



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 09:36 PM EDT

PDB ID : 5IRY  
Title : Crystal structure of human Desmocollin-1 ectodomain  
Authors : Brasch, J.; Harrison, O.J.; Shapiro, L.  
Deposited on : 2016-03-15  
Resolution : 3.10 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

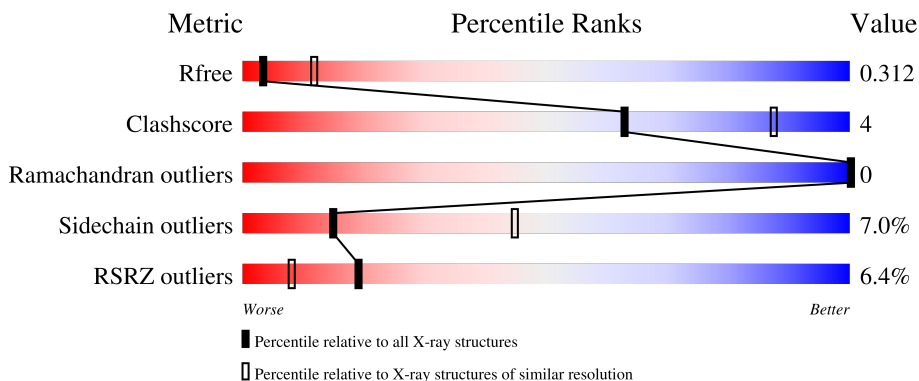
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	548	
1	B	548	
2	C	3	

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	CA	A	606	-	-	-	X
4	CA	B	602	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 17067 atoms, of which 8345 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.

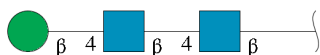
- Molecule 1 is a protein called Desmocollin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	539	8358	2679	4093	714	855	17	0	0	0
1	B	539	8359	2679	4094	714	855	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP Q08554
A	544	HIS	-	expression tag	UNP Q08554
A	545	HIS	-	expression tag	UNP Q08554
A	546	HIS	-	expression tag	UNP Q08554
A	547	HIS	-	expression tag	UNP Q08554
A	548	HIS	-	expression tag	UNP Q08554
B	543	HIS	-	expression tag	UNP Q08554
B	544	HIS	-	expression tag	UNP Q08554
B	545	HIS	-	expression tag	UNP Q08554
B	546	HIS	-	expression tag	UNP Q08554
B	547	HIS	-	expression tag	UNP Q08554
B	548	HIS	-	expression tag	UNP Q08554

- Molecule 2 is an oligosaccharide called beta-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
			Total	C	H	N	O			
2	C	3	78	22	39	2	15	0	0	0

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

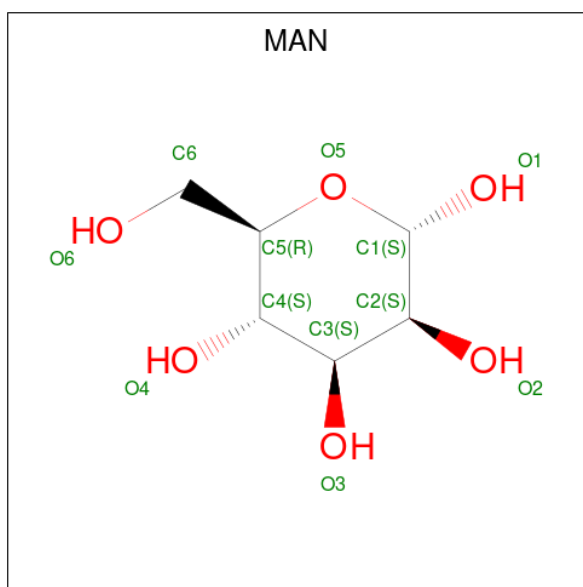


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	12	12	12	0	0
4	B	12	12	12	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	22	6	11	5	0	0
5	A	1	22	6	11	5	0	0
5	A	1	22	6	11	5	0	0
5	A	1	22	6	11	5	0	0
5	B	1	22	6	11	5	0	0
5	B	1	22	6	11	5	0	0
5	B	1	22	6	11	5	0	0
5	B	1	22	6	11	5	0	0
5	B	1	22	6	11	5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	10	2	6	2	0	0

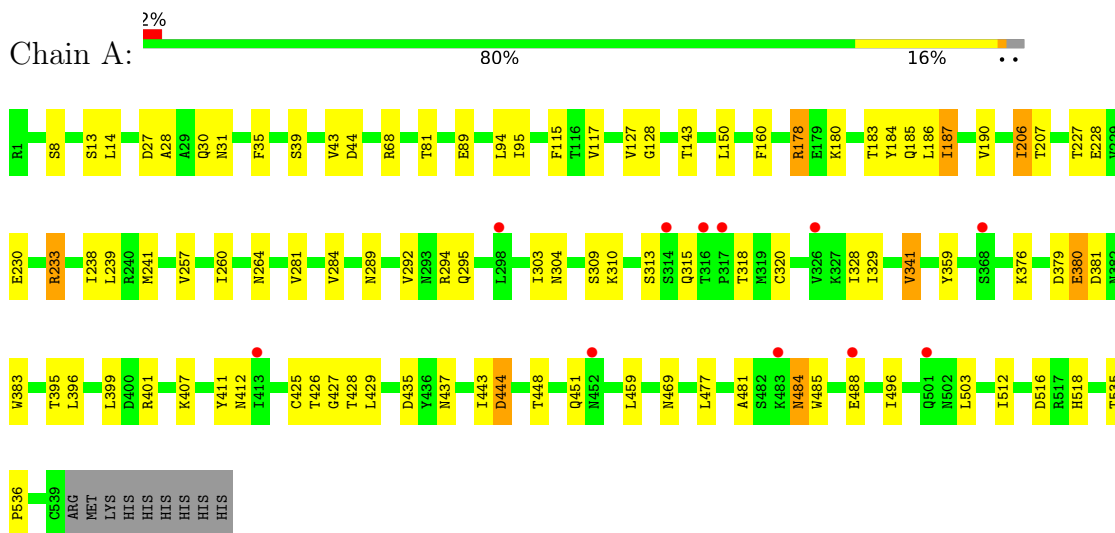
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0
7	B	3	Total O 3 3	0	0

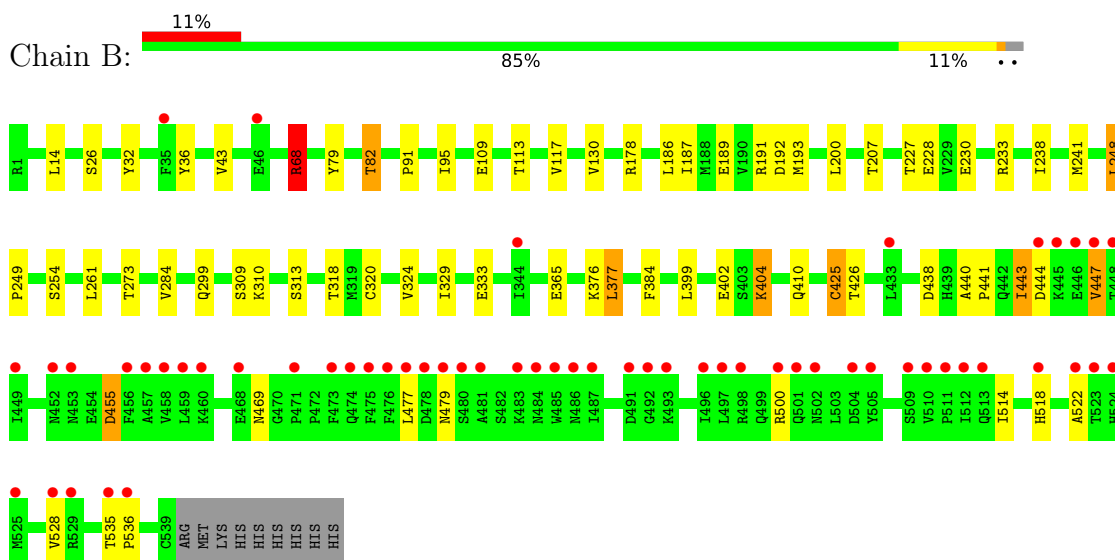
### 3 Residue-property plots [i](#)

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: Desmocollin-1

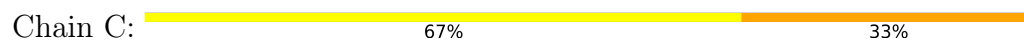


- Molecule 1: Desmocollin-1



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





MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.81Å 66.17Å 141.63Å 90.00° 127.15° 90.00°	Depositor
Resolution (Å)	19.99 – 3.10 112.89 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.99-3.10) 85.3 (112.89-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 3.07Å)	Xtrriage
Refinement program	PHENIX dev_1810	Depositor
R, $R_{free}$	0.249 , 0.302 0.261 , 0.312	Depositor DCC
$R_{free}$ test set	1422 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.2	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 101.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	187.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MAN, EDO, BMA, CA

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	0.31	0/4363	0.53	0/5946
1	B	0.29	0/4363	0.54	2/5946 (0.0%)
All	All	0.30	0/8726	0.54	2/11892 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	178	ARG	NE-CZ-NH1	6.28	123.44	120.30

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	4265	4093	4089	43	0
1	B	4265	4094	4092	30	0
2	C	39	39	34	4	0
3	A	14	14	13	1	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
5	A	44	44	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	55	55	50	0	0
6	A	4	6	6	0	0
7	A	9	0	0	1	0
7	B	3	0	0	0	0
All	All	8722	8345	8324	74	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 4.

All (74) 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:B:402:GLU:OE2	1:B:438:ASP:OD1	2.04	0.74
1:B:425:CYS:SG	1:B:426:THR:N	2.62	0.73
2:C:1:NAG:O6	2:C:2:NAG:N2	2.23	0.70
1:B:313:SER:O	1:B:318:THR:OG1	2.09	0.69
1:A:412:ASN:OD1	2:C:1:NAG:N2	2.26	0.69
1:A:380:GLU:N	1:A:380:GLU:OE2	2.28	0.66
1:A:35:PHE:N	1:A:81:THR:O	2.30	0.63
1:B:333:GLU:N	1:B:365:GLU:OE2	2.31	0.62
1:A:294:ARG:O	1:A:295:GLN:NE2	2.34	0.61
1:A:178:ARG:NH2	7:A:701:HOH:O	2.35	0.59
1:B:376:LYS:NZ	1:B:384:PHE:O	2.34	0.59
1:A:412:ASN:OD1	2:C:1:NAG:C7	2.54	0.56
1:B:376:LYS:HG2	1:B:377:LEU:N	2.21	0.55
1:A:313:SER:O	1:A:318:THR:OG1	2.22	0.55
1:B:68:ARG:HH11	1:B:68:ARG:CG	2.20	0.55
1:A:31:ASN:OD1	3:A:604:NAG:O5	2.25	0.54
1:B:455:ASP:OD1	1:B:455:ASP:N	2.38	0.54
1:A:160:PHE:HE2	1:A:184:TYR:HD1	1.55	0.53
1:A:230:GLU:HA	1:A:329:ILE:HG13	1.91	0.52
1:B:192:ASP:OD1	1:B:200:LEU:N	2.43	0.52
1:B:109:GLU:OE1	1:B:109:GLU:N	2.40	0.51
1:B:189:GLU:OE1	1:B:191:ARG:NH1	2.43	0.51
1:B:230:GLU:HA	1:B:329:ILE:HG13	1.92	0.51
1:A:481:ALA:HB1	1:A:485:TRP:HB2	1.93	0.50
1:B:227:THR:OG1	1:B:228:GLU:N	2.45	0.50
1:A:43:VAL:HG23	1:A:44:ASP:H	1.76	0.50
1:A:484:ASN:N	1:A:484:ASN:OD1	2.44	0.50
1:B:26:SER:N	1:B:36:TYR:OH	2.45	0.49
1:A:150:LEU:HB3	1:A:187:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HG21	1:A:264:ASN:HB2	1.95	0.48
1:A:381:ASP:HB3	1:A:383:TRP:NE1	2.29	0.47
1:A:379:ASP:OD2	1:A:411:TYR:OH	2.31	0.47
1:B:443:ILE:HD11	1:B:514:ILE:CD1	2.45	0.47
1:A:443:ILE:HD11	1:A:459:LEU:HB2	1.97	0.47
1:B:535:THR:HB	1:B:536:PRO:CD	2.46	0.46
1:A:407:LYS:HD2	2:C:1:NAG:H81	1.98	0.46
1:B:404:LYS:H	1:B:404:LYS:CD	2.28	0.46
1:B:227:THR:HG21	1:B:238:ILE:CG2	2.46	0.46
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.81	0.45
1:B:440:ALA:HB3	1:B:522:ALA:HB2	1.99	0.45
1:A:341:VAL:HG12	1:A:428:THR:HB	1.97	0.45
1:A:451:GLN:NE2	1:A:503:LEU:HD13	2.31	0.45
1:A:230:GLU:HG2	1:A:233:ARG:HG3	1.98	0.44
1:A:535:THR:HB	1:A:536:PRO:CD	2.47	0.44
1:A:315:GLN:OE1	1:A:315:GLN:N	2.41	0.44
1:B:447:VAL:HG22	1:B:528:VAL:HA	1.98	0.44
1:B:469:ASN:OD1	1:B:518:HIS:NE2	2.51	0.44
1:A:426:THR:HG21	5:A:618:MAN:H5	1.98	0.44
1:A:401:ARG:CZ	1:A:435:ASP:OD2	2.64	0.44
1:A:185:GLN:HG2	1:A:207:THR:HG22	1.99	0.43
1:A:289:ASN:O	1:A:292:VAL:HG12	2.19	0.43
1:A:186:LEU:HB2	1:A:206:ILE:HG23	2.00	0.43
1:A:227:THR:OG1	1:A:228:GLU:N	2.51	0.43
1:A:115:PHE:CE1	1:A:128:GLY:HA3	2.54	0.42
1:A:444:ASP:N	1:A:444:ASP:OD1	2.53	0.42
1:A:257:VAL:N	1:A:303:ILE:O	2.52	0.42
1:A:469:ASN:OD1	1:A:518:HIS:NE2	2.50	0.42
1:B:68:ARG:CG	1:B:68:ARG:NH1	2.82	0.42
1:B:32:TYR:HE1	1:B:82:THR:HG21	1.85	0.42
1:B:309:SER:O	1:B:310:LYS:HB3	2.20	0.42
1:A:27:ASP:OD1	1:A:28:ALA:N	2.53	0.41
1:A:238:ILE:HD11	1:A:284:VAL:HG22	2.03	0.41
1:A:309:SER:O	1:A:310:LYS:HB3	2.20	0.41
1:A:437:ASN:ND2	1:A:516:ASP:OD2	2.49	0.41
1:A:381:ASP:HB3	1:A:383:TRP:HE1	1.85	0.41
1:A:359:TYR:CE2	1:A:427:GLY:HA3	2.55	0.41
1:B:261:LEU:N	1:B:299:GLN:O	2.41	0.41
1:B:440:ALA:HB1	1:B:441:PRO:HD2	2.02	0.41
1:B:79:TYR:CE1	1:B:91:PRO:HB3	2.55	0.41
1:B:443:ILE:HG22	1:B:444:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD23	1:B:249:PRO:HD2	2.04	0.40
1:A:488:GLU:HB2	1:A:496:ILE:HD11	2.03	0.40
1:A:303:ILE:CG2	1:A:304:ASN:N	2.84	0.40
1:A:230:GLU:HG2	1:A:233:ARG:CG	2.51	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 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	537/548 (98%)	485 (90%)	52 (10%)	0	100	100
1	B	537/548 (98%)	486 (90%)	51 (10%)	0	100	100
All	All	1074/1096 (98%)	971 (90%)	103 (10%)	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 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	485/494 (98%)	448 (92%)	37 (8%)	13	41
1	B	485/494 (98%)	454 (94%)	31 (6%)	17	48
All	All	970/988 (98%)	902 (93%)	68 (7%)	15	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	13	SER
1	A	14	LEU
1	A	30	GLN
1	A	39	SER
1	A	68	ARG
1	A	89	GLU
1	A	94	LEU
1	A	95	ILE
1	A	117	VAL
1	A	127	VAL
1	A	143	THR
1	A	178	ARG
1	A	180	LYS
1	A	183	THR
1	A	187	ILE
1	A	190	VAL
1	A	206	ILE
1	A	233	ARG
1	A	239	LEU
1	A	241	MET
1	A	281	VAL
1	A	320	CYS
1	A	328	ILE
1	A	341	VAL
1	A	376	LYS
1	A	380	GLU
1	A	395	THR
1	A	396	LEU
1	A	399	LEU
1	A	425	CYS
1	A	429	LEU
1	A	444	ASP
1	A	448	THR
1	A	477	LEU
1	A	484	ASN
1	A	512	ILE
1	B	14	LEU
1	B	43	VAL
1	B	68	ARG
1	B	82	THR
1	B	95	ILE

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Mol	Chain	Res	Type
1	B	113	THR
1	B	117	VAL
1	B	130	VAL
1	B	186	LEU
1	B	187	ILE
1	B	193	MET
1	B	207	THR
1	B	233	ARG
1	B	241	MET
1	B	248	LEU
1	B	254	SER
1	B	273	THR
1	B	284	VAL
1	B	320	CYS
1	B	324	VAL
1	B	377	LEU
1	B	399	LEU
1	B	404	LYS
1	B	410	GLN
1	B	425	CYS
1	B	443	ILE
1	B	447	VAL
1	B	455	ASP
1	B	477	LEU
1	B	479	ASN
1	B	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

3 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	C	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.61	0
2	BMA	C	3	2	11,11,12	0.88	1 (9%)	15,15,17	0.95	1 (6%)

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	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.86	1.39	1.43
2	C	3	BMA	C1-C2	2.35	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	3.34	116.72	112.19
2	C	3	BMA	O2-C2-C3	-2.01	106.12	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

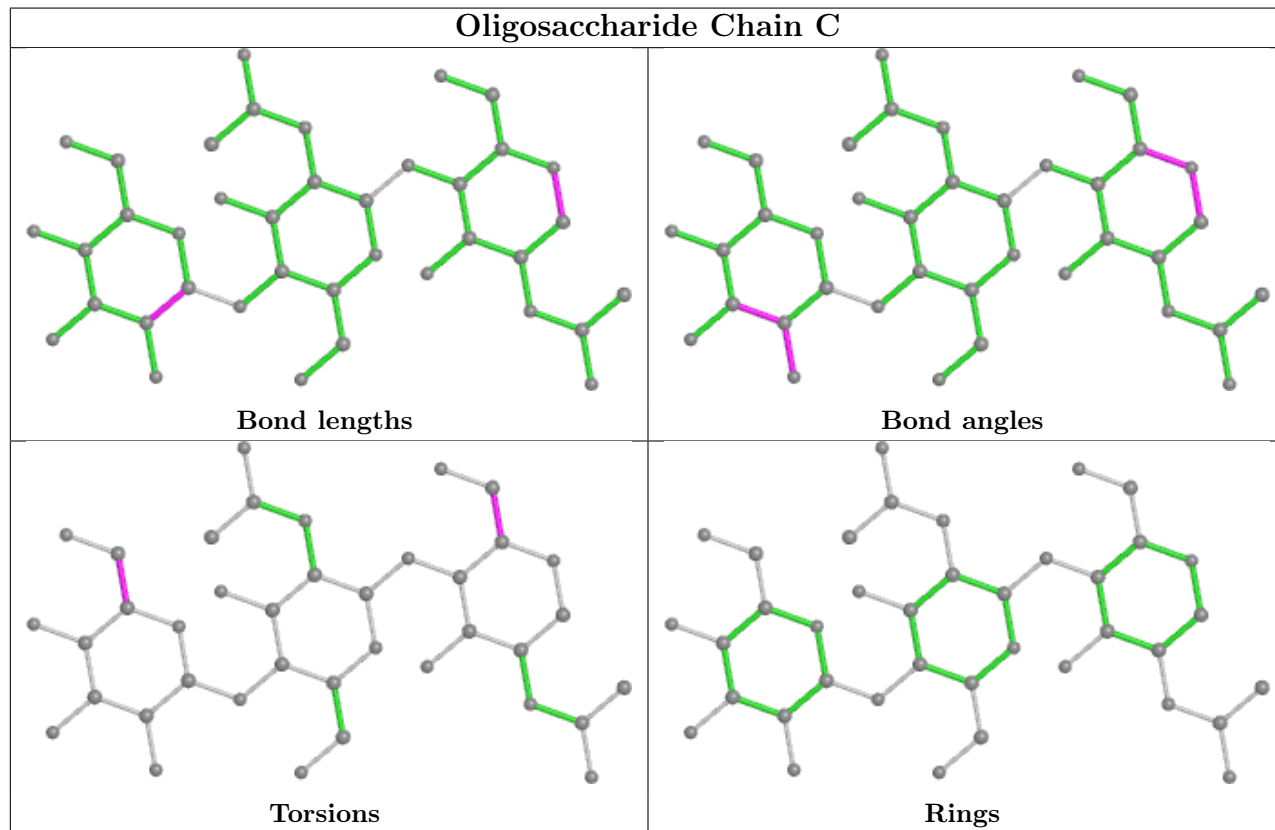
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	1	NAG	4	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 35 ligands modelled in this entry, 24 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
5	MAN	A	619	1	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
6	EDO	A	621	-	3,3,3	0.48	0	2,2,2	0.25	0
5	MAN	A	617	1	11,11,12	1.15	1 (9%)	15,15,17	1.59	3 (20%)
3	NAG	A	604	1	14,14,15	0.86	1 (7%)	17,19,21	0.94	1 (5%)
5	MAN	B	616	1	11,11,12	0.81	0	15,15,17	1.18	2 (13%)
5	MAN	B	615	1	11,11,12	0.70	0	15,15,17	1.23	2 (13%)
5	MAN	B	617	1	11,11,12	0.96	1 (9%)	15,15,17	1.13	1 (6%)
5	MAN	A	620	1	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
5	MAN	B	613	1	11,11,12	0.76	1 (9%)	15,15,17	0.94	1 (6%)
5	MAN	B	614	1	11,11,12	0.67	0	15,15,17	1.43	2 (13%)
5	MAN	A	618	1	11,11,12	0.85	1 (9%)	15,15,17	1.73	2 (13%)

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	MAN	A	619	1	-	2/2/19/22	0/1/1/1
6	EDO	A	621	-	-	0/1/1/1	-
5	MAN	A	617	1	-	2/2/19/22	0/1/1/1
3	NAG	A	604	1	-	4/6/23/26	0/1/1/1
5	MAN	B	616	1	-	2/2/19/22	0/1/1/1
5	MAN	B	615	1	-	0/2/19/22	0/1/1/1
5	MAN	B	617	1	-	0/2/19/22	0/1/1/1
5	MAN	A	620	1	-	0/2/19/22	0/1/1/1
5	MAN	B	613	1	-	0/2/19/22	0/1/1/1
5	MAN	B	614	1	-	0/2/19/22	0/1/1/1
5	MAN	A	618	1	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	NAG	O5-C1	-3.13	1.38	1.43
5	A	617	MAN	O5-C1	-2.48	1.39	1.43
5	A	618	MAN	O5-C5	2.28	1.48	1.43
5	B	613	MAN	O5-C1	-2.28	1.40	1.43
5	B	617	MAN	O5-C1	-2.15	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	618	MAN	C1-O5-C5	5.26	119.32	112.19
5	B	614	MAN	C1-O5-C5	4.52	118.31	112.19
5	A	617	MAN	O5-C1-C2	3.88	116.76	110.77
5	A	617	MAN	C1-O5-C5	3.47	116.89	112.19
3	A	604	NAG	C1-O5-C5	3.23	116.57	112.19
5	A	618	MAN	O5-C1-C2	3.15	115.64	110.77
5	A	619	MAN	C1-O5-C5	2.99	116.25	112.19
5	B	615	MAN	C1-O5-C5	2.97	116.21	112.19
5	A	620	MAN	C1-O5-C5	2.84	116.04	112.19
5	B	616	MAN	C1-O5-C5	2.68	115.82	112.19
5	B	613	MAN	O2-C2-C3	-2.36	105.40	110.14
5	B	615	MAN	O2-C2-C3	-2.33	105.48	110.14
5	A	619	MAN	O2-C2-C3	-2.31	105.52	110.14
5	B	617	MAN	O2-C2-C3	-2.31	105.52	110.14
5	B	614	MAN	O2-C2-C3	-2.28	105.56	110.14
5	B	616	MAN	O2-C2-C3	-2.23	105.68	110.14
5	A	620	MAN	O2-C2-C3	-2.19	105.75	110.14
5	A	617	MAN	C1-C2-C3	-2.18	106.99	109.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	616	MAN	O5-C5-C6-O6
5	A	619	MAN	O5-C5-C6-O6
5	B	616	MAN	C4-C5-C6-O6
5	A	619	MAN	C4-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
5	A	617	MAN	O5-C5-C6-O6
5	A	617	MAN	C4-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
3	A	604	NAG	C1-C2-N2-C7
3	A	604	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	NAG	1	0
5	A	618	MAN	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	539/548 (98%)	-0.00	11 (2%) 65 44	116, 152, 214, 303	0
1	B	539/548 (98%)	0.59	58 (10%) 5 2	108, 159, 303, 387	0
All	All	1078/1096 (98%)	0.29	69 (6%) 19 8	108, 155, 291, 387	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	LEU	19.3
1	B	480	SER	18.8
1	B	478	ASP	11.6
1	B	512	ILE	11.0
1	B	447	VAL	10.4
1	B	448	THR	9.4
1	B	493	LYS	8.9
1	B	479	ASN	8.0
1	B	492	GLY	7.1
1	B	525	MET	6.6
1	B	453	ASN	6.5
1	B	474	GLN	6.2
1	B	444	ASP	5.9
1	B	485	TRP	5.6
1	B	475	PHE	5.6
1	B	483	LYS	5.5
1	B	487	ILE	5.4
1	B	513	GLN	5.1
1	B	500	ARG	4.8
1	B	511	PRO	4.8
1	A	317	PRO	4.6
1	B	476	PHE	4.6
1	B	471	PRO	4.5
1	B	504	ASP	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	445	LYS	4.3
1	B	522	ALA	4.2
1	B	528	VAL	4.1
1	B	491	ASP	3.9
1	B	497	LEU	3.9
1	B	484	ASN	3.9
1	B	459	LEU	3.7
1	B	481	ALA	3.7
1	B	498	ARG	3.7
1	B	473	PHE	3.7
1	B	536	PRO	3.7
1	B	486	ASN	3.7
1	B	456	PHE	3.7
1	A	316	THR	3.6
1	B	523	THR	3.6
1	B	446	GLU	3.3
1	A	452	ASN	3.3
1	B	496	ILE	3.3
1	A	501	GLN	3.2
1	B	510	VAL	3.1
1	B	524	HIS	3.1
1	A	314	SER	3.0
1	B	501	GLN	3.0
1	B	449	ILE	2.9
1	B	35	PHE	2.8
1	B	452	ASN	2.7
1	B	460	LYS	2.7
1	A	326	VAL	2.7
1	A	368	SER	2.6
1	B	509	SER	2.6
1	B	505	TYR	2.5
1	B	458	VAL	2.5
1	B	457	ALA	2.5
1	B	535	THR	2.4
1	B	433	LEU	2.4
1	B	344	ILE	2.4
1	B	529	ARG	2.3
1	A	413	ILE	2.3
1	B	502	ASN	2.2
1	B	468	GLU	2.2
1	B	46	GLU	2.2
1	B	518	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	298	LEU	2.0
1	A	488	GLU	2.0
1	A	483	LYS	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.

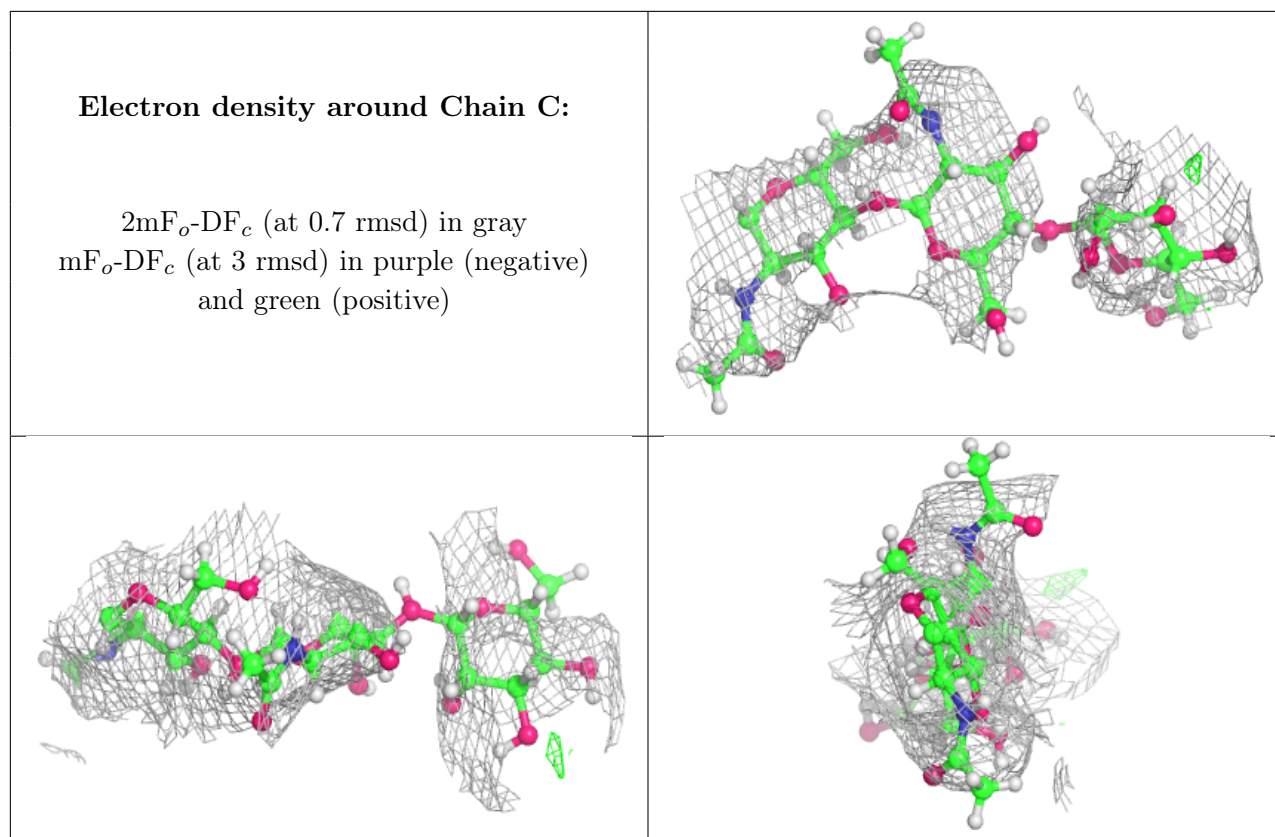
## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	BMA	C	3	11/12	0.32	0.30	224,245,286,294	0
2	NAG	C	2	14/15	0.76	0.30	228,244,283,293	0
2	NAG	C	1	14/15	0.82	0.21	188,225,258,281	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.





## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	CA	A	606	1/1	0.10	0.46	327,327,327,327	0
4	CA	B	607	1/1	0.19	0.16	256,256,256,256	0
4	CA	A	616	1/1	0.41	0.23	132,132,132,132	0
4	CA	B	601	1/1	0.51	0.21	171,171,171,171	0
4	CA	A	605	1/1	0.54	0.34	175,175,175,175	0
4	CA	A	608	1/1	0.55	0.14	175,175,175,175	0
4	CA	B	603	1/1	0.59	0.29	139,139,139,139	0
3	NAG	A	604	14/15	0.59	0.31	184,216,251,259	0
4	CA	A	615	1/1	0.60	0.18	143,143,143,143	0
5	MAN	B	615	11/12	0.66	0.19	154,189,222,228	0
4	CA	A	613	1/1	0.68	0.11	190,190,190,190	0
4	CA	B	602	1/1	0.69	0.43	252,252,252,252	0
4	CA	B	609	1/1	0.69	0.24	154,154,154,154	0
4	CA	A	611	1/1	0.69	0.25	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	A	612	1/1	0.70	0.17	194,194,194,194	0
6	EDO	A	621	4/4	0.73	0.34	153,184,190,199	0
5	MAN	B	617	11/12	0.76	0.31	178,204,229,237	0
4	CA	B	604	1/1	0.78	0.26	147,147,147,147	0
5	MAN	A	618	11/12	0.81	0.16	162,195,224,242	0
4	CA	B	608	1/1	0.85	0.13	254,254,254,254	0
4	CA	B	610	1/1	0.85	0.26	174,174,174,174	0
4	CA	B	611	1/1	0.86	0.19	147,147,147,147	0
4	CA	B	612	1/1	0.86	0.21	171,171,171,171	0
4	CA	A	610	1/1	0.86	0.31	162,162,162,162	0
5	MAN	A	620	11/12	0.88	0.22	144,174,215,231	0
5	MAN	A	619	11/12	0.89	0.22	136,174,189,227	0
4	CA	B	605	1/1	0.90	0.22	144,144,144,144	0
5	MAN	B	613	11/12	0.91	0.23	140,165,195,198	0
5	MAN	B	616	11/12	0.92	0.16	135,163,184,196	0
5	MAN	A	617	11/12	0.92	0.17	153,183,203,220	0
4	CA	B	606	1/1	0.92	0.10	236,236,236,236	0
4	CA	A	614	1/1	0.93	0.25	128,128,128,128	0
4	CA	A	609	1/1	0.94	0.23	168,168,168,168	0
5	MAN	B	614	11/12	0.94	0.20	146,176,197,222	0
4	CA	A	607	1/1	0.99	0.29	129,129,129,129	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.