72	0.52
1:A:310:HIS:ND1	1:A:331:HIS:HD2	2.07	0.52
1:A:349:PRO:HG3	1:A:375:TYR:CE2	2.43	0.52
1:A:385:SER:HA	1:A:408:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:CE2	1:A:160:ALA:HB2	2.44	0.52
1:A:228:VAL:HB	1:A:229:PRO:CD	2.40	0.52
1:A:194:ALA:O	1:A:222:THR:HA	2.10	0.51
1:A:333:THR:OG1	1:A:338:CYS:HB3	2.10	0.51
1:A:308:HIS:HD2	1:A:337:SER:O	1.94	0.51
1:A:177:LEU:HD22	1:A:237:VAL:HG21	1.93	0.51
1:A:185:HIS:O	1:A:187:TYR:N	2.44	0.50
1:A:68:THR:O	1:A:134:GLN:O	2.30	0.50
1:A:155:GLN:N	1:A:155:GLN:NE2	2.49	0.50
1:A:164:ILE:HD13	1:A:266:LEU:HD13	1.93	0.50
1:A:182:ASP:OD2	1:A:186:THR:HB	2.11	0.50
1:A:287:THR:O	1:A:287:THR:HG22	2.11	0.50
1:A:54:TYR:HE2	1:A:160:ALA:HB2	1.75	0.49
1:A:50:LEU:O	1:A:309:GLY:HA2	2.12	0.49
1:A:349:PRO:HG3	1:A:375:TYR:CZ	2.48	0.49
1:A:146:GLU:HG2	1:A:269:LEU:HA	1.95	0.49
1:A:221:THR:HG22	1:A:222:THR:H	1.78	0.49
1:A:419:ARG:HG2	1:A:419:ARG:NH1	2.27	0.49
3:A:2003:NAG:O3	3:A:2003:NAG:H83	2.13	0.48
1:A:310:HIS:ND1	1:A:331:HIS:CD2	2.81	0.48
1:A:331:HIS:HB3	1:A:360:GLU:HB3	1.95	0.48
1:A:304:ARG:NE	4:A:2004:PO4:O1	2.47	0.48
1:A:145:ASN:OD1	1:A:271:THR:HG23	2.14	0.48
1:A:147:VAL:HG22	1:A:268:PHE:HB2	1.94	0.47
1:A:127:ASP:OD2	1:A:129:THR:HG23	2.13	0.47
1:A:242:GLY:O	1:A:243:ARG:C	2.57	0.47
1:A:209:LEU:HD12	1:A:209:LEU:O	2.13	0.47
1:A:222:THR:O	1:A:223:GLU:C	2.57	0.47
1:A:226:ARG:O	1:A:229:PRO:HD2	2.15	0.47
1:A:134:GLN:NE2	1:A:168:ASN:HD21	2.13	0.47
1:A:135:SER:HB2	1:A:136:PRO:HD2	1.97	0.47
1:A:402:GLN:O	1:A:403:HIS:HB2	2.14	0.46
1:A:158:HIS:HE2	4:A:2005:PO4:P	2.38	0.46
1:A:161:TYR:CD1	1:A:161:TYR:C	2.93	0.46
1:A:366:CYS:O	1:A:367:HIS:C	2.59	0.46
1:A:274:LEU:O	1:A:275:LEU:CB	2.63	0.46
1:A:167:ALA:HB2	1:A:297:LYS:HB3	1.98	0.46
1:A:347:GLN:HG2	1:A:364:CYS:CA	2.39	0.45
1:A:196:SER:O	1:A:199:ASP:N	2.46	0.45
1:A:347:GLN:NE2	1:A:394:GLY:HA3	2.32	0.45
1:A:222:THR:O	1:A:224:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:ND2	2:B:1:NAG:C7	2.80	0.45
1:A:212:ILE:HG13	1:A:219:ILE:CD1	2.47	0.44
1:A:227:ILE:HG23	1:A:228:VAL:N	2.32	0.44
1:A:225:SER:O	1:A:272:ASN:ND2	2.50	0.44
1:A:376:ASP:OD1	1:A:379:VAL:HG23	2.17	0.44
1:A:247:LEU:HG	1:A:248:ASN:N	2.32	0.43
1:A:143:GLU:C	1:A:145:ASN:H	2.25	0.43
1:A:369:HIS:NE2	1:A:425:LEU:O	2.42	0.43
1:A:356:ASP:OD1	1:A:356:ASP:N	2.52	0.43
1:A:387:ASN:HD21	1:A:391:VAL:HB	1.83	0.43
1:A:227:ILE:HG22	1:A:274:LEU:HD13	2.00	0.43
1:A:369:HIS:CE1	1:A:403:HIS:HD1	2.33	0.42
1:A:297:LYS:O	1:A:298:ASP:HB2	2.19	0.42
1:A:242:GLY:O	1:A:243:ARG:O	2.37	0.42
1:A:125:ALA:O	1:A:298:ASP:HA	2.19	0.42
1:A:374:TYR:HD2	1:A:399:LEU:HD21	1.84	0.42
1:A:64:THR:HG22	1:A:65:ALA:N	2.35	0.41
1:A:146:GLU:HA	1:A:268:PHE:O	2.20	0.41
1:A:172:PRO:HG2	1:A:175:TRP:CD1	2.55	0.41
1:A:159:VAL:HG21	1:A:264:ILE:HD11	2.02	0.41
1:A:163:LEU:C	1:A:163:LEU:CD2	2.89	0.41
1:A:158:HIS:NE2	4:A:2005:PO4:O1	2.51	0.41
1:A:345:PHE:HA	1:A:363:SER:HA	2.02	0.41
1:A:427:SER:C	1:A:429:HIS:N	2.78	0.41
1:A:285:ASP:HA	1:A:286:PRO:HD3	1.90	0.41
1:A:329:CYS:HB3	1:A:333:THR:OG1	2.21	0.41
1:A:148:ASN:ND2	2:B:1:NAG:C8	2.84	0.40
1:A:284:ARG:HH11	1:A:284:ARG:CG	2.35	0.40
1:A:161:TYR:CE2	1:A:302:GLY:HA3	2.57	0.40
1:A:214:GLN:O	1:A:216:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	338/403 (84%)	269 (80%)	52 (15%)	17 (5%)	1	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	186	THR
1	A	223	GLU
1	A	228	VAL
1	A	215	ASP
1	A	243	ARG
1	A	275	LEU
1	A	337	SER
1	A	59	GLU
1	A	284	ARG
1	A	154	GLY
1	A	273	THR
1	A	425	LEU
1	A	208	THR
1	A	227	ILE
1	A	184	GLY
1	A	286	PRO

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	286/341 (84%)	266 (93%)	20 (7%)	14	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	127	ASP

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	156	VAL
1	A	171	ARG
1	A	190	TRP
1	A	199	ASP
1	A	203	ARG
1	A	218	VAL
1	A	219	ILE
1	A	230	LEU
1	A	247	LEU
1	A	255	LEU
1	A	274	LEU
1	A	293	TYR
1	A	313	VAL
1	A	348	GLN
1	A	363	SER
1	A	378	GLU
1	A	408	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	155	GLN
1	A	168	ASN
1	A	191	GLN
1	A	232	ASN
1	A	308	HIS
1	A	331	HIS
1	A	362	GLN
1	A	404	HIS
1	A	409	ASN
1	A	429	HIS

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 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	B	1	2,1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	B	2	2	14,14,15	0.54	0	17,19,21	0.89	1 (5%)

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	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C2-N2-C7	-2.70	119.29	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

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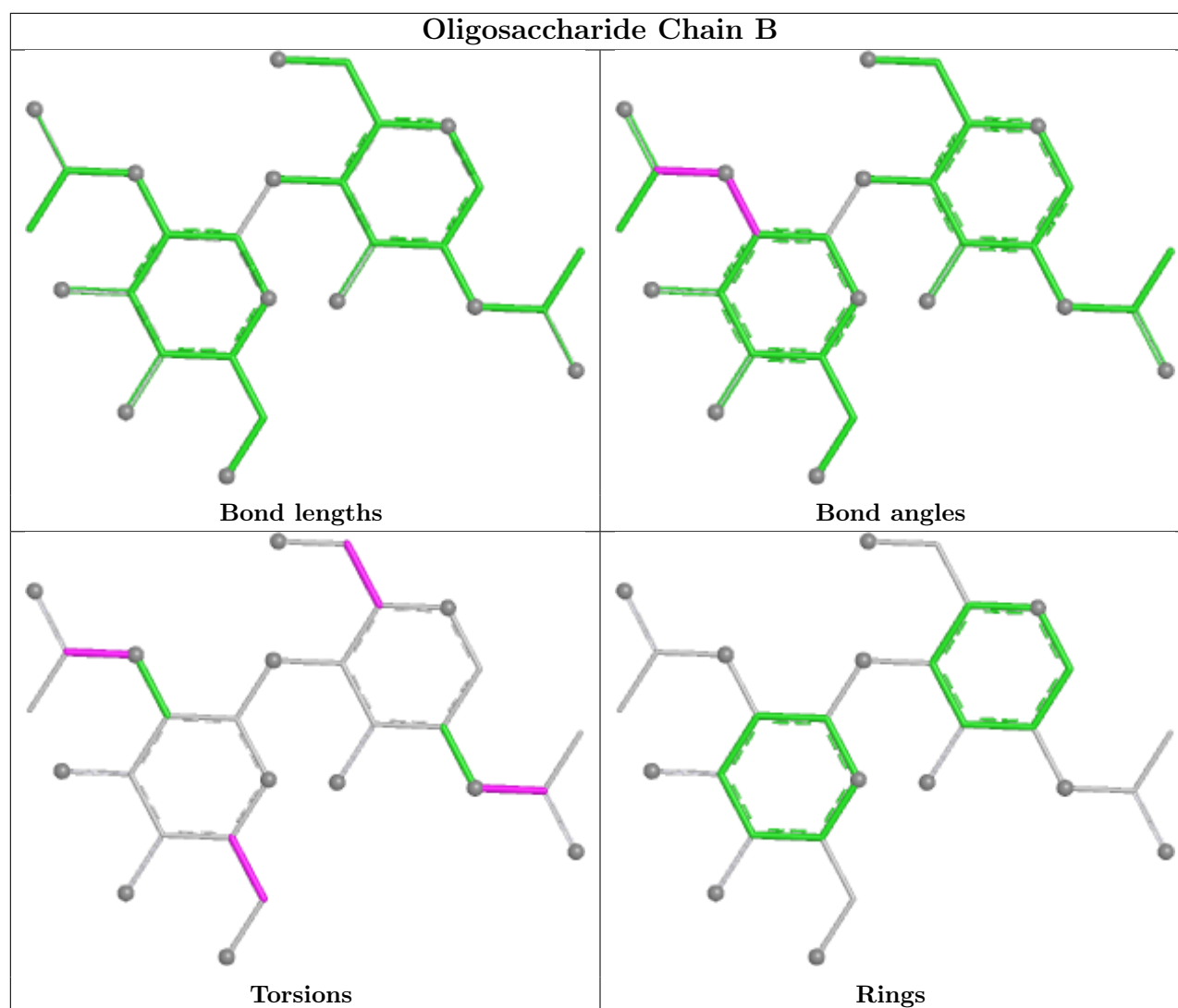
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	3	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](#)

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	$\# Z > 2$
4	PO4	A	2009	-	4,4,4	1.68	0	6,6,6	0.45	0
4	PO4	A	2006	-	4,4,4	1.71	1 (25%)	6,6,6	0.46	0
4	PO4	A	2008	-	4,4,4	1.72	2 (50%)	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2003	1	14,14,15	0.65	0	17,19,21	0.77	1 (5%)
4	PO4	A	2005	-	4,4,4	1.74	0	6,6,6	0.50	0
4	PO4	A	2004	-	4,4,4	1.91	2 (50%)	6,6,6	0.50	0
4	PO4	A	2007	-	4,4,4	1.58	0	6,6,6	0.50	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	2003	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2004	PO4	P-O3	-2.19	1.48	1.54
4	A	2004	PO4	P-O4	-2.17	1.48	1.54
4	A	2008	PO4	P-O3	-2.11	1.48	1.54
4	A	2006	PO4	P-O3	-2.05	1.48	1.54
4	A	2008	PO4	P-O2	-2.01	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2003	NAG	C2-N2-C7	-2.49	119.56	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	A	2003	NAG	O5-C5-C6-O6
3	A	2003	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	NAG	1	0
4	A	2005	PO4	3	0
4	A	2004	PO4	2	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/403 (84%)	0.86	51 (14%) 5 4	38, 75, 110, 117	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	MET	4.7
1	A	142	LEU	4.4
1	A	393	GLN	4.4
1	A	274	LEU	4.1
1	A	194	ALA	3.9
1	A	221	THR	3.5
1	A	287	THR	3.4
1	A	144	TYR	3.4
1	A	273	THR	3.4
1	A	207	ARG	3.3
1	A	288	VAL	3.3
1	A	220	CYS	3.2
1	A	188	GLN	3.1
1	A	364	CYS	3.1
1	A	210	GLU	3.0
1	A	120	HIS	3.0
1	A	218	VAL	2.9
1	A	275	LEU	2.9
1	A	276	GLY	2.8
1	A	293	TYR	2.7
1	A	186	THR	2.7
1	A	49	SER	2.6
1	A	229	PRO	2.6
1	A	206	PRO	2.6
1	A	247	LEU	2.6
1	A	143	GLU	2.6
1	A	422	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	TYR	2.5
1	A	228	VAL	2.5
1	A	171	ARG	2.5
1	A	200	CYS	2.4
1	A	68	THR	2.3
1	A	185	HIS	2.3
1	A	295	SER	2.3
1	A	209	LEU	2.3
1	A	136	PRO	2.3
1	A	69	CYS	2.2
1	A	174	LEU	2.2
1	A	251	TYR	2.2
1	A	48	PHE	2.2
1	A	197	LYS	2.2
1	A	158	HIS	2.2
1	A	204	PHE	2.2
1	A	286	PRO	2.1
1	A	201	LEU	2.1
1	A	134	GLN	2.1
1	A	131	ARG	2.1
1	A	292	TYR	2.1
1	A	230	LEU	2.1
1	A	146	GLU	2.0
1	A	135	SER	2.0

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

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

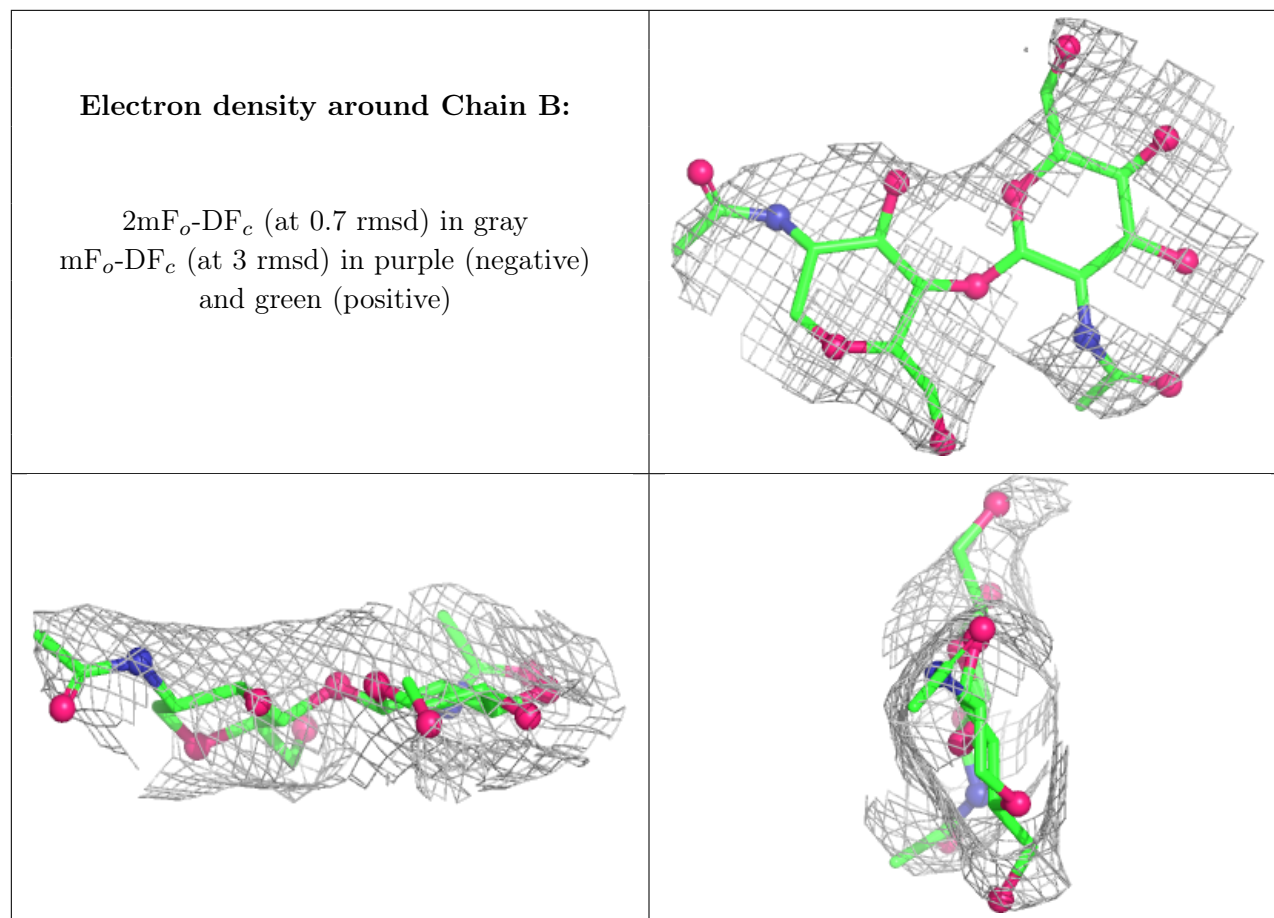
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.74	0.15	109,112,112,113	0
2	NAG	B	1	14/15	0.83	0.15	106,108,109,110	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	2003	14/15	0.76	0.14	93,97,98,98	0
4	PO4	A	2009	5/5	0.85	0.26	140,140,141,141	0
4	PO4	A	2006	5/5	0.88	0.15	110,110,110,110	0
4	PO4	A	2007	5/5	0.89	0.26	87,89,91,91	0
4	PO4	A	2008	5/5	0.90	0.12	93,93,94,94	0
4	PO4	A	2005	5/5	0.96	0.12	104,104,105,105	0
4	PO4	A	2004	5/5	0.97	0.09	58,59,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.