



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:15 AM GMT

PDB ID : 4C2S  
Title : Crystal structure of the fucosylgalactoside alpha N- acetylgalactosaminyltransferase(GTA P156L mutant) in complex with UDP and deoxy-H-antigen acceptor  
Authors : Weadge, J.T.; Palcic, M.; Henriksen, A.  
Deposited on : 2013-08-19  
Resolution : 2.48 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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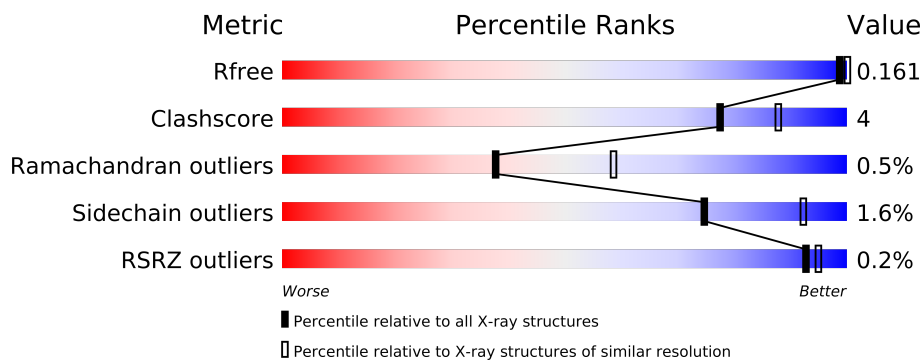
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.48 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))
$R_{free}$	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4959 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HISTO-BLOOD GROUP ABO SYSTEM TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2370	1529	415	414	12			
1	B	290	Total	C	N	O	S	0	0	0
			2356	1523	408	413	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	EXPRESSION TAG	UNP P16442
A	156	LEU	PRO	ENGINEERED MUTATION	UNP P16442
B	63	MET	-	EXPRESSION TAG	UNP P16442
B	156	LEU	PRO	ENGINEERED MUTATION	UNP P16442

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

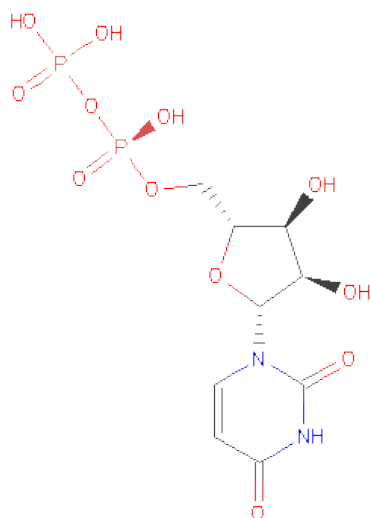
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			27	18	9		
3	B	2	Total	C	O	0	0
			27	18	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	EXPRESSION TAG	UNP P16442
A	156	LEU	PRO	ENGINEERED MUTATION	UNP P16442
B	63	MET	-	EXPRESSION TAG	UNP P16442
B	156	LEU	PRO	ENGINEERED MUTATION	UNP P16442

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is water.

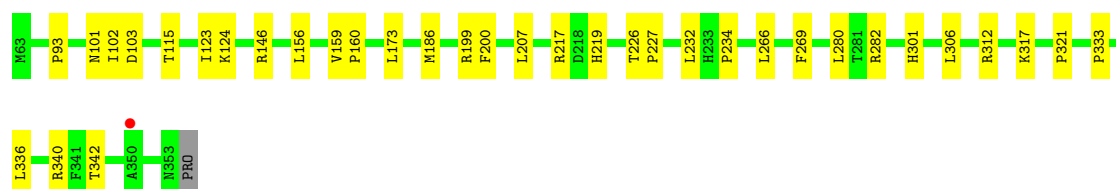
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	58	Total	O	0	0
			58	58		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: HISTO-BLOOD GROUP ABO SYSTEM TRANSFERASE

Chain A: 



- Molecule 1: HISTO-BLOOD GROUP ABO SYSTEM TRANSFERASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.51Å 52.61Å 80.27Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	36.88 – 2.48 36.88 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.88-2.48) 98.9 (36.88-2.48)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.84 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.145 , 0.182 0.134 , 0.161	Depositor DCC
$R_{free}$ test set	1118 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 12.2	EDS
Estimated twinning fraction	0.938 for H, K, L 0.062 for H, -K, -L 0.286 for -h,-k,l	Xtriage
Reported twinning fraction	0.938 for H, K, L 0.062 for H, -K, -L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22069 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MN, DLG, FUC

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	0.78	0/2435	0.70	0/3305
1	B	0.76	0/2421	0.68	0/3289
All	All	0.77	0/4856	0.69	0/6594

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2370	0	2336	23	0
1	B	2356	0	2320	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	33	0	0
3	B	27	0	33	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	A	69	0	0	1	0
5	B	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4959	0	4744	35	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:ARG:NH1	5:A:2039:HOH:O	2.10	0.83
1:B:226:THR:HG21	1:B:317:LYS:HB2	1.66	0.78
1:A:226:THR:HG21	1:A:317:LYS:HB2	1.79	0.65
1:B:75:LYS:HG3	1:B:78:THR:HB	1.82	0.61
1:A:199:ARG:HG3	1:A:199:ARG:O	2.02	0.60
1:B:353:ASN:HB3	5:B:2059:HOH:O	2.03	0.59
1:A:173:LEU:HD21	1:A:199:ARG:HH22	1.68	0.58
1:A:173:LEU:HD21	1:A:199:ARG:NH2	2.18	0.57
1:A:93:PRO:HG2	1:A:317:LYS:HG2	1.87	0.56
1:A:186:MET:HG3	1:A:301:HIS:HB3	1.91	0.53
1:A:333:PRO:HD2	1:A:336:LEU:HD12	1.92	0.51
1:A:280:LEU:HD21	1:A:306:LEU:HD13	1.93	0.51
1:B:156:LEU:HD21	1:B:174:GLU:HB2	1.93	0.51
1:A:186:MET:CG	1:A:301:HIS:HB3	2.41	0.51
1:A:219:HIS:O	1:A:340:ARG:HD3	2.11	0.51
1:B:333:PRO:HD2	1:B:336:LEU:HD12	1.94	0.50
1:B:123:ILE:HD13	1:B:153:THR:HA	1.94	0.49
1:A:312:ARG:HD2	1:B:66:LEU:O	2.13	0.49
1:A:115:THR:OG1	1:A:146:ARG:NH1	2.46	0.48
1:B:269:PHE:HB2	1:B:324:LEU:HD12	1.94	0.48
1:A:101:ASN:OD1	1:A:103:ASP:HB2	2.15	0.46
1:B:261:GLY:HA2	1:B:311:LEU:HD13	1.96	0.46
1:A:156:LEU:H	1:A:156:LEU:HD12	1.79	0.46
1:B:233:HIS:HA	1:B:266:LEU:HG	1.98	0.46
1:A:226:THR:OG1	1:A:227:PRO:HD2	2.17	0.45
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.89	0.44
1:A:217:ARG:HD3	1:A:342:THR:OG1	2.18	0.44
1:B:153:THR:O	1:B:174:GLU:HA	2.18	0.43
1:A:232:LEU:HD12	1:A:321:PRO:HD3	2.01	0.42
1:A:234:PRO:HD3	1:A:266:LEU:HD11	2.00	0.42
1:B:186:MET:HA	1:B:302:ASP:HB3	2.01	0.42
1:B:75:LYS:HG2	1:B:75:LYS:H	1.59	0.41
1:A:232:LEU:HB2	1:A:321:PRO:HD3	2.02	0.41
1:A:102:ILE:HD12	1:A:102:ILE:HA	1.90	0.41
1:A:123:ILE:HG22	1:A:124:LYS:HG3	2.02	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/292 (99%)	274 (95%)	14 (5%)	1 (0%)	50	71
1	B	288/292 (99%)	276 (96%)	10 (4%)	2 (1%)	30	48
All	All	577/584 (99%)	550 (95%)	24 (4%)	3 (0%)	38	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	PHE
1	B	201	LEU
1	B	202	SER

### 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	253/260 (97%)	251 (99%)	2 (1%)	89	97
1	B	252/260 (97%)	246 (98%)	6 (2%)	61	85
All	All	505/520 (97%)	497 (98%)	8 (2%)	75	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LEU
1	A	269	PHE
1	B	80	CYS

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Mol	Chain	Res	Type
1	B	113	ASN
1	B	269	PHE
1	B	296	ILE
1	B	324	LEU
1	B	353	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 carbohydrates 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$
3	DLG	A	452	3	17,17,17	1.19	3 (17%)	21,21,21	1.10	1 (4%)
3	FUC	A	453	3	9,10,11	0.71	0	10,14,16	0.86	0
3	DLG	B	452	3	17,17,17	1.19	2 (11%)	21,21,21	1.14	3 (14%)
3	FUC	B	453	3	9,10,11	0.81	0	10,14,16	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DLG	A	452	3	-	0/9/25/25	0/1/1/1
3	FUC	A	453	3	-	0/0/17/20	0/1/1/1
3	DLG	B	452	3	-	0/9/25/25	0/1/1/1
3	FUC	B	453	3	-	0/0/17/20	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	452	DLG	O1-C1	3.02	1.45	1.40
3	A	452	DLG	O1-C1	2.45	1.44	1.40
3	A	452	DLG	C3-C2	2.42	1.56	1.52
3	B	452	DLG	C15-C14	-2.18	1.33	1.51
3	A	452	DLG	C15-C14	-2.14	1.34	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	DLG	C4-C3-C2	-3.41	107.68	111.64
3	B	452	DLG	O5-C1-C2	-2.66	107.66	111.06
3	B	452	DLG	O1-C1-C2	2.30	111.05	108.16
3	B	452	DLG	C4-C3-C2	-2.16	109.14	111.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	UDP	A	475	2	26,26,26	1.19	2 (7%)	36,40,40	1.34	4 (11%)
4	UDP	B	475	2	26,26,26	1.20	2 (7%)	36,40,40	1.40	4 (11%)

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	UDP	A	475	2	-	0/14/32/32	0/2/2/2
4	UDP	B	475	2	-	0/14/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	475	UDP	C2-N1	3.44	1.42	1.38
4	A	475	UDP	C6-C5	2.84	1.40	1.36
4	B	475	UDP	C6-C5	2.69	1.40	1.36
4	A	475	UDP	C2'-C1'	-2.26	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	475	UDP	N3-C2-N1	4.52	119.74	115.97
4	A	475	UDP	N3-C2-N1	4.43	119.67	115.97
4	B	475	UDP	C2-N1-C1'	3.91	120.66	118.21
4	A	475	UDP	PA-O3A-PB	-3.39	121.75	131.68
4	B	475	UDP	PA-O3A-PB	-3.30	122.02	131.68
4	A	475	UDP	O4'-C1'-N1	2.66	113.67	108.06
4	A	475	UDP	C2-N1-C1'	2.35	119.68	118.21
4	B	475	UDP	C5-C4-N3	2.08	120.62	116.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	291/292 (99%)	-0.64	1 (0%) 91 94	2, 11, 21, 32	0
1	B	290/292 (99%)	-0.65	0 100 100	6, 12, 21, 30	0
All	All	581/584 (99%)	-0.64	1 (0%) 93 95	2, 12, 21, 32	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	ALA	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DLG	A	452	17/17	0.09	-0.54	4,4,15,17	0
3	DLG	B	452	17/17	0.10	-0.58	10,11,17,18	0
3	FUC	B	453	10/11	0.08	-1.18	8,8,9,9	0
3	FUC	A	453	10/11	0.07	-2.22	2,3,3,3	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	UDP	A	475	25/25	0.09	-1.08	2,2,8,9	0
4	UDP	B	475	25/25	0.09	-1.29	6,9,11,14	0
2	MN	A	406	1/1	0.06	-2.61	12,12,12,12	0
2	MN	B	406	1/1	0.06	-4.76	14,14,14,14	0

## 6.5 Other polymers

There are no such residues in this entry.