



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:20 PM BST

PDB ID : 6NWX  
Title : Structure of mouse GILT, an enzyme involved in antigen processing  
Authors : Li, Y.  
Deposited on : 2019-02-07  
Resolution : 2.00 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.

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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 : 2.13.1  
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) : 2.13.1



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	C	3	-	-	-	X
2	BMA	D	3	-	-	-	X
3	NAG	A	304	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3653 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 Gamma-interferon-inducible lysosomal thiol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	189	1530	979	240	289	22	0	8	0
1	B	193	1562	999	247	291	25	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	-	expression tag	UNP Q9ESY9
B	48	ALA	-	expression tag	UNP Q9ESY9

- 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.



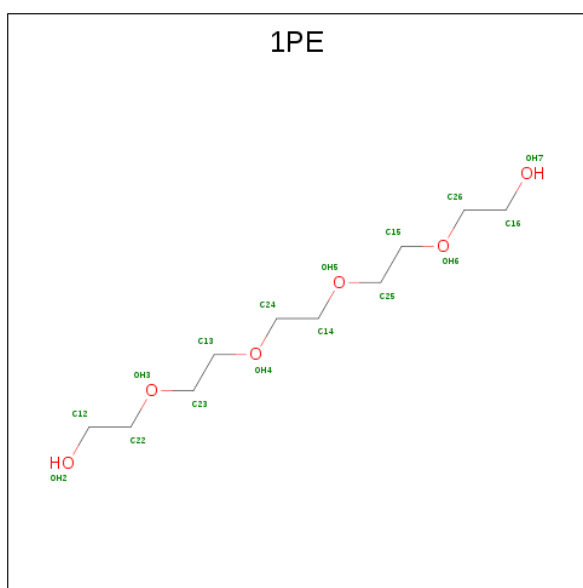
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



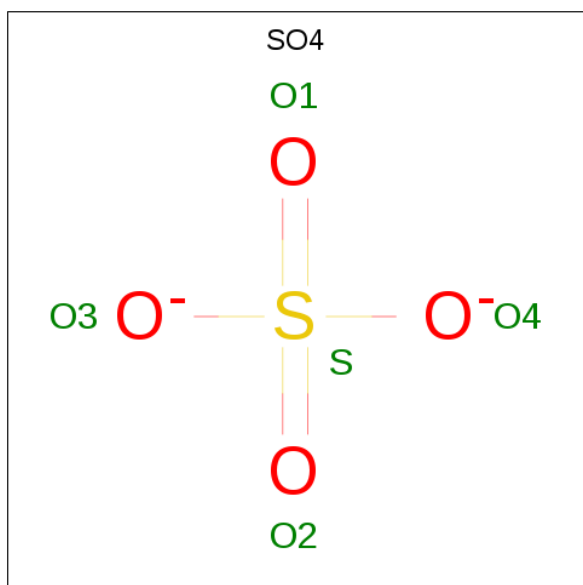
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

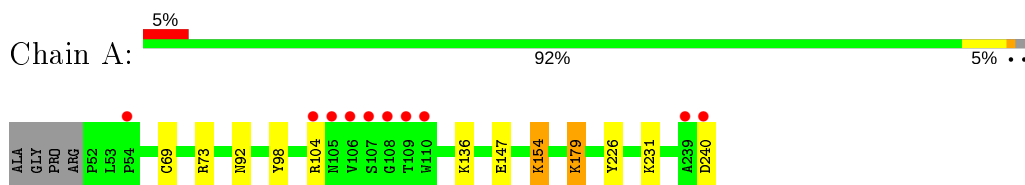
- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	182	Total 182	O 182	0	0
6	B	174	Total 174	O 174	0	0

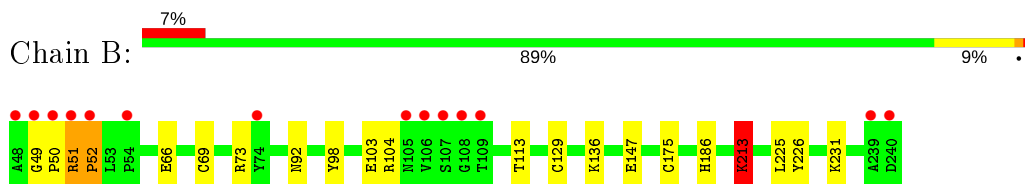
### 3 Residue-property plots [i](#)

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.

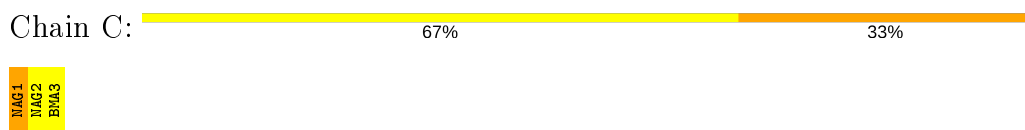
- Molecule 1: Gamma-interferon-inducible lysosomal thiol reductase



- Molecule 1: Gamma-interferon-inducible lysosomal thiol reductase



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



- Molecule 2: beta-D-mannopyranose-(1-4)-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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.44Å 44.72Å 78.17Å 90.00° 111.07° 90.00°	Depositor
Resolution (Å)	29.39 – 2.00 29.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.39-2.00) 92.4 (29.39-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.168 , 0.202 0.168 , 0.204	Depositor DCC
$R_{free}$ test set	1867 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% 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: BMA, 1PE, SO4, 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	0/1588	0.42	0/2161
1	B	0.28	0/1627	0.48	2/2214 (0.1%)
All	All	0.27	0/3215	0.45	2/4375 (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	213	LYS	CD-CE-NZ	-5.95	98.03	111.70
1	B	213	LYS	CB-CG-CD	-5.02	98.55	111.60

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	1530	0	1512	9	0
1	B	1562	0	1551	15	0
2	C	39	0	34	2	0
2	D	39	0	34	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	32	0	44	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	44	3	0
5	A	25	0	0	1	0
5	B	10	0	0	0	0
6	A	182	0	0	4	0
6	B	174	0	0	1	0
All	All	3653	0	3245	30	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.

All (30) 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:213:LYS:H	1:B:213:LYS:HD2	1.05	1.13
1:B:213:LYS:HD2	1:B:213:LYS:N	1.75	0.96
1:A:104:ARG:NH2	6:A:401:HOH:O	2.18	0.76
1:A:136:LYS:HD3	4:A:306:1PE:H241	1.75	0.68
1:B:129:CYS:SG	1:B:175[C]:CYS:HB3	2.34	0.68
1:A:136:LYS:HE2	4:A:306:1PE:H261	1.85	0.59
1:B:103:GLU:OE2	1:B:186:HIS:ND1	2.30	0.56
4:A:306:1PE:H232	2:C:1:NAG:H82	1.88	0.55
1:A:92:ASN:OD1	1:A:136:LYS:NZ	2.42	0.53
1:B:226:TYR:O	1:B:231:LYS:NZ	2.43	0.51
1:B:50:PRO:O	1:B:51:ARG:HB2	2.10	0.50
1:A:179:LYS:HE3	6:A:505:HOH:O	2.12	0.49
1:B:49:GLY:HA2	1:B:50:PRO:C	2.33	0.48
4:A:306:1PE:H251	6:A:471:HOH:O	2.14	0.48
4:B:306:1PE:OH2	6:B:401:HOH:O	2.19	0.48
1:B:92:ASN:OD1	1:B:136:LYS:NZ	2.46	0.48
1:B:50:PRO:O	1:B:52:PRO:HD3	2.13	0.47
1:A:226:TYR:O	1:A:231:LYS:NZ	2.47	0.47
1:B:136:LYS:HD3	4:B:305:1PE:H142	1.97	0.47
1:B:73:ARG:HG2	1:B:147:GLU:OE1	2.15	0.47
4:B:306:1PE:H221	4:B:306:1PE:H131	1.65	0.47
1:B:66:GLU:HG3	1:B:69[B]:CYS:HB3	1.97	0.46
1:B:104:ARG:NH1	1:B:113:THR:OG1	2.50	0.44
1:B:103:GLU:O	1:B:104:ARG:HG3	2.20	0.42
5:A:310:SO4:O1	6:A:402:HOH:O	2.21	0.42
1:A:73:ARG:HG2	1:A:147:GLU:OE1	2.19	0.41
1:A:104:ARG:NE	1:A:104:ARG:HA	2.36	0.41
1:A:154:LYS:O	1:A:154:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:306:1PE:H222	2:C:1:NAG:H82	2.02	0.41
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.97	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	195/193 (101%)	192 (98%)	2 (1%)	1 (0%)	29	23
1	B	201/193 (104%)	194 (96%)	4 (2%)	3 (2%)	10	4
All	All	396/386 (103%)	386 (98%)	6 (2%)	4 (1%)	14	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ARG
1	B	98	TYR
1	A	98	TYR
1	B	52	PRO

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/173 (104%)	174 (97%)	5 (3%)	43	44
1	B	183/173 (106%)	182 (100%)	1 (0%)	88	92
All	All	362/346 (105%)	356 (98%)	6 (2%)	65	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69[A]	CYS
1	A	69[B]	CYS
1	A	154	LYS
1	A	179	LYS
1	A	240	ASP
1	B	213	LYS

Some 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](#)

6 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	2.09	4 (28%)	17,19,21	1.07	0
2	NAG	C	2	2	14,14,15	2.17	5 (35%)	17,19,21	1.09	2 (11%)
2	BMA	C	3	2	11,11,12	1.26	1 (9%)	15,15,17	1.13	1 (6%)
2	NAG	D	1	1,2	14,14,15	2.13	3 (21%)	17,19,21	1.28	2 (11%)
2	NAG	D	2	2	14,14,15	2.08	3 (21%)	17,19,21	1.88	5 (29%)
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.78	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	4.79	1.51	1.43
2	D	1	NAG	O5-C1	4.66	1.51	1.43
2	C	1	NAG	O5-C1	4.52	1.50	1.43
2	D	1	NAG	C7-N2	4.35	1.49	1.34
2	D	2	NAG	O5-C1	4.31	1.50	1.43
2	C	1	NAG	C7-N2	4.30	1.49	1.34
2	D	2	NAG	C7-N2	4.29	1.49	1.34
2	C	2	NAG	C7-N2	4.28	1.49	1.34
2	C	3	BMA	C1-C2	3.37	1.59	1.52
2	D	1	NAG	C2-N2	2.96	1.51	1.46
2	D	2	NAG	C2-N2	2.92	1.51	1.46
2	C	1	NAG	C2-N2	2.87	1.51	1.46
2	C	2	NAG	C2-N2	2.85	1.51	1.46
2	C	2	NAG	C3-C2	-2.30	1.47	1.52
2	C	1	NAG	C3-C2	-2.18	1.47	1.52
2	C	2	NAG	O5-C5	2.01	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	4.48	117.58	111.02
2	C	3	BMA	O2-C2-C3	-2.90	104.34	110.14
2	D	2	NAG	C3-C4-C5	2.85	115.32	110.24
2	D	2	NAG	O4-C4-C3	-2.77	103.96	110.35
2	D	1	NAG	C8-C7-N2	2.53	120.39	116.10
2	D	1	NAG	C4-C3-C2	2.31	114.40	111.02
2	C	2	NAG	C8-C7-N2	2.26	119.92	116.10
2	D	2	NAG	C8-C7-N2	2.25	119.91	116.10
2	C	2	NAG	C2-N2-C7	-2.23	119.72	122.90
2	D	2	NAG	C2-N2-C7	-2.03	120.01	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

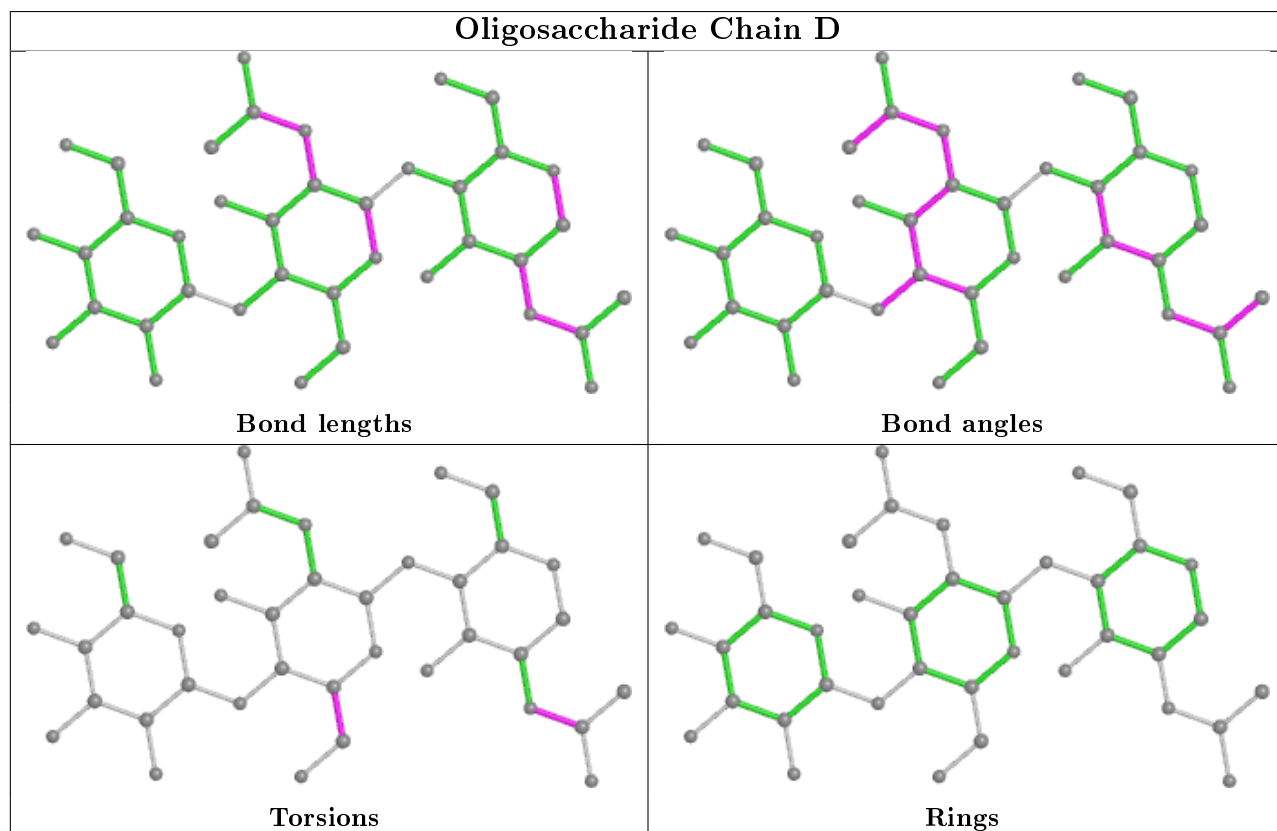
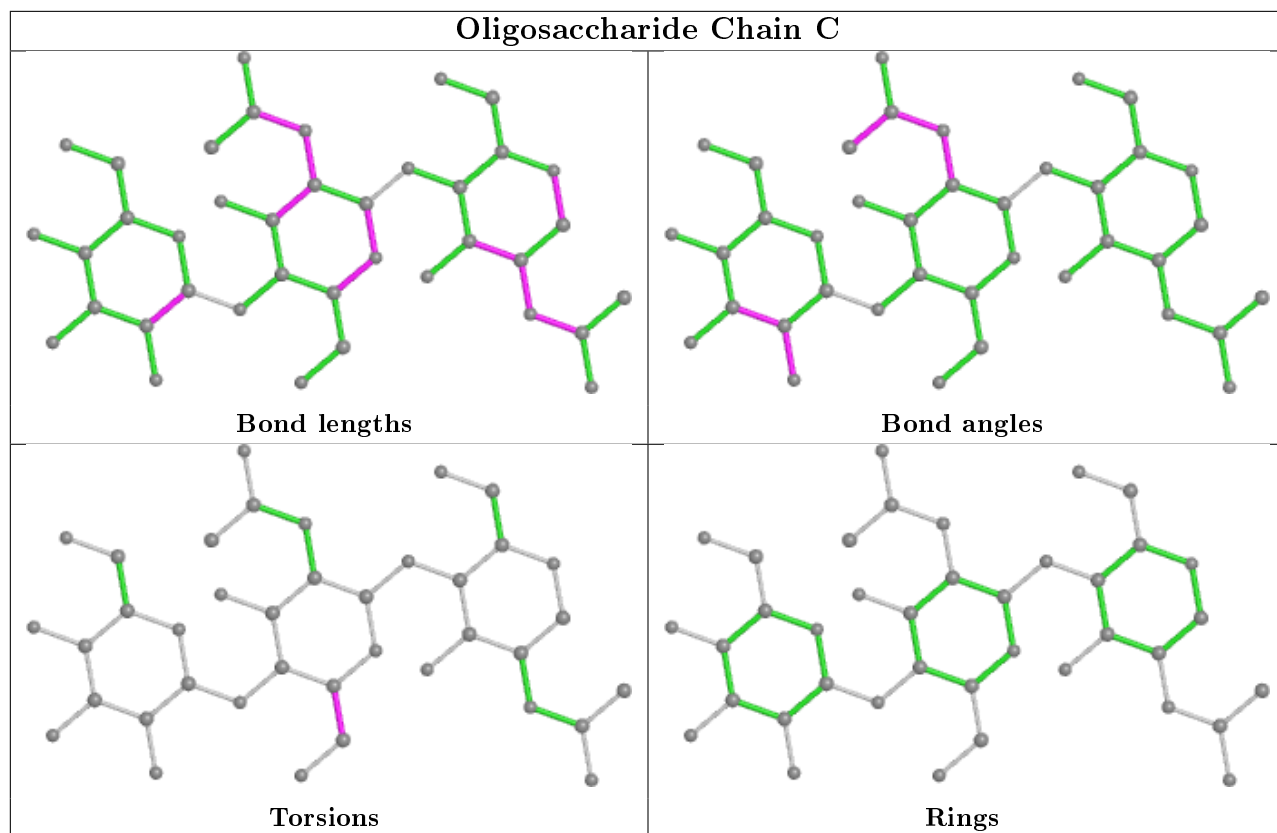
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	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

13 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
5	SO4	A	311	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	309	-	4,4,4	0.14	0	6,6,6	0.06	0
4	1PE	A	306	-	15,15,15	0.52	0	14,14,14	0.27	0
4	1PE	B	306	-	15,15,15	0.53	0	14,14,14	0.28	0
5	SO4	A	310	-	4,4,4	0.13	0	6,6,6	0.05	0
4	1PE	B	305	-	15,15,15	0.53	0	14,14,14	0.26	0
5	SO4	B	307	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	307	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	308	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	308	-	4,4,4	0.15	0	6,6,6	0.05	0
3	NAG	B	304	1	14,14,15	2.18	3 (21%)	17,19,21	1.37	3 (17%)
3	NAG	A	304	1	14,14,15	2.21	5 (35%)	17,19,21	1.67	5 (29%)
4	1PE	A	305	-	15,15,15	0.53	0	14,14,14	0.20	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
4	1PE	A	306	-	-	11/13/13/13	-
4	1PE	B	306	-	-	6/13/13/13	-
4	1PE	B	305	-	-	5/13/13/13	-
3	NAG	B	304	1	-	4/6/23/26	0/1/1/1
3	NAG	A	304	1	-	1/6/23/26	0/1/1/1
4	1PE	A	305	-	-	6/13/13/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	304	NAG	O5-C1	5.02	1.51	1.43
3	A	304	NAG	O5-C1	4.84	1.51	1.43
3	A	304	NAG	C7-N2	4.33	1.49	1.34
3	B	304	NAG	C7-N2	4.30	1.49	1.34
3	B	304	NAG	C2-N2	3.00	1.51	1.46
3	A	304	NAG	C2-N2	2.91	1.51	1.46
3	A	304	NAG	O5-C5	2.39	1.48	1.43
3	A	304	NAG	C3-C2	-2.11	1.48	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	NAG	C3-C4-C5	3.21	115.97	110.24
3	A	304	NAG	C2-N2-C7	-2.91	118.77	122.90
3	A	304	NAG	C8-C7-N2	2.39	120.15	116.10
3	B	304	NAG	C4-C3-C2	2.23	114.29	111.02
3	B	304	NAG	C8-C7-N2	2.18	119.78	116.10
3	A	304	NAG	O5-C5-C4	2.12	115.99	110.83
3	A	304	NAG	C4-C3-C2	2.06	114.04	111.02
3	B	304	NAG	C2-N2-C7	-2.06	119.97	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	304	NAG	O5-C5-C6-O6
4	A	306	1PE	OH5-C14-C24-OH4
4	A	305	1PE	OH4-C13-C23-OH3
4	A	305	1PE	OH5-C14-C24-OH4
3	B	304	NAG	C4-C5-C6-O6
3	B	304	NAG	C8-C7-N2-C2
3	B	304	NAG	O7-C7-N2-C2
4	A	306	1PE	OH4-C13-C23-OH3
4	B	306	1PE	OH5-C14-C24-OH4
4	B	306	1PE	OH6-C15-C25-OH5
4	B	305	1PE	OH5-C14-C24-OH4
4	A	306	1PE	OH2-C12-C22-OH3
4	B	306	1PE	C13-C23-OH3-C22
3	A	304	NAG	C4-C5-C6-O6
4	A	306	1PE	C25-C15-OH6-C26
4	B	305	1PE	OH6-C15-C25-OH5
4	B	306	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
4	A	306	1PE	C13-C23-OH3-C22
4	A	306	1PE	C12-C22-OH3-C23
4	B	305	1PE	C24-C14-OH5-C25
4	A	305	1PE	C23-C13-OH4-C24
4	A	305	1PE	OH7-C16-C26-OH6
4	A	306	1PE	OH7-C16-C26-OH6
4	B	306	1PE	C14-C24-OH4-C13
4	A	306	1PE	C24-C14-OH5-C25
4	B	305	1PE	OH2-C12-C22-OH3
4	A	306	1PE	OH6-C15-C25-OH5
4	A	305	1PE	C12-C22-OH3-C23
4	B	305	1PE	C25-C15-OH6-C26
4	A	306	1PE	C14-C24-OH4-C13
4	A	305	1PE	C16-C26-OH6-C15
4	A	306	1PE	C15-C25-OH5-C14
4	B	306	1PE	OH7-C16-C26-OH6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	1PE	5	0
4	B	306	1PE	2	0
5	A	310	SO4	1	0
4	B	305	1PE	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	189/193 (97%)	-0.09	10 (5%) 26 25	24, 38, 74, 120	0
1	B	193/193 (100%)	0.17	14 (7%) 15 14	24, 39, 89, 133	0
All	All	382/386 (98%)	0.04	24 (6%) 20 19	24, 39, 77, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	PRO	12.2
1	B	48	ALA	9.3
1	B	49	GLY	7.8
1	B	51	ARG	6.7
1	B	52	PRO	6.2
1	B	108	GLY	5.6
1	B	109	THR	4.8
1	A	108	GLY	4.8
1	A	107	SER	4.5
1	B	107	SER	4.4
1	B	106	VAL	4.2
1	B	239	ALA	4.2
1	A	106	VAL	3.9
1	A	104	ARG	3.8
1	A	240	ASP	3.8
1	B	240	ASP	3.5
1	A	109	THR	3.3
1	B	105	ASN	3.2
1	A	54	PRO	2.7
1	B	54	PRO	2.7
1	A	239	ALA	2.6
1	A	105	ASN	2.3
1	A	110	TRP	2.1
1	B	74[A]	TYR	2.0

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

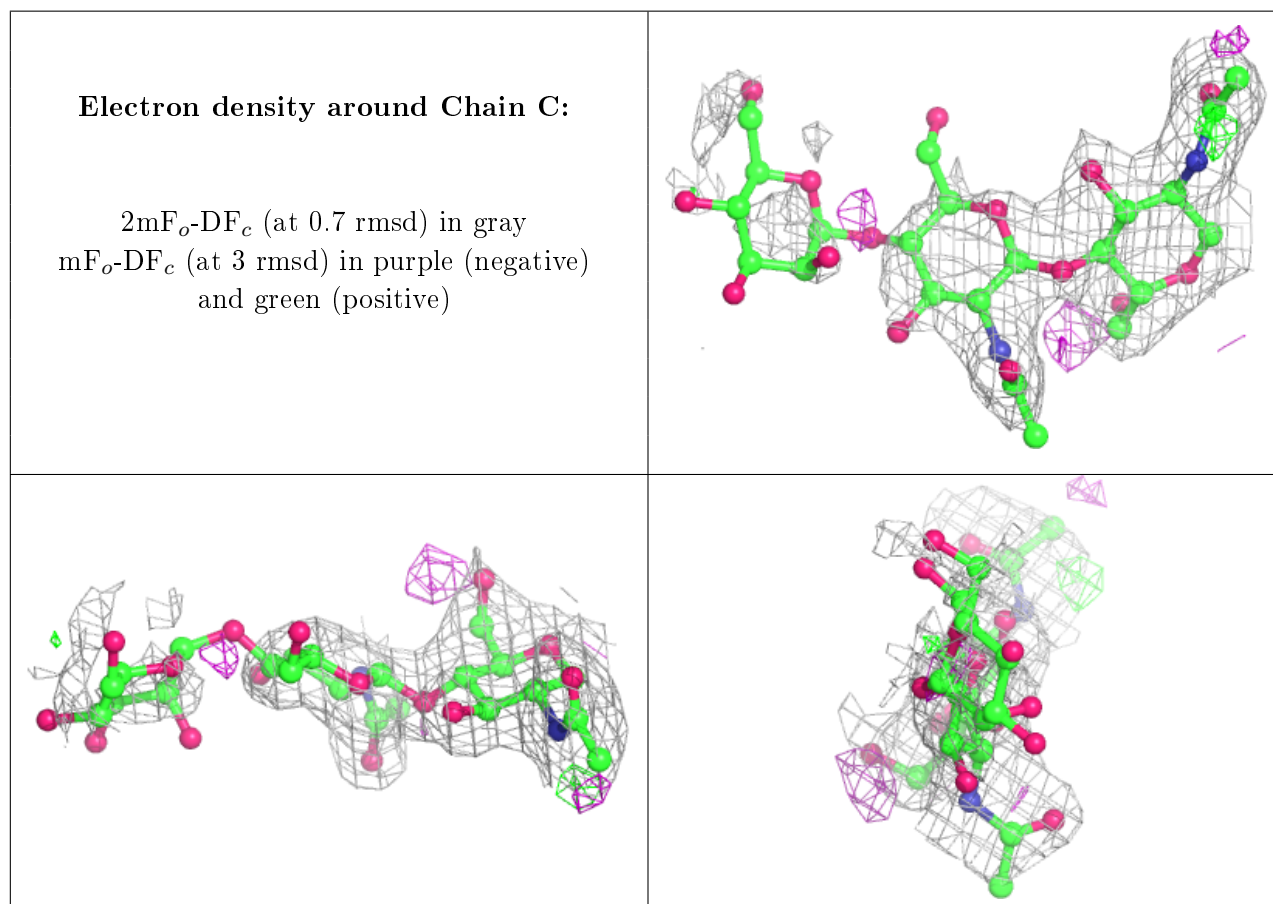
There are no non-standard protein/DNA/RNA residues in this entry.

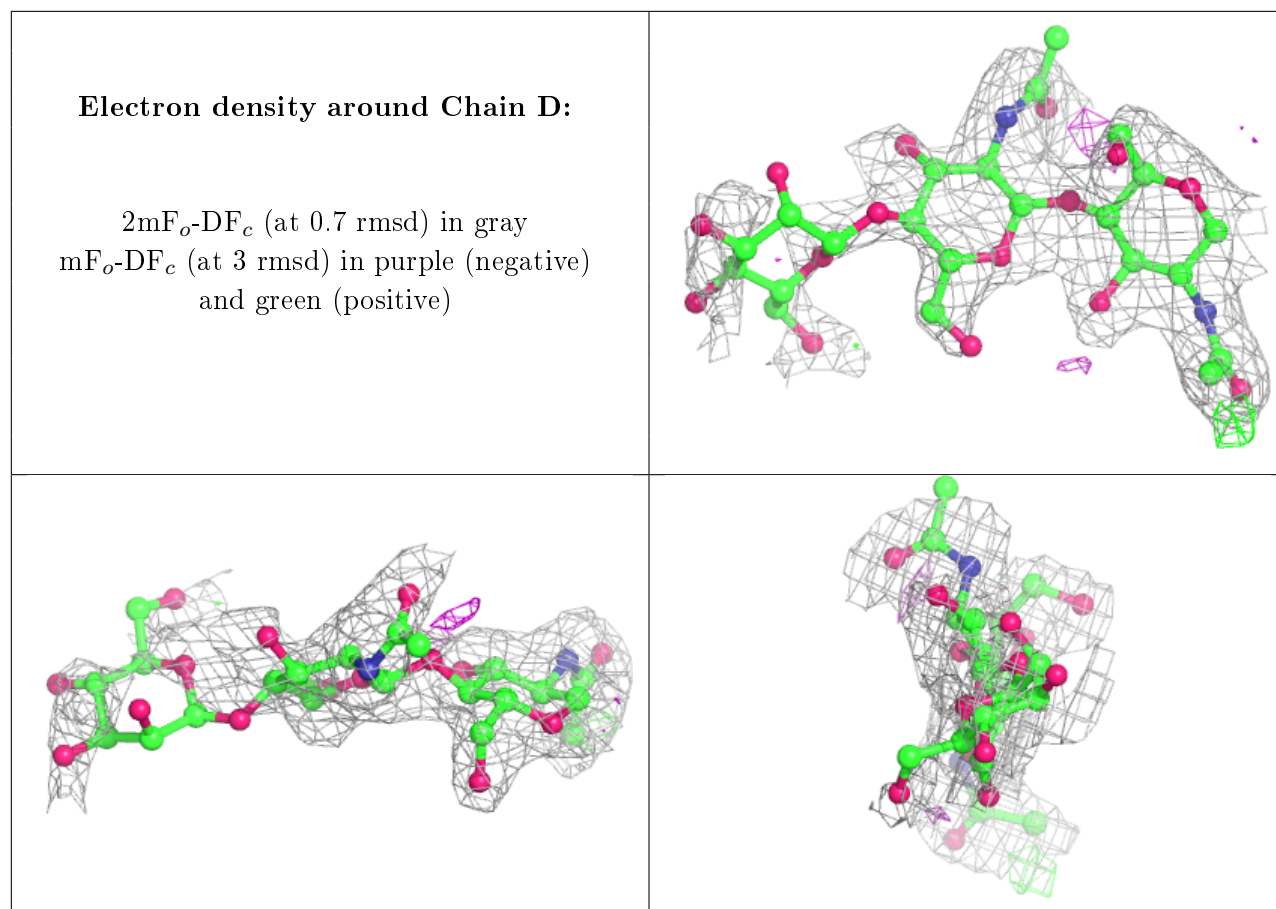
## 6.3 Carbohydrates [i](#)

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	D	3	11/12	<a href="#">0.34</a>	<a href="#">0.62</a>	126,138,140,141	0
2	BMA	C	3	11/12	<a href="#">0.40</a>	<a href="#">0.65</a>	129,142,144,144	0
2	NAG	D	2	14/15	0.71	0.32	69,91,111,124	0
2	NAG	C	2	14/15	0.77	0.40	65,95,116,135	0
2	NAG	D	1	14/15	0.92	0.13	39,56,67,74	0
2	NAG	C	1	14/15	0.92	0.14	41,52,68,78	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
3	NAG	A	304	14/15	0.67	0.45	102,113,121,123	0
3	NAG	B	304	14/15	0.71	0.39	101,117,127,127	0
5	SO4	A	309	5/5	0.83	0.23	110,117,120,124	0
5	SO4	A	311	5/5	0.87	0.30	151,152,153,153	0
5	SO4	B	308	5/5	0.88	0.16	74,85,96,110	0
5	SO4	B	307	5/5	0.91	0.12	81,83,92,93	0
4	1PE	A	306	16/16	0.91	0.12	33,55,72,77	0
5	SO4	A	310	5/5	0.93	0.15	79,85,98,112	0
4	1PE	B	305	16/16	0.93	0.12	37,47,66,72	0
4	1PE	B	306	16/16	0.93	0.15	42,56,71,77	0
4	1PE	A	305	16/16	0.93	0.16	44,58,68,73	0
5	SO4	A	308	5/5	0.94	0.11	79,83,94,96	0
5	SO4	A	307	5/5	0.98	0.11	39,47,54,62	0

## 6.5 Other polymers

There are no such residues in this entry.