



# Full wwPDB X-ray Structure Validation Report i

Nov 11, 2021 – 11:08 am GMT

PDB ID : 7P39  
Title : 4,6-alpha-glucanotransferase GtfB from Limosilactobacillus reuteri NCC 2613 complexed with acarbose  
Authors : Pijning, T.; te Poele, E.; Gangoiti, J.; Boerner, T.; Dijkhuizen, L.  
Deposited on : 2021-07-07  
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](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 i symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

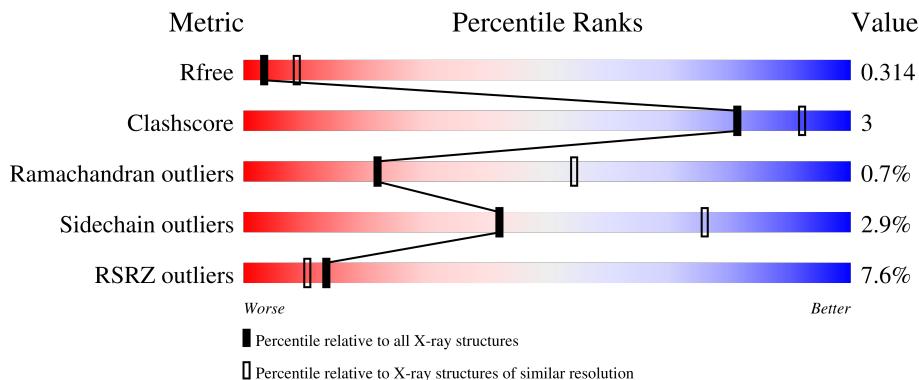
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

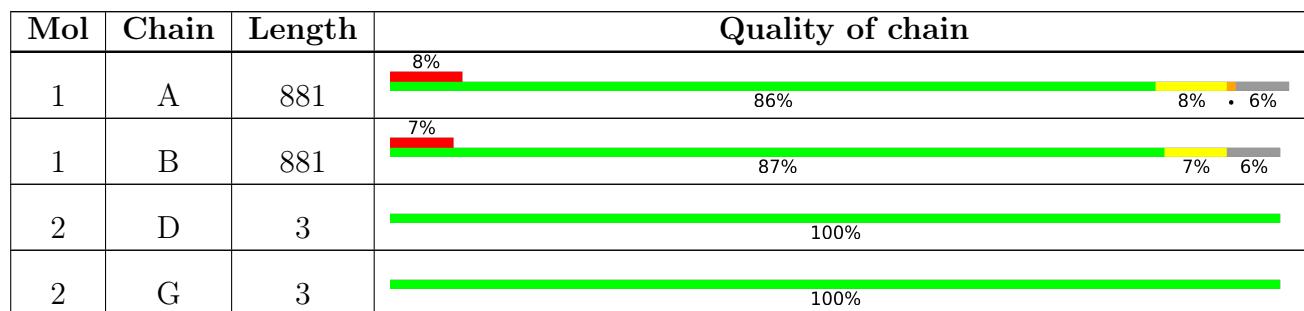
The reported resolution of this entry is 2.90 Å.

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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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.



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13136 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 Dextranucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C 6511	N 4054	O 1101	S 1334	22	0	0
1	B	832	Total	C 6511	N 4054	O 1101	S 1334	22	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
A	398	ALA	-	expression tag	UNP A0A1Z2RUH3
A	399	HIS	-	expression tag	UNP A0A1Z2RUH3
A	400	HIS	-	expression tag	UNP A0A1Z2RUH3
A	401	HIS	-	expression tag	UNP A0A1Z2RUH3
A	402	HIS	-	expression tag	UNP A0A1Z2RUH3
A	403	HIS	-	expression tag	UNP A0A1Z2RUH3
A	404	HIS	-	expression tag	UNP A0A1Z2RUH3
A	405	SER	-	expression tag	UNP A0A1Z2RUH3
A	406	ALA	-	expression tag	UNP A0A1Z2RUH3
A	407	ALA	-	expression tag	UNP A0A1Z2RUH3
A	408	LEU	-	expression tag	UNP A0A1Z2RUH3
A	409	GLU	-	expression tag	UNP A0A1Z2RUH3
A	410	VAL	-	expression tag	UNP A0A1Z2RUH3
A	411	LEU	-	expression tag	UNP A0A1Z2RUH3
A	412	PHE	-	expression tag	UNP A0A1Z2RUH3
A	413	GLN	-	expression tag	UNP A0A1Z2RUH3
A	414	GLY	-	expression tag	UNP A0A1Z2RUH3
A	415	PRO	-	expression tag	UNP A0A1Z2RUH3
A	416	GLY	-	expression tag	UNP A0A1Z2RUH3
B	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
B	398	ALA	-	expression tag	UNP A0A1Z2RUH3
B	399	HIS	-	expression tag	UNP A0A1Z2RUH3
B	400	HIS	-	expression tag	UNP A0A1Z2RUH3
B	401	HIS	-	expression tag	UNP A0A1Z2RUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	402	HIS	-	expression tag	UNP A0A1Z2RUH3
B	403	HIS	-	expression tag	UNP A0A1Z2RUH3
B	404	HIS	-	expression tag	UNP A0A1Z2RUH3
B	405	SER	-	expression tag	UNP A0A1Z2RUH3
B	406	ALA	-	expression tag	UNP A0A1Z2RUH3
B	407	ALA	-	expression tag	UNP A0A1Z2RUH3
B	408	LEU	-	expression tag	UNP A0A1Z2RUH3
B	409	GLU	-	expression tag	UNP A0A1Z2RUH3
B	410	VAL	-	expression tag	UNP A0A1Z2RUH3
B	411	LEU	-	expression tag	UNP A0A1Z2RUH3
B	412	PHE	-	expression tag	UNP A0A1Z2RUH3
B	413	GLN	-	expression tag	UNP A0A1Z2RUH3
B	414	GLY	-	expression tag	UNP A0A1Z2RUH3
B	415	PRO	-	expression tag	UNP A0A1Z2RUH3
B	416	GLY	-	expression tag	UNP A0A1Z2RUH3

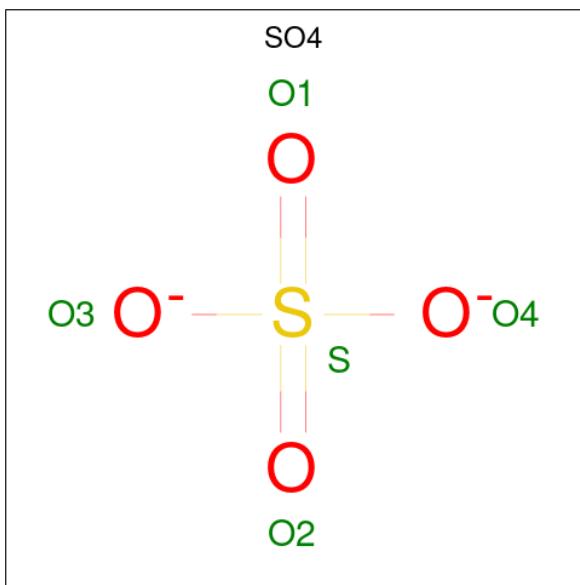
- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{|(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-e-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	3	Total C N O 44 25 1 18	0	0	0
2	G	3	Total C N O 44 25 1 18	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

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



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

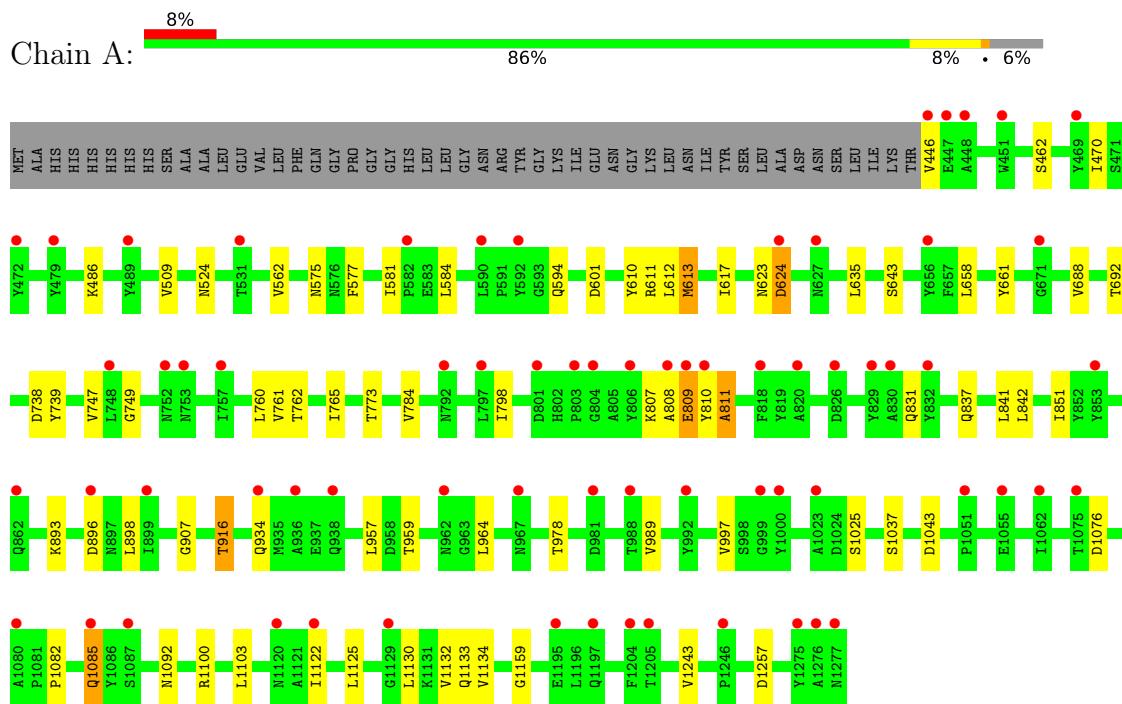
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total    O 10    10	0	0
5	B	9	Total    O 9    9	0	0

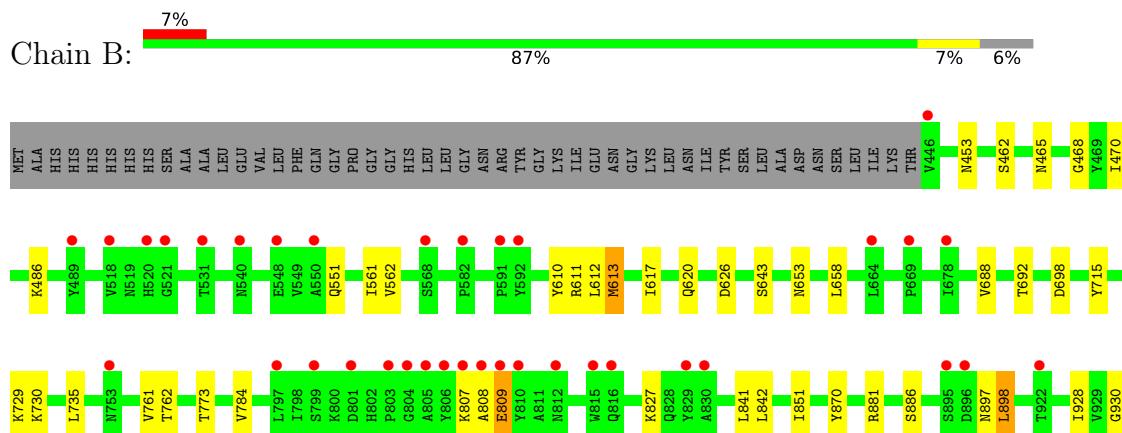
### 3 Residue-property plots

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: Dextransucrase



- Molecule 1: Dextransucrase





- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 100%

BGC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G: 100%

BGC1  
GLC2  
AC13

## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.22Å    133.81Å    147.87Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	49.29 – 2.90 47.16 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.29-2.90) 97.8 (47.16-2.90)	Depositor EDS
$R_{merge}$	0.43	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.83 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
$R$ , $R_{free}$	0.293 , 0.315 0.295 , 0.314	Depositor DCC
$R_{free}$ test set	2250 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	13136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1296e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  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: AC1, SO4, BGC, CA, GLC

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	0.37	0/6653	0.57	0/9063
1	B	0.37	0/6653	0.57	0/9063
All	All	0.37	0/13306	0.57	0/18126

There are no bond length outliers.

There are no bond angle outliers.

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	6511	0	6129	40	0
1	B	6511	0	6129	26	0
2	D	44	0	30	0	0
2	G	44	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
5	A	10	0	0	0	0
5	B	9	0	0	0	0
All	All	13136	0	12318	66	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 3.

All (66) 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:1122:ILE:HG23	1:A:1132:VAL:HG11	1.61	0.83
1:B:1122:ILE:HG23	1:B:1132:VAL:HG11	1.61	0.82
1:A:577:PHE:CZ	1:A:581:ILE:HD11	2.15	0.82
1:B:1076:ASP:HB3	1:B:1133:GLN:HE22	1.52	0.74
1:A:1076:ASP:HB3	1:A:1133:GLN:HE22	1.51	0.73
1:A:661:TYR:CE1	1:A:1103:LEU:HD23	2.28	0.69
1:A:581:ILE:HD12	1:A:584:LEU:HD12	1.75	0.67
1:B:1043:ASP:OD2	1:B:1079:MET:HA	1.95	0.67
1:B:1232:THR:HG21	1:B:1235:GLN:HE21	1.61	0.66
1:B:653:ASN:HD21	1:B:1192:TYR:H	1.43	0.65
1:B:784:VAL:HG23	1:B:841:LEU:HD22	1.80	0.63
1:A:898:LEU:HD21	1:A:989:VAL:HG21	1.81	0.62
1:B:1122:ILE:HG23	1:B:1132:VAL:CG1	2.29	0.62
1:A:784:VAL:HG23	1:A:841:LEU:HD22	1.80	0.61
1:A:1122:ILE:HG23	1:A:1132:VAL:CG1	2.29	0.61
1:B:761:VAL:HG23	1:B:762:THR:HG23	1.83	0.61
1:B:827:LYS:NZ	1:B:870:TYR:OH	2.35	0.59
1:A:761:VAL:HG23	1:A:762:THR:HG23	1.83	0.59
1:A:1085:GLN:NE2	1:A:1092:ASN:OD1	2.35	0.59
1:B:453:ASN:HD21	1:B:551:GLN:HE22	1.51	0.58
1:A:957:LEU:HD21	1:A:964:LEU:HD22	1.86	0.57
1:B:620:GLN:HE22	1:B:730:LYS:NZ	2.03	0.57
1:A:747:VAL:HG11	1:A:760:LEU:CD1	2.35	0.56
1:A:747:VAL:HG11	1:A:760:LEU:HD11	1.88	0.56
1:A:658:LEU:HD13	1:A:1134:VAL:HG11	1.90	0.54
1:A:610:TYR:O	1:A:612:LEU:HD12	2.08	0.53
1:B:610:TYR:O	1:B:612:LEU:N	2.42	0.53
1:B:658:LEU:HD13	1:B:1134:VAL:HG11	1.90	0.52
1:A:738:ASP:OD2	1:A:765:ILE:HG22	2.11	0.50
1:A:807:LYS:O	1:A:809:GLU:N	2.44	0.49
1:A:624:ASP:OD1	1:A:624:ASP:N	2.45	0.49
1:A:959:THR:CG2	1:A:997:VAL:HG21	2.43	0.49
1:A:907:GLY:O	1:A:916:THR:HG23	2.13	0.48
1:A:831:GLN:HE21	1:A:837:GLN:HE22	1.61	0.48
1:B:807:LYS:O	1:B:809:GLU:N	2.46	0.48
1:A:688:VAL:O	1:A:692:THR:HG23	2.14	0.47
1:A:842:LEU:HD21	1:A:851:ILE:HD11	1.97	0.47
1:B:688:VAL:O	1:B:692:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:LEU:HD11	1:B:928:ILE:HG23	1.95	0.47
1:B:842:LEU:HD21	1:B:851:ILE:HD11	1.97	0.47
1:A:1082:PRO:HG2	1:A:1103:LEU:HD12	1.98	0.46
1:B:715:TYR:HB3	1:B:735:LEU:HB2	1.99	0.45
1:A:798:ILE:HD12	1:A:811:ALA:HB1	1.98	0.45
1:B:465:ASN:HD22	1:B:468:GLY:HA2	1.82	0.45
1:B:957:LEU:HD11	1:B:964:LEU:HB3	1.98	0.45
1:A:893:LYS:HE3	1:A:896:ASP:HA	1.99	0.45
1:A:661:TYR:HE1	1:A:1103:LEU:HD23	1.78	0.44
1:B:613:MET:HG2	1:B:1159:GLY:HA3	1.98	0.44
1:A:577:PHE:CE2	1:A:581:ILE:HD11	2.51	0.44
1:A:509:VAL:HG13	1:A:581:ILE:HD13	2.00	0.44
1:A:446:VAL:O	1:A:446:VAL:HG13	2.19	0.43
1:A:613:MET:HG2	1:A:1159:GLY:HA3	2.01	0.43
1:A:959:THR:HG21	1:A:997:VAL:HG11	2.01	0.42
1:A:959:THR:HG22	1:A:997:VAL:HG21	2.00	0.42
1:B:1043:ASP:OD1	1:B:1043:ASP:C	2.57	0.42
1:A:749:GLY:HA3	1:A:831:GLN:NE2	2.34	0.42
1:B:470:ILE:HD12	1:B:470:ILE:N	2.35	0.42
1:A:1125:LEU:HD12	1:A:1130:LEU:HD22	2.02	0.42
1:A:470:ILE:N	1:A:470:ILE:HD12	2.34	0.41
1:A:749:GLY:HA3	1:A:831:GLN:HE22	1.85	0.41
1:B:897:ASN:O	1:B:930:GLY:HA2	2.20	0.41
1:A:810:TYR:CG	1:A:811:ALA:N	2.88	0.41
1:A:810:TYR:O	1:A:811:ALA:CB	2.68	0.41
1:B:1125:LEU:HD12	1:B:1130:LEU:HD22	2.03	0.41
1:A:738:ASP:OD1	1:A:739:TYR:N	2.54	0.41
1:B:881:ARG:NH2	1:B:1038:HIS:O	2.53	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	830/881 (94%)	793 (96%)	30 (4%)	7 (1%)	19 51
1	B	830/881 (94%)	791 (95%)	34 (4%)	5 (1%)	25 58
All	All	1660/1762 (94%)	1584 (95%)	64 (4%)	12 (1%)	22 54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	808	ALA
1	A	809	GLU
1	A	811	ALA
1	A	1243	VAL
1	B	808	ALA
1	A	611	ARG
1	B	809	GLU
1	A	617	ILE
1	B	617	ILE
1	A	1025	SER
1	B	611	ARG
1	B	886	SER

### 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	702/741 (95%)	681 (97%)	21 (3%)	41 75
1	B	702/741 (95%)	682 (97%)	20 (3%)	43 76
All	All	1404/1482 (95%)	1363 (97%)	41 (3%)	42 76

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	SER
1	A	486	LYS
1	A	524	ASN
1	A	562	VAL

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Mol	Chain	Res	Type
1	A	575	ASN
1	A	594	GLN
1	A	601	ASP
1	A	613	MET
1	A	623	ASN
1	A	624	ASP
1	A	635	LEU
1	A	643	SER
1	A	773	THR
1	A	916	THR
1	A	934	GLN
1	A	978	THR
1	A	1037	SER
1	A	1043	ASP
1	A	1085	GLN
1	A	1100	ARG
1	A	1257	ASP
1	B	462	SER
1	B	486	LYS
1	B	561	ILE
1	B	562	VAL
1	B	613	MET
1	B	626	ASP
1	B	643	SER
1	B	698	ASP
1	B	729	LYS
1	B	773	THR
1	B	898	LEU
1	B	969	ASP
1	B	1037	SER
1	B	1043	ASP
1	B	1056	ASN
1	B	1100	ARG
1	B	1210	SER
1	B	1245	LEU
1	B	1257	ASP
1	B	1264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	ASN

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Mol	Chain	Res	Type
1	A	524	ASN
1	A	551	GLN
1	A	575	ASN
1	A	594	GLN
1	A	599	ASN
1	A	623	ASN
1	A	625	ASN
1	A	642	ASN
1	A	711	ASN
1	A	746	ASN
1	A	753	ASN
1	A	780	ASN
1	A	831	GLN
1	A	950	ASN
1	A	1056	ASN
1	A	1133	GLN
1	B	453	ASN
1	B	620	GLN
1	B	625	ASN
1	B	653	ASN
1	B	683	HIS
1	B	746	ASN
1	B	759	ASN
1	B	780	ASN
1	B	792	ASN
1	B	862	GLN
1	B	948	HIS
1	B	973	ASN
1	B	1012	GLN
1	B	1056	ASN
1	B	1085	GLN
1	B	1133	GLN
1	B	1277	ASN

### 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.

There are no bond length outliers.

There are no bond angle outliers.

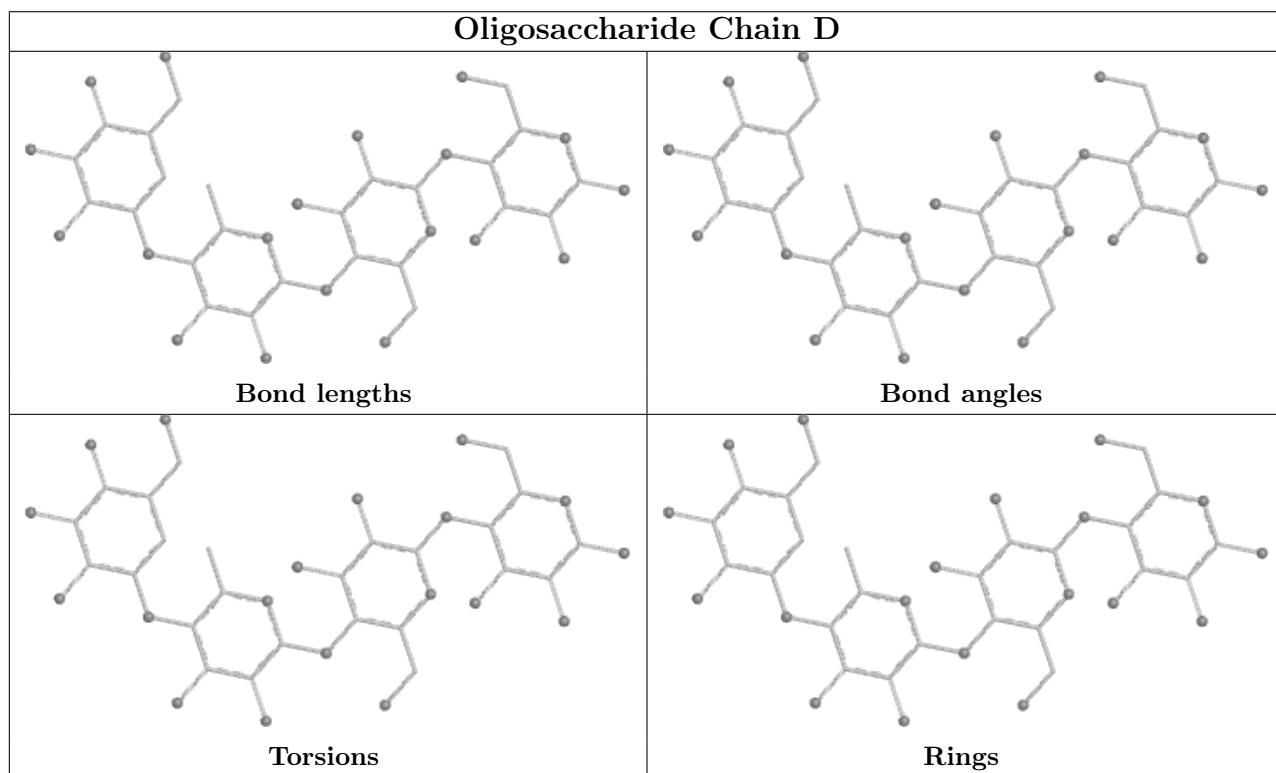
There are no chirality outliers.

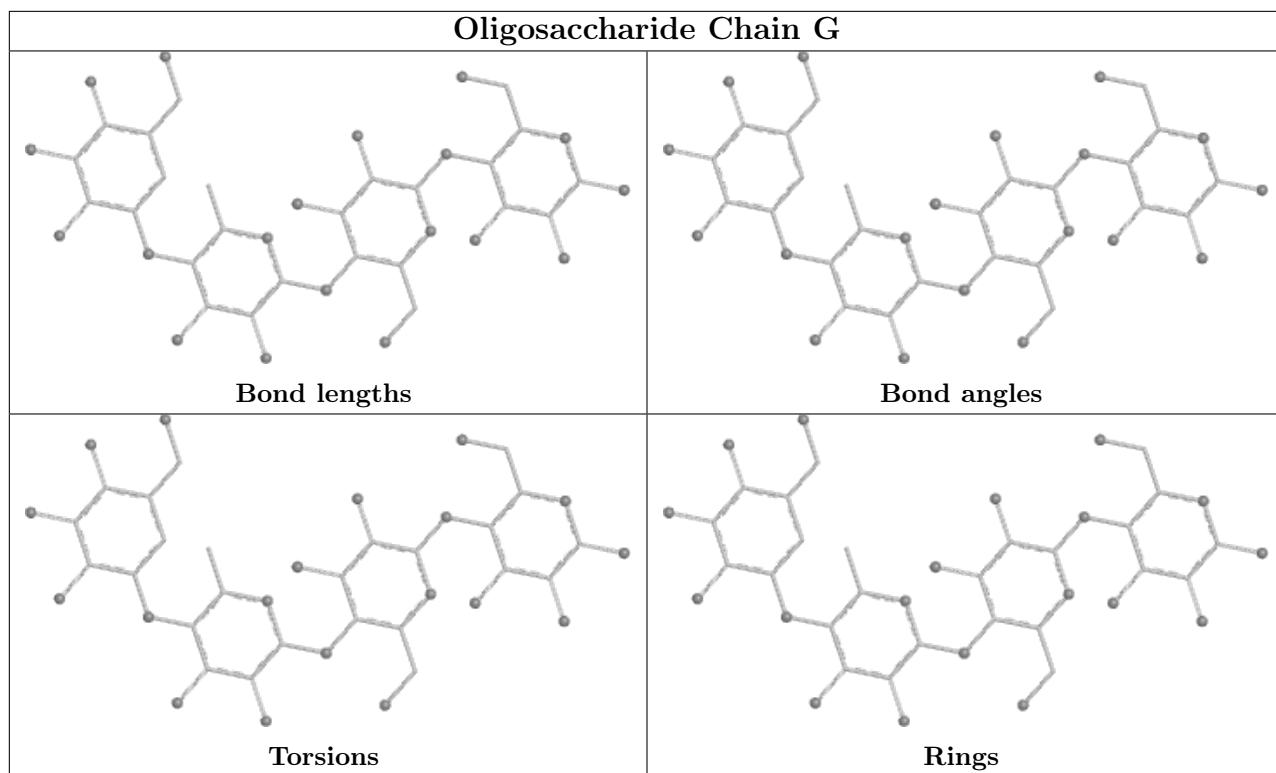
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 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, 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	832/881 (94%)	0.95	68 (8%) 11 9	30, 41, 66, 102	0
1	B	832/881 (94%)	0.91	58 (6%) 16 12	29, 41, 56, 96	0
All	All	1664/1762 (94%)	0.93	126 (7%) 13 10	29, 41, 62, 102	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	808	ALA	8.6
1	A	1275	TYR	6.4
1	A	806	TYR	5.4
1	B	810	TYR	5.4
1	A	810	TYR	5.2
1	B	797	LEU	5.1
1	A	809	GLU	5.0
1	B	753	ASN	4.8
1	A	803	PRO	4.5
1	B	1275	TYR	4.5
1	A	797	LEU	4.2
1	B	807	LYS	4.1
1	B	806	TYR	4.0
1	B	803	PRO	4.0
1	B	799	SER	3.9
1	A	999	GLY	3.9
1	A	981	ASP	3.9
1	B	1120	ASN	3.9
1	B	808	ALA	3.8
1	A	489	TYR	3.7
1	B	804	GLY	3.6
1	B	896	ASP	3.5
1	A	801	ASP	3.5
1	B	812	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	829	TYR	3.4
1	B	592	TYR	3.3
1	A	1080	ALA	3.3
1	A	804	GLY	3.3
1	B	531	THR	3.2
1	B	489	TYR	3.2
1	A	752	ASN	3.1
1	B	809	GLU	3.0
1	A	992	TYR	3.0
1	B	992	TYR	3.0
1	A	1062	ILE	3.0
1	A	531	THR	2.9
1	A	1246	PRO	2.9
1	B	981	ASP	2.8
1	A	936	ALA	2.8
1	B	1023	ALA	2.8
1	A	826	ASP	2.8
1	B	521	GLY	2.8
1	A	896	ASP	2.8
1	A	624	ASP	2.7
1	B	816	GLN	2.7
1	A	1023	ALA	2.7
1	A	934	GLN	2.7
1	B	801	ASP	2.6
1	A	938	GLN	2.6
1	A	1120	ASN	2.6
1	B	1257	ASP	2.6
1	B	582	PRO	2.6
1	B	1062	ILE	2.6
1	B	520	HIS	2.6
1	A	1000	TYR	2.6
1	B	830	ALA	2.6
1	A	592	TYR	2.5
1	A	820	ALA	2.5
1	B	934	GLN	2.5
1	A	627	ASN	2.5
1	A	1122	ILE	2.5
1	B	895	SER	2.5
1	B	518	VAL	2.5
1	A	1205	THR	2.5
1	A	1085	GLN	2.4
1	B	805	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	479	TYR	2.4
1	B	1261	PHE	2.4
1	B	1165	ASN	2.4
1	B	568	SER	2.4
1	B	1267	GLU	2.4
1	B	936	ALA	2.4
1	B	982	ASN	2.4
1	A	899	ILE	2.4
1	B	922	THR	2.3
1	A	962	ASN	2.3
1	A	671	GLY	2.3
1	A	1129	GLY	2.3
1	A	1051	PRO	2.3
1	B	1176	ALA	2.3
1	A	1276	ALA	2.3
1	A	753	ASN	2.3
1	B	815	TRP	2.3
1	B	548	GLU	2.3
1	A	967	ASN	2.3
1	A	829	TYR	2.3
1	A	988	THR	2.3
1	A	656	TYR	2.3
1	A	832	TYR	2.2
1	A	830	ALA	2.2
1	A	1197	GLN	2.2
1	A	792	ASN	2.2
1	B	1052	THR	2.2
1	B	591	PRO	2.2
1	B	446	VAL	2.2
1	A	1195	GLU	2.2
1	A	1277	ASN	2.2
1	A	757	ILE	2.2
1	B	550	ALA	2.2
1	B	1047	TYR	2.2
1	A	447	GLU	2.2
1	A	446	VAL	2.2
1	A	818	PHE	2.2
1	A	1204	PHE	2.1
1	B	1024	ASP	2.1
1	B	976	THR	2.1
1	A	590	LEU	2.1
1	B	669	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	469	TYR	2.1
1	A	862	GLN	2.1
1	B	1210	SER	2.1
1	A	472	TYR	2.1
1	A	748	LEU	2.1
1	B	664	LEU	2.1
1	A	448	ALA	2.1
1	A	1055	GLU	2.1
1	A	1075	THR	2.1
1	B	1262	ASN	2.1
1	A	853	TYR	2.1
1	A	451	TRP	2.0
1	B	1079	MET	2.0
1	B	969	ASP	2.0
1	A	582	PRO	2.0
1	B	540	ASN	2.0
1	B	678	ILE	2.0
1	A	1087	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 [\(i\)](#)

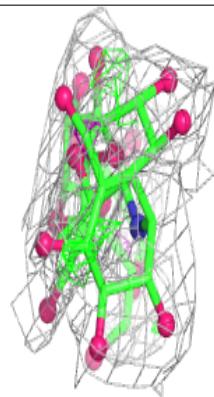
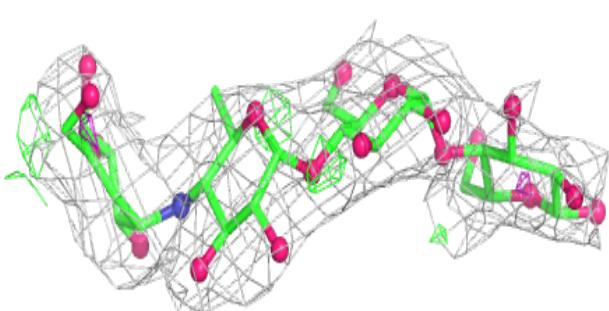
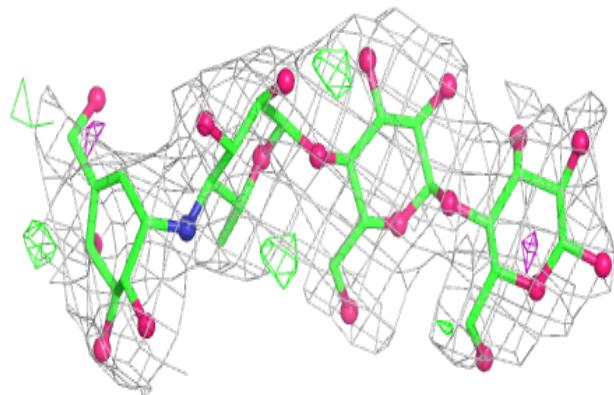
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	BGC	D	1	12/12	0.70	0.34	51,53,53,54	0
2	BGC	G	1	12/12	0.81	0.31	46,47,47,47	0
2	AC1	D	3	21/22	0.82	0.28	45,46,47,47	0
2	AC1	G	3	21/22	0.82	0.26	45,45,46,46	0
2	GLC	D	2	11/12	0.83	0.22	47,49,49,49	0
2	GLC	G	2	11/12	0.87	0.22	43,45,45,45	0

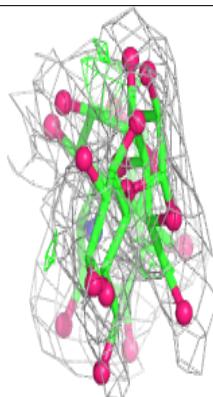
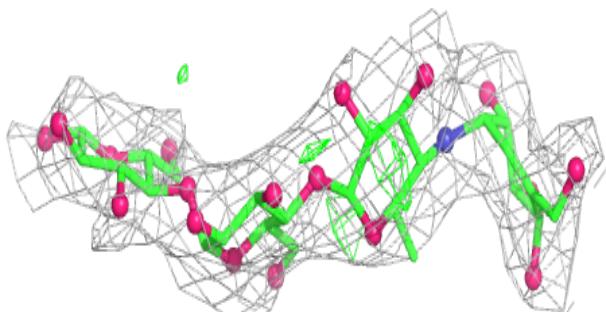
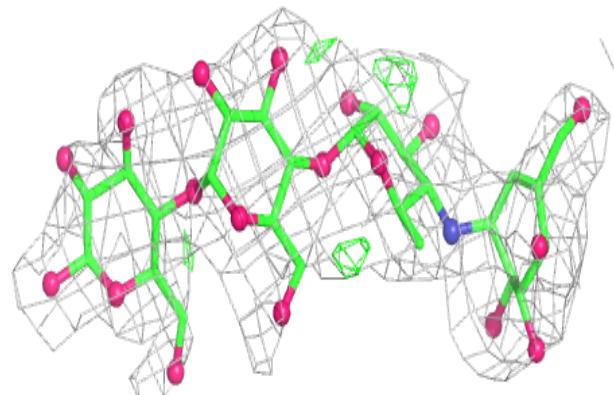
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain D:**

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

**Electron density around Chain G:**

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



## 6.4 Ligands [\(i\)](#)

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	CA	B	1301	1/1	0.69	0.14	27,27,27,27	0
4	SO4	A	1302	5/5	0.74	0.34	72,73,73,73	0
3	CA	A	1301	1/1	0.79	0.14	29,29,29,29	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.