



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 3NIG / pdb_00003nig
Title : The Closed Headpiece of Integrin Iib 3 and its Complex with an Iib 3 -Specific Antagonist That Does Not Induce Opening
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2010-06-15
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

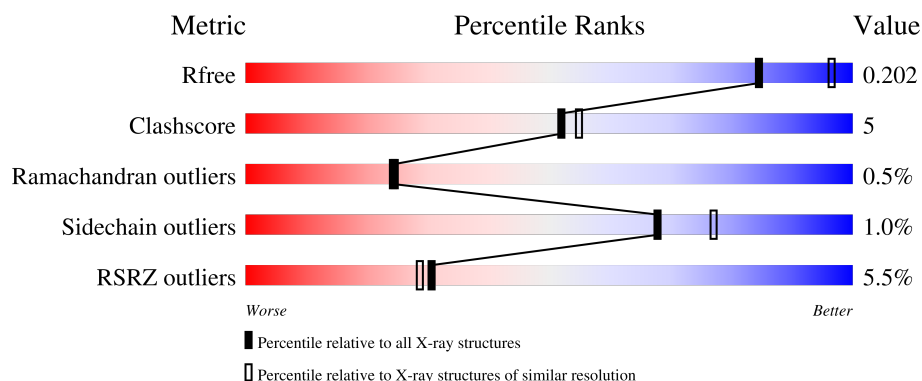
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	457	95% ..
1	C	457	92% 7% .
2	B	471	6% 84% 14% .
2	D	471	3% 87% 12% .
3	E	221	27% 73% 22% ..

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	3	
5	J	3	
6	I	2	
6	K	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
5	MAN	G	3	X	-	-	-
5	MAN	J	3	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22226 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	3	0
			3515	2235	605	667	8			
1	C	453	Total	C	N	O	S	0	3	0
			3489	2217	601	663	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	0	0
			3590	2236	613	708	33			
2	D	471	Total	C	N	O	S	0	1	0
			3634	2265	620	715	34			

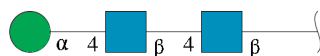
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

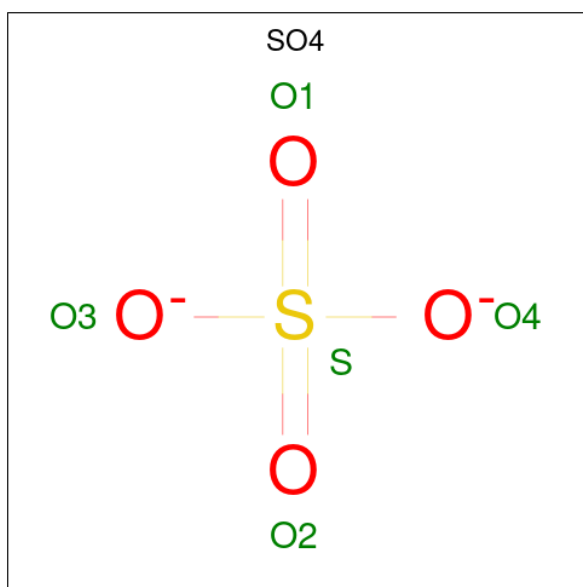
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Ca	0	0
			4	4		
7	B	2	Total	Ca	0	0
			2	2		
7	C	4	Total	Ca	0	0
			4	4		
7	D	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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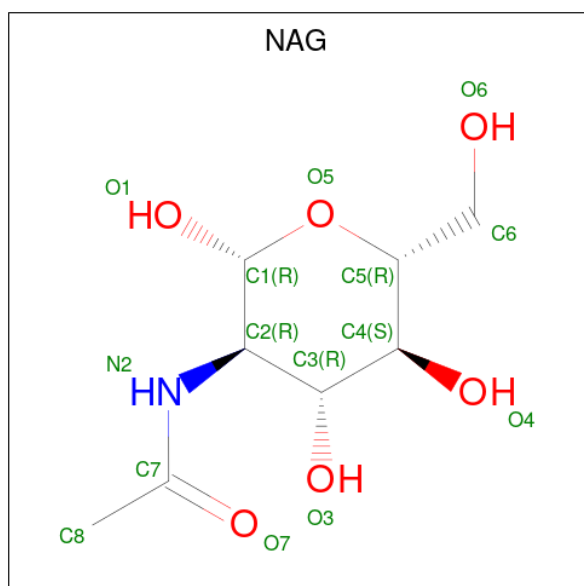
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	446	Total 446	O 446	0	0
12	B	231	Total 231	O 231	0	0
12	C	259	Total 259	O 259	0	0
12	D	191	Total 191	O 191	0	0
12	E	9	Total 9	O 9	0	0
12	F	12	Total 12	O 12	0	0
12	H	32	Total 32	O 32	0	0
12	L	47	Total 47	O 47	0	0

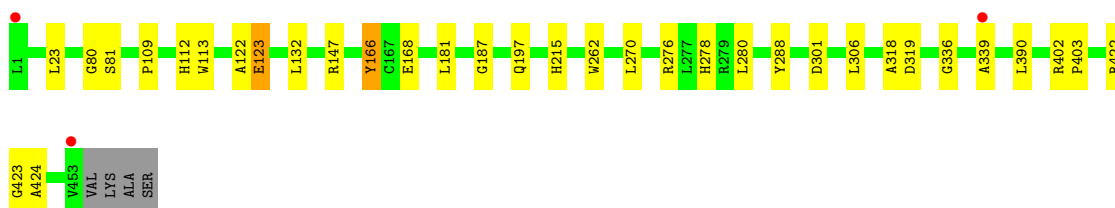
3 Residue-property plots [i](#)

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 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.

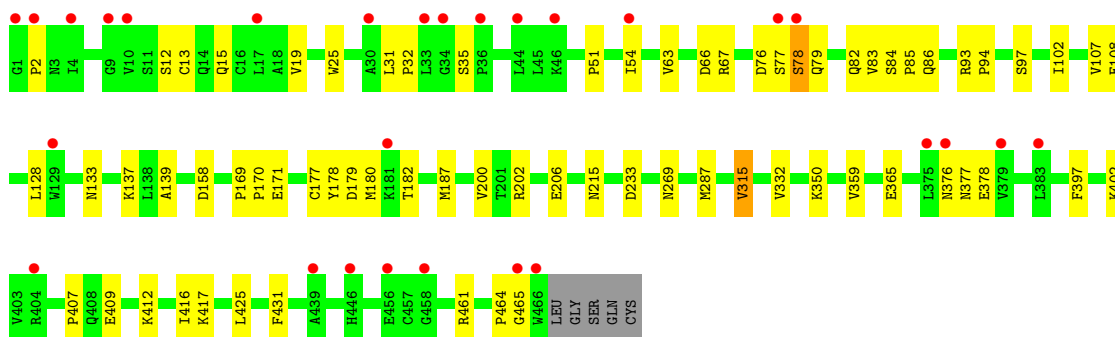
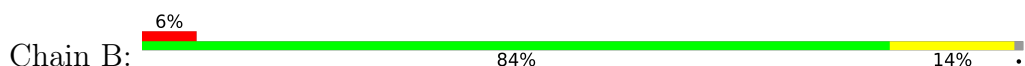
- Molecule 1: Integrin alpha-IIb



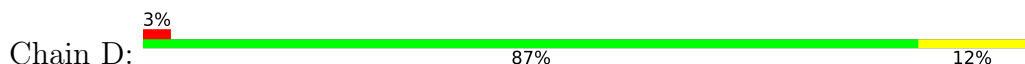
- Molecule 1: Integrin alpha-IIb

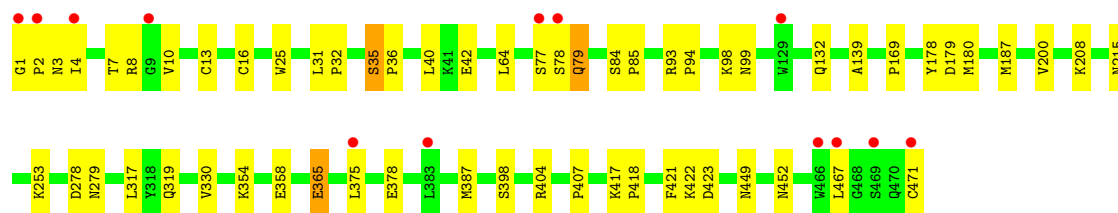


- Molecule 2: Integrin beta-3

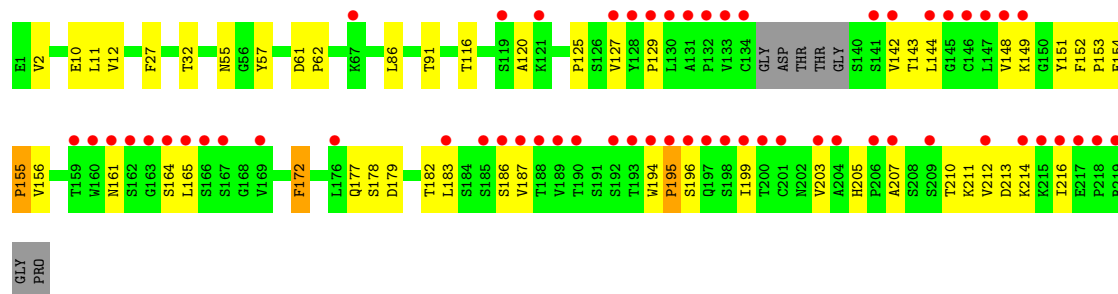
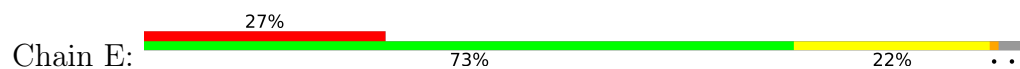


- Molecule 2: Integrin beta-3

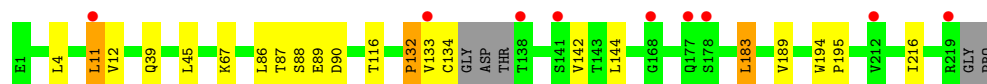
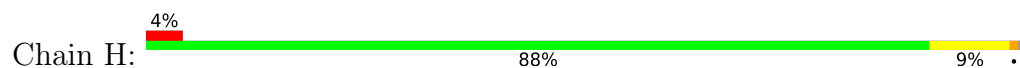




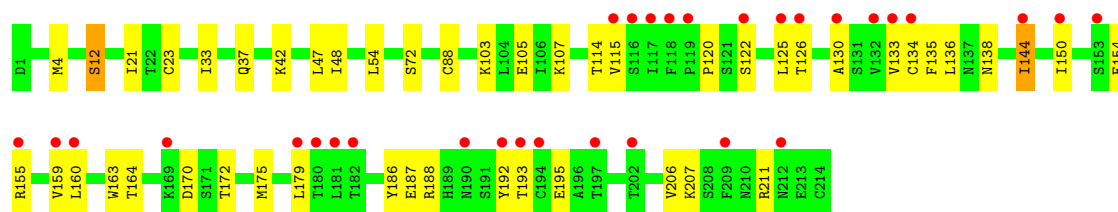
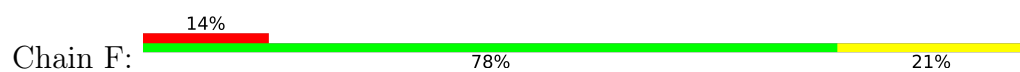
• Molecule 3: Monoclonal antibody 10E5 heavy chain



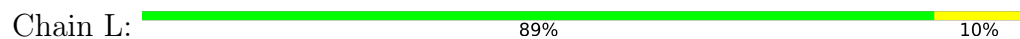
• Molecule 3: Monoclonal antibody 10E5 heavy chain



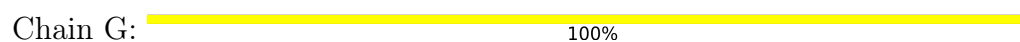
• Molecule 4: Monoclonal antibody 10E5 light chain



• Molecule 4: Monoclonal antibody 10E5 light chain



• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
MAN3

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2
MAN3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	260.67Å 145.17Å 104.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.25 48.49 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.49-2.25) 99.9 (48.49-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.172 , 0.212 0.162 , 0.202	Depositor DCC
R_{free} test set	1009 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22226	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, MAN, MG, CA, SO4

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	0.75	0/3621	0.86	2/4934 (0.0%)
1	C	0.59	0/3595	0.81	2/4899 (0.0%)
2	B	0.63	0/3657	0.82	3/4959 (0.1%)
2	D	0.58	0/3706	0.78	2/5026 (0.0%)
3	E	0.38	0/1673	0.72	2/2290 (0.1%)
3	H	0.46	0/1684	0.70	0/2305
4	F	0.37	0/1673	0.70	0/2269
4	L	0.44	0/1673	0.72	0/2269
All	All	0.58	0/21282	0.78	11/28951 (0.0%)

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
2	B	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	THR	N-CA-C	6.31	116.40	108.45
1	C	336	GLY	CA-C-N	6.18	125.88	119.82
1	C	336	GLY	C-N-CA	6.18	125.88	119.82
2	D	79	GLN	N-CA-C	-6.18	105.32	112.92
2	D	180	MET	N-CA-C	-5.27	102.39	110.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	78	SER	Peptide

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	3515	0	3361	10	0
1	C	3489	0	3327	24	0
2	B	3590	0	3511	41	0
2	D	3634	0	3551	35	0
3	E	1631	0	1590	38	0
3	H	1642	0	1600	15	0
4	F	1637	0	1553	34	0
4	L	1637	0	1553	14	0
5	G	39	0	34	0	0
5	J	39	0	34	2	0
6	I	28	0	25	1	0
6	K	28	0	25	1	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	A	12	0	16	3	0
8	C	6	0	8	2	0
9	A	10	0	0	1	0
9	C	10	0	0	0	0
9	D	5	0	0	0	0
9	L	5	0	0	1	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	446	0	0	1	0
12	B	231	0	0	1	0
12	C	259	0	0	2	0
12	D	191	0	0	2	0
12	E	9	0	0	2	0
12	F	12	0	0	0	0
12	H	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	47	0	0	1	0
All	All	22226	0	20214	211	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 5.

The worst 5 of 211 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)
2:D:365:GLU:HG3	2:D:407:PRO:HG3	1.66	0.76
2:D:78:SER:HB3	2:D:422:LYS:HE2	1.75	0.68
3:E:161:ASN:HB2	3:E:164:SER:HB2	1.77	0.66
2:D:375:LEU:O	2:D:378:GLU:HB2	1.95	0.65
1:C:402:ARG:HD2	12:C:574:HOH:O	1.98	0.64

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 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	458/457 (100%)	440 (96%)	16 (4%)	2 (0%)	30	31
1	C	454/457 (99%)	439 (97%)	14 (3%)	1 (0%)	43	50
2	B	464/471 (98%)	439 (95%)	22 (5%)	3 (1%)	21	21
2	D	470/471 (100%)	455 (97%)	14 (3%)	1 (0%)	43	50
3	E	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	9	5
3	H	212/221 (96%)	195 (92%)	16 (8%)	1 (0%)	24	24
4	F	212/214 (99%)	194 (92%)	18 (8%)	0	100	100
4	L	212/214 (99%)	204 (96%)	6 (3%)	2 (1%)	14	12
All	All	2692/2726 (99%)	2549 (95%)	130 (5%)	13 (0%)	24	24

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	GLU
3	E	178	SER
1	A	123	GLU
2	B	2	PRO
2	B	76	ASP

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	367/364 (101%)	361 (98%)	6 (2%)	55	66
1	C	364/364 (100%)	361 (99%)	3 (1%)	73	80
2	B	412/416 (99%)	406 (98%)	6 (2%)	57	68
2	D	417/416 (100%)	412 (99%)	5 (1%)	63	74
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	185 (99%)	2 (1%)	65	75
4	F	188/188 (100%)	186 (99%)	2 (1%)	65	75
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2309/2316 (100%)	2285 (99%)	24 (1%)	68	77

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	TYR
2	D	187	MET
2	D	64	LEU
2	D	215	ASN
2	B	63	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	274	HIS
3	H	39	GLN
4	L	38	GLN
3	H	82	GLN
2	B	440	GLN

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 ⓘ

10 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	$\# Z > 2$
5	NAG	G	1	5,2	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
5	NAG	G	2	5	14,14,15	0.63	0	17,19,21	3.13	6 (35%)
5	MAN	G	3	5	11,11,12	0.52	0	15,15,17	1.17	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.57	0	17,19,21	1.13	2 (11%)
6	NAG	I	2	6	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
5	NAG	J	1	5,2	14,14,15	0.49	0	17,19,21	1.18	2 (11%)
5	NAG	J	2	5	14,14,15	0.52	0	17,19,21	1.39	1 (5%)
5	MAN	J	3	5	11,11,12	0.50	0	15,15,17	1.23	1 (6%)
6	NAG	K	1	6,2	14,14,15	0.69	0	17,19,21	0.97	1 (5%)
6	NAG	K	2	6	14,14,15	0.53	0	17,19,21	0.95	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
5	NAG	J	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	MAN	J	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	C1-O5-C5	10.19	125.84	112.19
5	G	2	NAG	O5-C5-C6	-5.02	97.89	107.66
5	J	2	NAG	C1-O5-C5	4.82	118.64	112.19
5	G	3	MAN	C1-O5-C5	3.23	116.52	112.19
5	J	3	MAN	C1-O5-C5	3.17	116.44	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	3	MAN	C1
5	J	3	MAN	C1

5 of 12 torsion outliers are listed below:

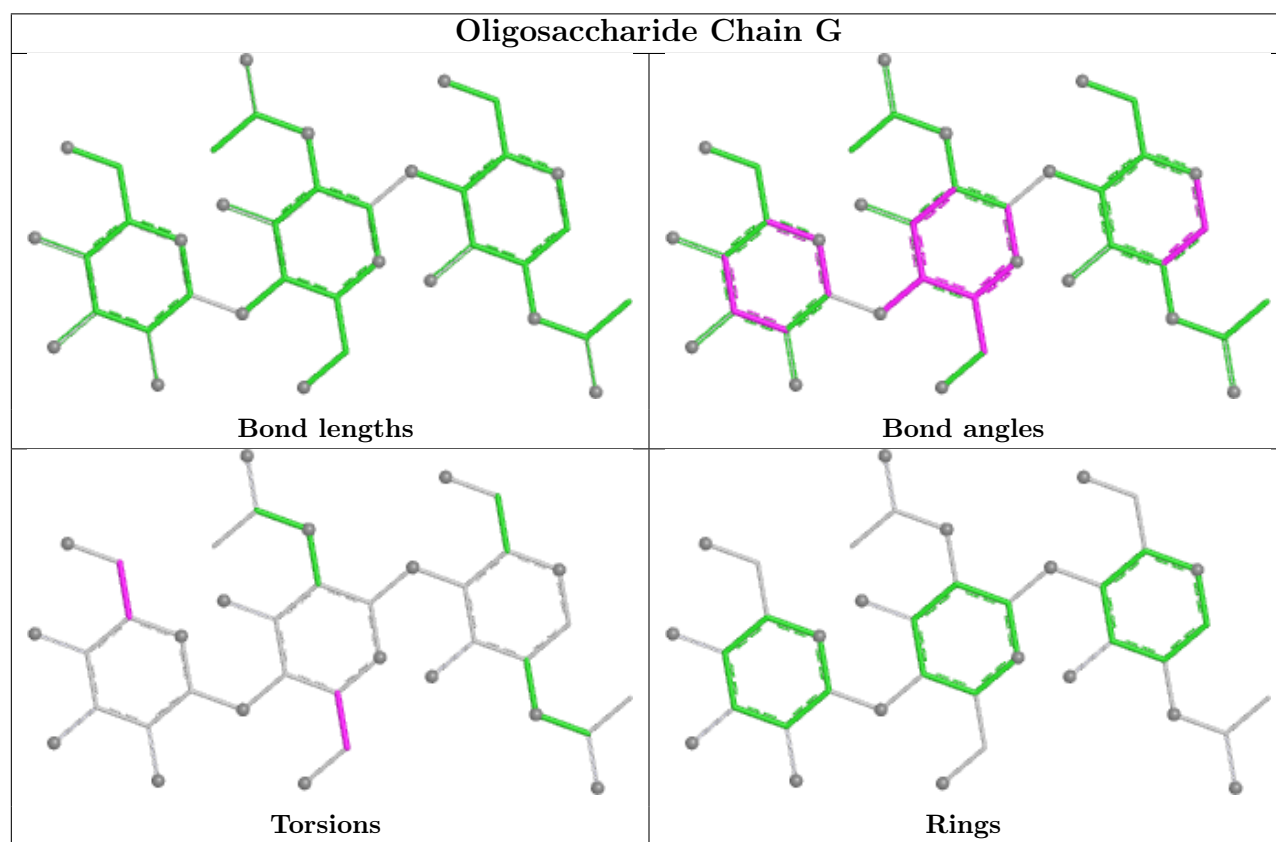
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
5	G	3	MAN	C4-C5-C6-O6
5	J	3	MAN	O5-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
5	G	3	MAN	O5-C5-C6-O6

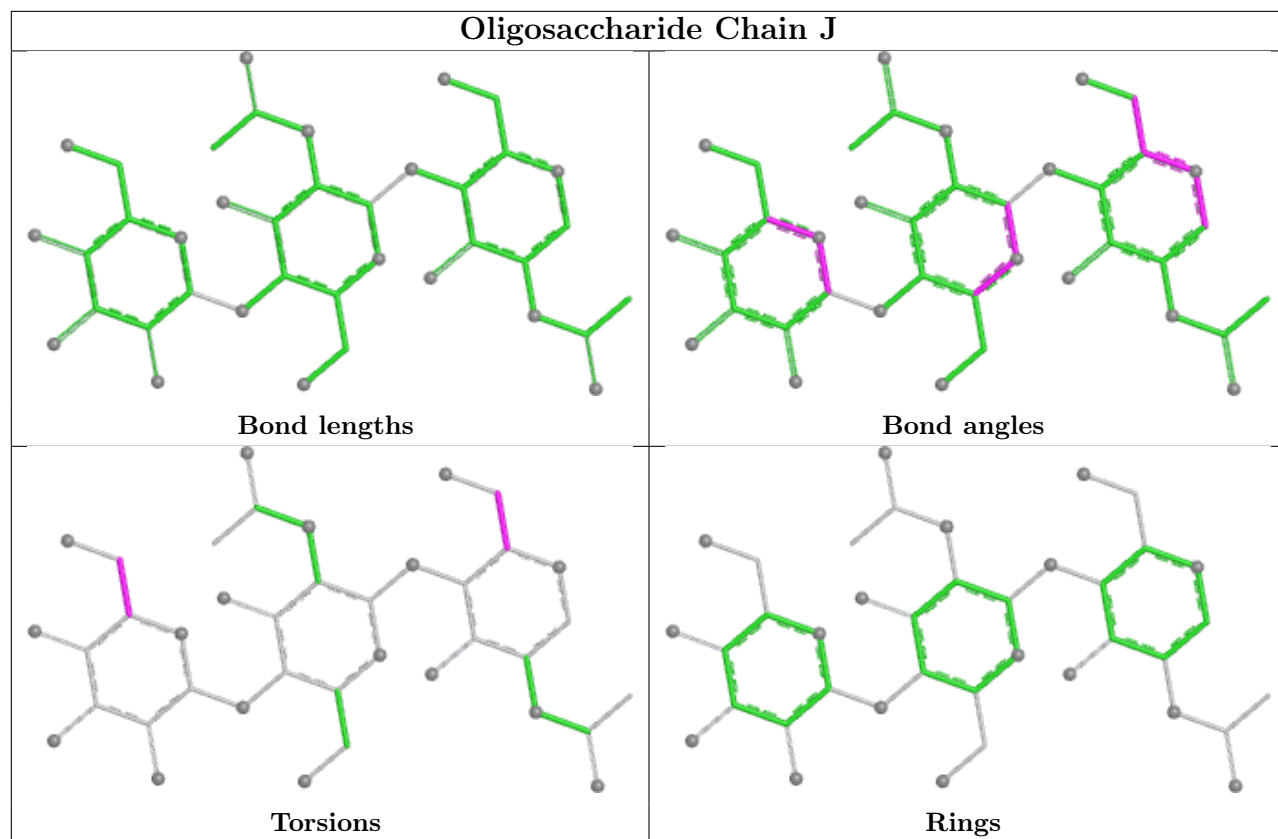
There are no ring outliers.

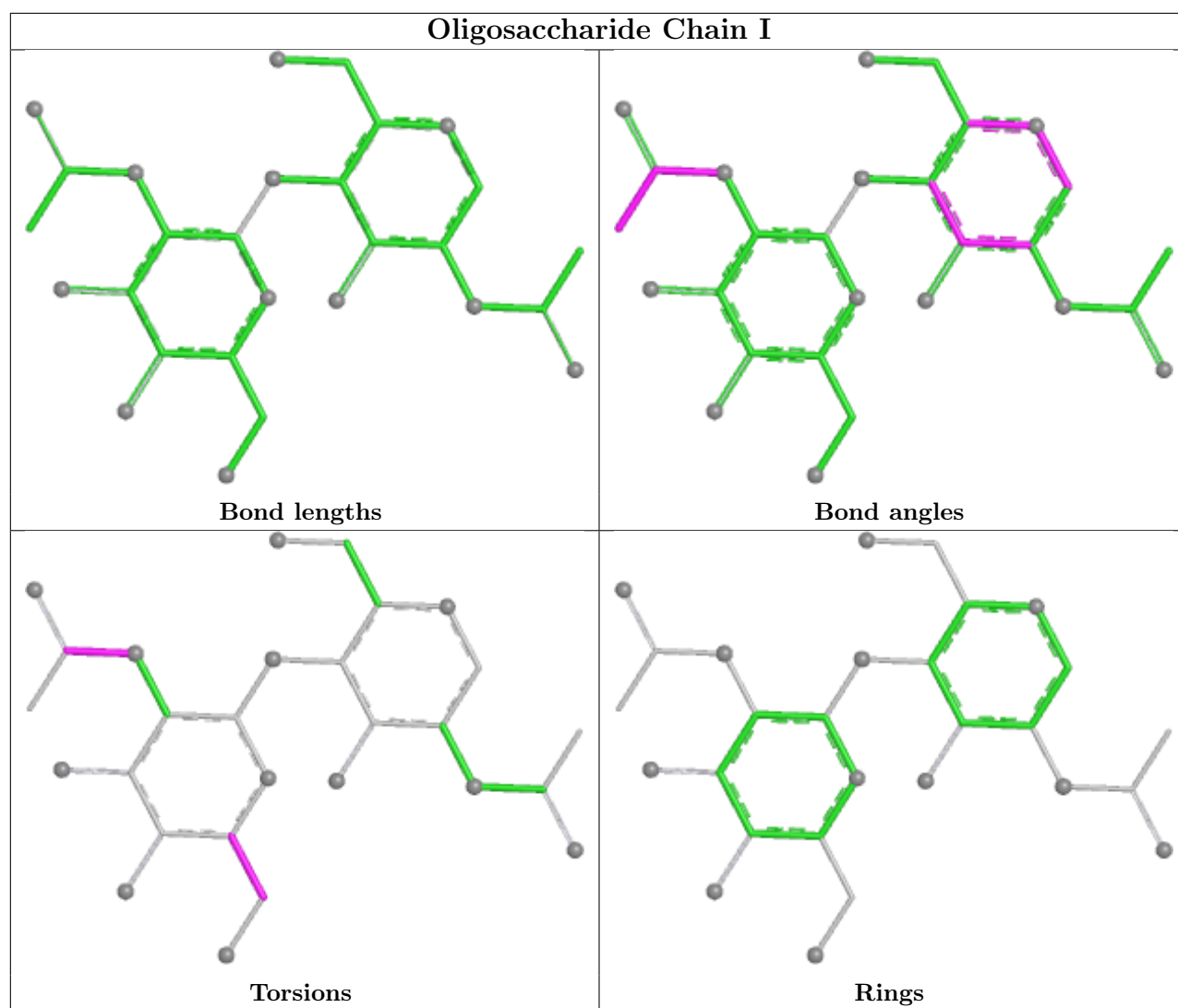
6 monomers are involved in 4 short contacts:

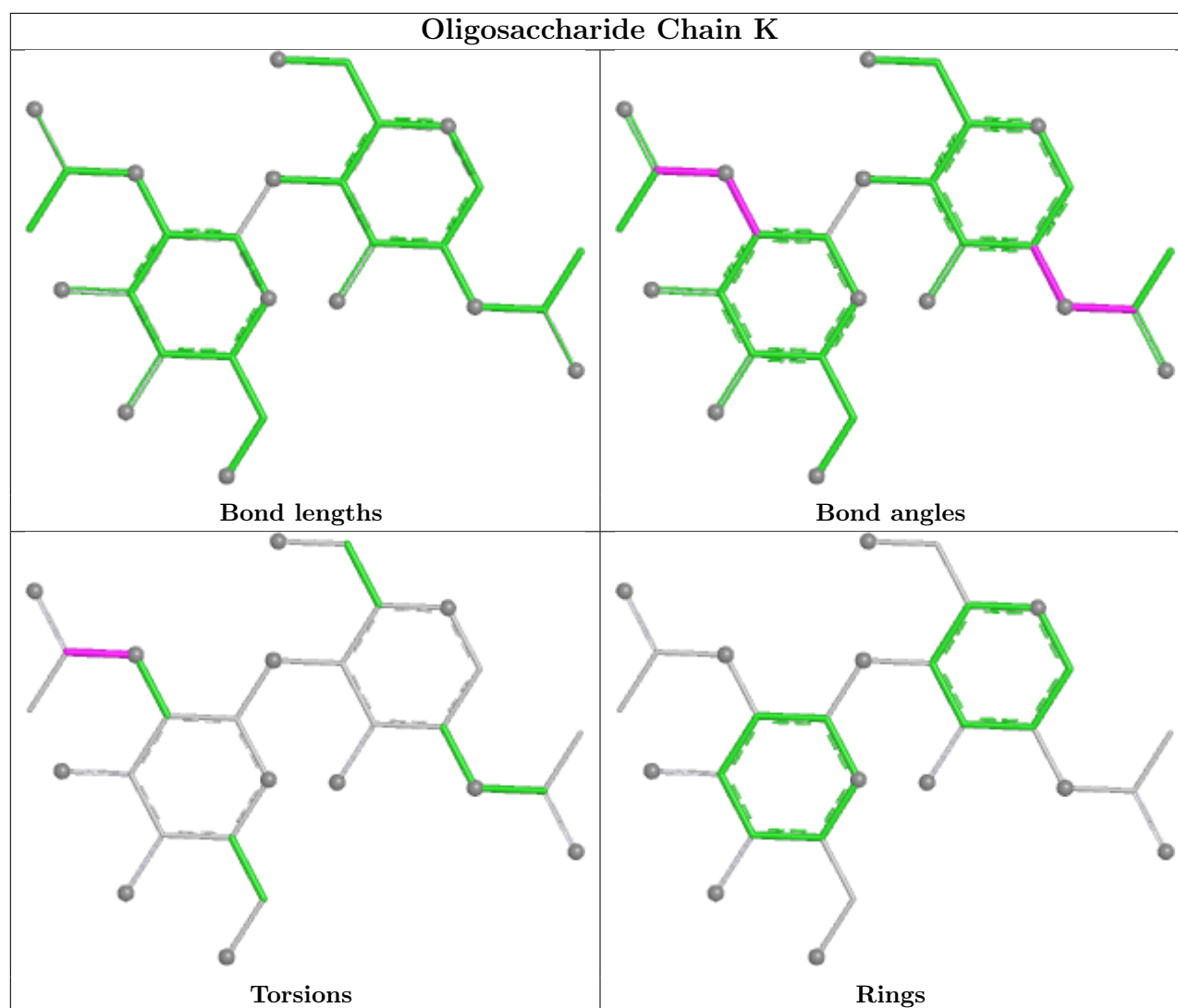
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0
6	K	1	NAG	1	0
5	J	2	NAG	2	0
6	I	2	NAG	1	0
5	J	1	NAG	1	0
5	J	3	MAN	1	0

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](#)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	$\# Z > 2$
9	SO4	D	472	-	4,4,4	0.33	0	6,6,6	0.56	0
9	SO4	A	460	-	4,4,4	0.35	0	6,6,6	0.38	0
9	SO4	C	460	-	4,4,4	0.36	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	A	461	-	4,4,4	0.35	0	6,6,6	1.09	0
9	SO4	C	459	-	4,4,4	0.29	0	6,6,6	0.45	0
9	SO4	L	215	-	4,4,4	0.29	0	6,6,6	0.28	0
11	NAG	B	3099	2	14,14,15	0.54	0	17,19,21	0.60	0
8	GOL	A	459	-	5,5,5	0.45	0	5,5,5	0.35	0
11	NAG	D	3099	2	14,14,15	0.59	0	17,19,21	0.75	0
8	GOL	A	458	-	5,5,5	0.23	0	5,5,5	0.50	0
8	GOL	C	458	-	5,5,5	0.25	0	5,5,5	0.85	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
11	NAG	B	3099	2	-	4/6/23/26	0/1/1/1
8	GOL	A	459	-	-	4/4/4/4	-
11	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
8	GOL	A	458	-	-	0/4/4/4	-
8	GOL	C	458	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	459	GOL	O1-C1-C2-C3
8	C	458	GOL	O1-C1-C2-O2
8	C	458	GOL	O1-C1-C2-C3
11	B	3099	NAG	O5-C5-C6-O6
8	A	459	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	461	SO4	1	0
9	L	215	SO4	1	0
8	A	459	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	458	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	457/457 (100%)	-0.79	5 (1%) 78 79	14, 27, 61, 131	3 (0%)
1	C	453/457 (99%)	-0.47	3 (0%) 84 85	18, 42, 76, 121	3 (0%)
2	B	466/471 (98%)	-0.02	28 (6%) 27 25	18, 56, 134, 196	0
2	D	471/471 (100%)	-0.08	13 (2%) 55 55	24, 54, 118, 159	1 (0%)
3	E	214/221 (96%)	1.32	59 (27%) 1 1	47, 110, 196, 236	0
3	H	216/221 (97%)	0.35	9 (4%) 40 40	30, 77, 138, 181	0
4	F	214/214 (100%)	0.79	31 (14%) 6 5	49, 98, 187, 249	1 (0%)
4	L	214/214 (100%)	-0.03	1 (0%) 87 88	36, 67, 102, 164	1 (0%)
All	All	2705/2726 (99%)	-0.04	149 (5%) 30 29	14, 55, 142, 249	9 (0%)

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	165	LEU	7.5
3	E	212	VAL	6.7
2	B	33	LEU	6.4
2	D	78	SER	6.3
3	E	199	ILE	5.7

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

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

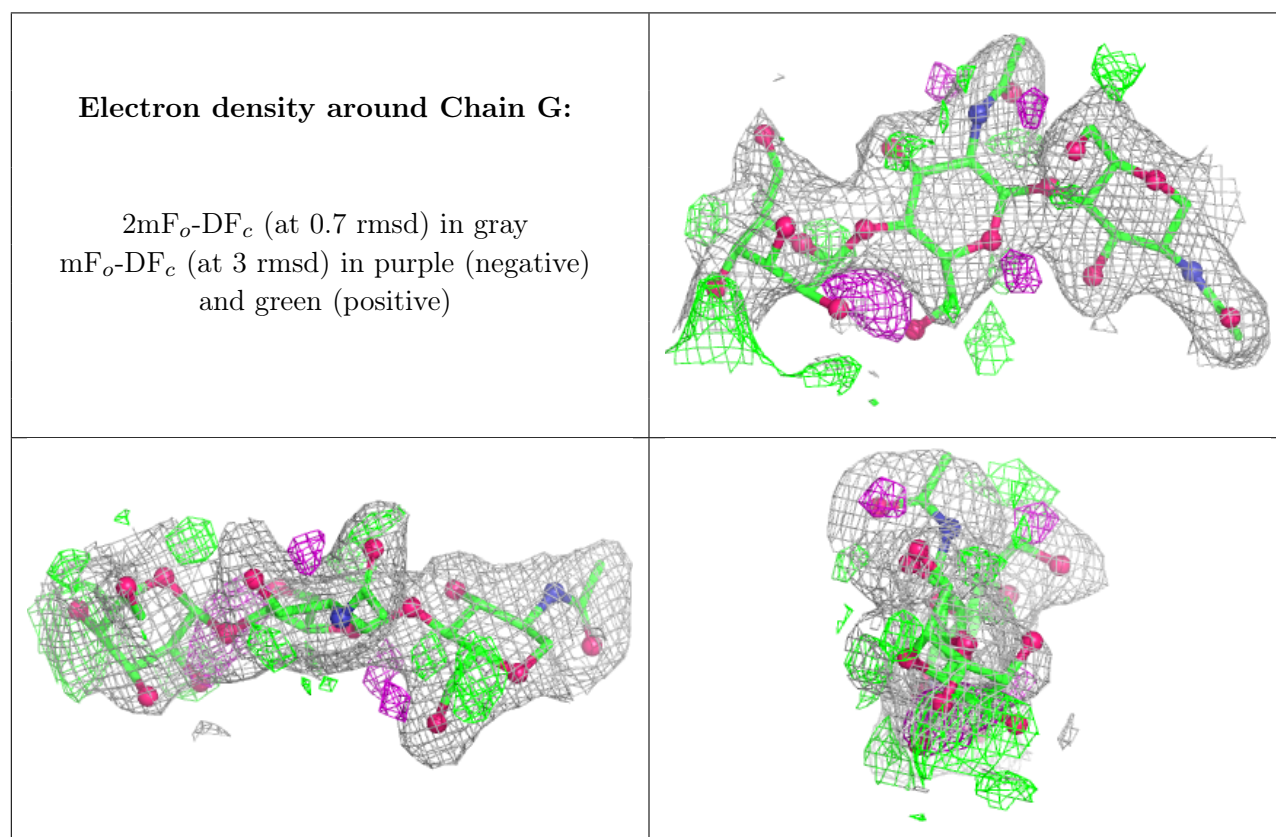
6.3 Carbohydrates [i](#)

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.

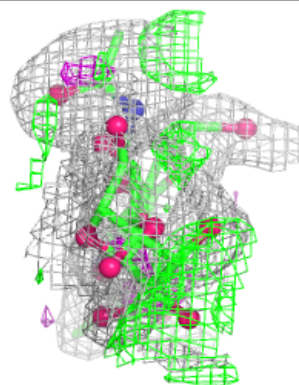
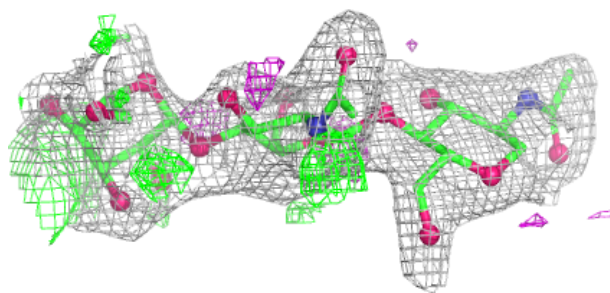
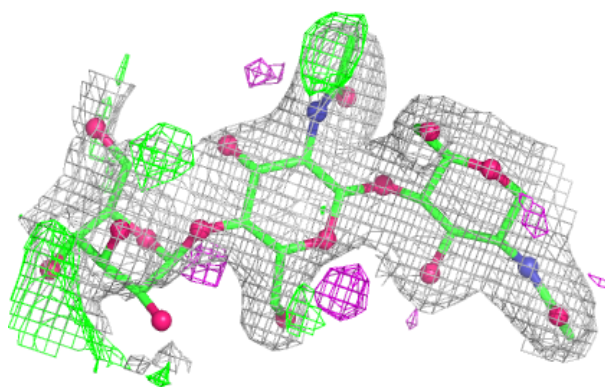
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1	14/15	-	-	23,35,51,52	0
5	NAG	G	2	14/15	-	-	47,74,105,108	0
5	MAN	G	3	11/12	-	-	132,140,144,145	0
5	NAG	J	2	14/15	0.51	0.17	58,95,109,117	0
6	NAG	K	2	14/15	0.81	0.15	134,139,145,145	0
5	MAN	J	3	11/12	-	-	125,131,134,134	0
5	NAG	J	1	14/15	0.84	0.13	44,54,71,72	0
6	NAG	I	2	14/15	0.87	0.14	125,129,141,141	0
6	NAG	I	1	14/15	0.95	0.08	90,114,122,124	0
6	NAG	K	1	14/15	0.96	0.08	83,111,133,135	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

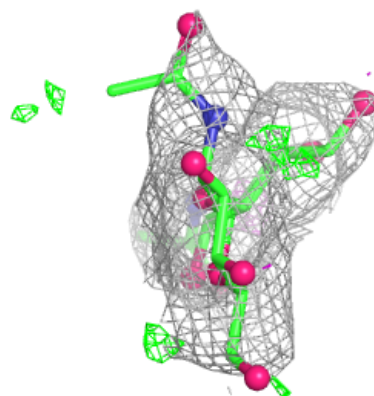
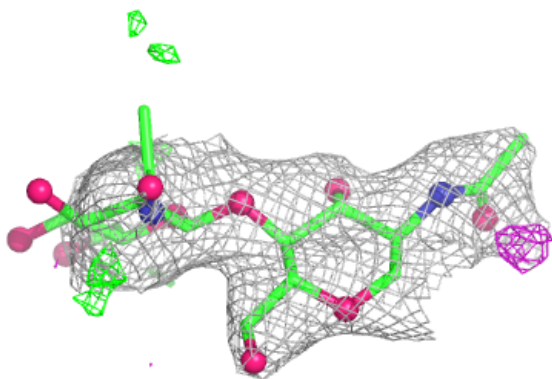
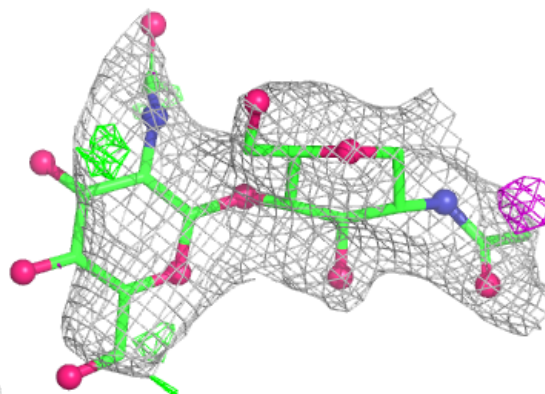


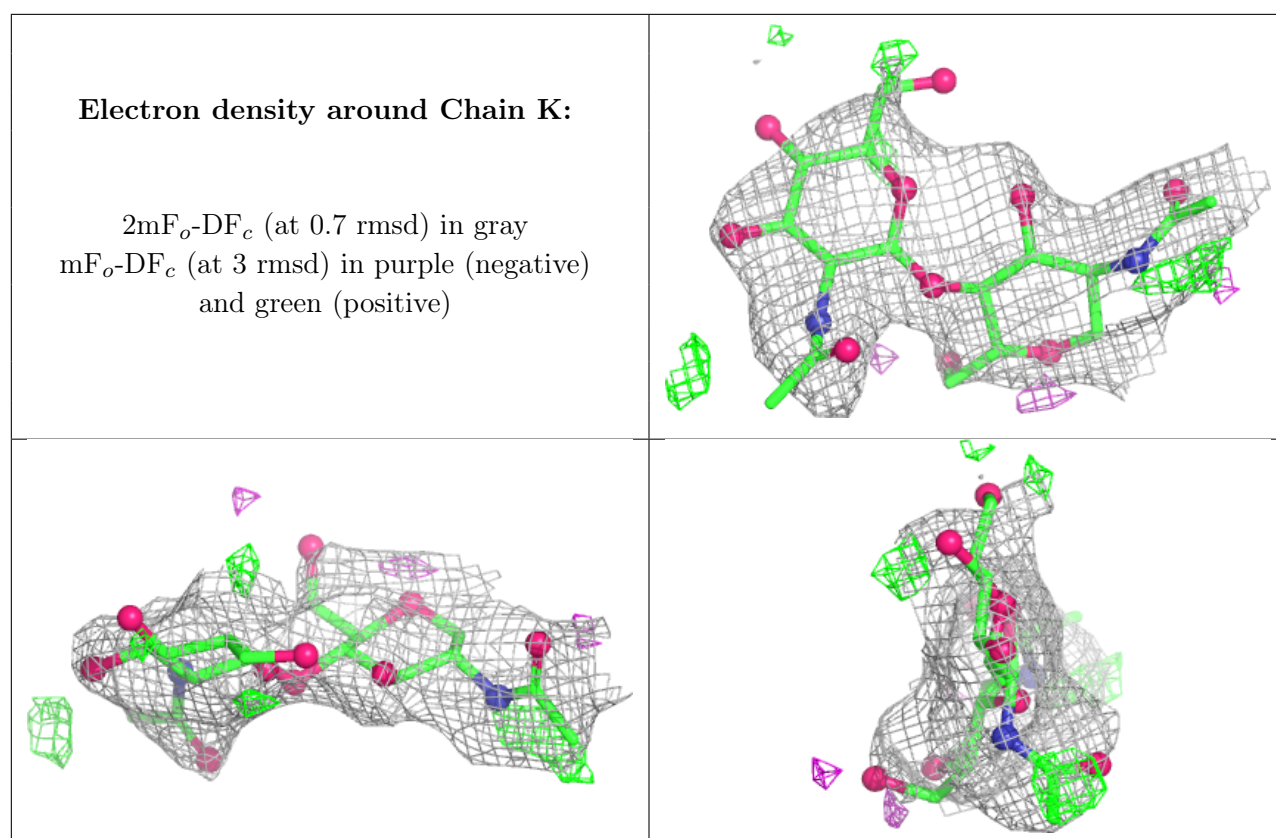
Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

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
11	NAG	D	3099	14/15	0.68	0.16	99,112,115,118	0
9	SO4	L	215	5/5	0.70	0.13	81,82,86,95	0
9	SO4	C	460	5/5	0.75	0.11	66,66,70,129	0
11	NAG	B	3099	14/15	0.80	0.12	108,118,123,123	0
9	SO4	D	472	5/5	0.83	0.13	62,66,72,133	0
9	SO4	A	461	5/5	0.83	0.15	48,49,63,70	0
9	SO4	C	459	5/5	0.90	0.12	56,71,86,96	0
9	SO4	A	460	5/5	0.90	0.12	57,67,89,90	0
8	GOL	A	459	6/6	0.90	0.13	34,51,67,74	0
8	GOL	A	458	6/6	0.92	0.13	44,55,69,77	0
8	GOL	C	458	6/6	0.95	0.11	43,61,65,68	0
7	CA	C	2004	1/1	0.97	0.04	58,58,58,58	0
7	CA	A	2004	1/1	0.98	0.03	35,35,35,35	0
10	MG	B	2001	1/1	0.98	0.03	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	A	2007	1/1	0.99	0.02	23,23,23,23	0
7	CA	B	2002	1/1	0.99	0.05	39,39,39,39	0
7	CA	A	2005	1/1	0.99	0.03	28,28,28,28	0
7	CA	C	2005	1/1	0.99	0.03	44,44,44,44	0
10	MG	D	2001	1/1	0.99	0.02	42,42,42,42	0
7	CA	C	2006	1/1	0.99	0.03	41,41,41,41	0
7	CA	C	2007	1/1	0.99	0.05	47,47,47,47	0
7	CA	B	2003	1/1	1.00	0.02	20,20,20,20	0
7	CA	D	2002	1/1	1.00	0.03	37,37,37,37	0
7	CA	D	2003	1/1	1.00	0.02	29,29,29,29	0
7	CA	A	2006	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.