



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2016 – 11:00 AM EDT

PDB ID : 5GGI  
Title : Crystal structure of human protein O-mannose beta-1,2-N-acetylglucosaminyltransferase in complex with Mn, UDP and Mannosyl-peptide  
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Deposited on : 2016-06-16  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

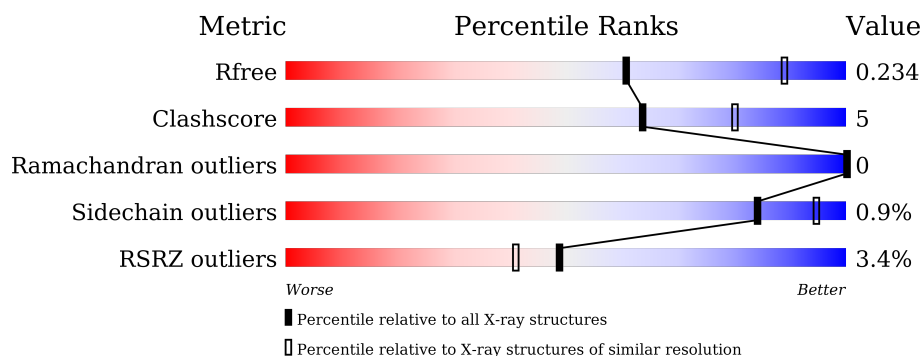
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	578	<div> <div>2%</div> <div>60%</div> <div>8%</div> <div>32%</div> </div>
1	B	578	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>
2	F	11	<div> <div>18%</div> <div>73%</div> <div>18%</div> <div>9%</div> </div>
2	G	11	<div> <div>18%</div> <div>45%</div> <div>55%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UDP	A	701	-	-	-	X
5	PO4	A	703	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7946 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 Protein O-linked-mannose beta-1,2-N-acetylglucosaminyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	2	0
			3231	2075	554	585	17			
1	B	551	Total	C	N	O	S	0	6	0
			4446	2844	767	814	21			

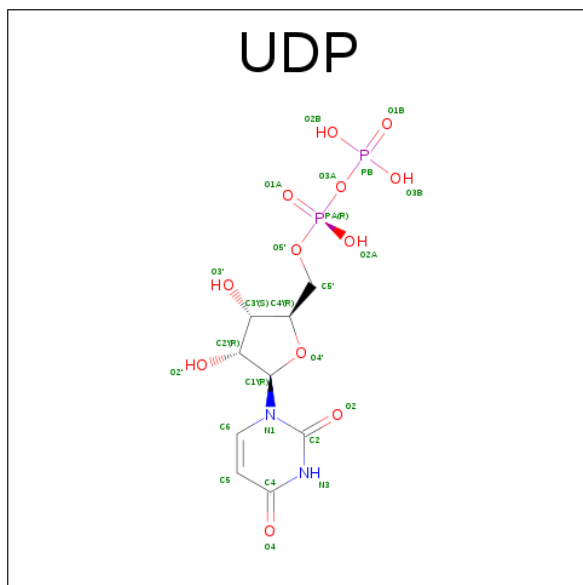
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	VAL	MET	variant	UNP Q8WZA1
A	661	LEU	-	expression tag	UNP Q8WZA1
A	662	GLU	-	expression tag	UNP Q8WZA1
A	663	LEU	-	expression tag	UNP Q8WZA1
A	664	GLU	-	expression tag	UNP Q8WZA1
A	665	VAL	-	expression tag	UNP Q8WZA1
A	666	LEU	-	expression tag	UNP Q8WZA1
A	667	PHE	-	expression tag	UNP Q8WZA1
A	668	GLN	-	expression tag	UNP Q8WZA1
A	669	GLY	-	expression tag	UNP Q8WZA1
B	623	VAL	MET	variant	UNP Q8WZA1
B	661	LEU	-	expression tag	UNP Q8WZA1
B	662	GLU	-	expression tag	UNP Q8WZA1
B	663	LEU	-	expression tag	UNP Q8WZA1
B	664	GLU	-	expression tag	UNP Q8WZA1
B	665	VAL	-	expression tag	UNP Q8WZA1
B	666	LEU	-	expression tag	UNP Q8WZA1
B	667	PHE	-	expression tag	UNP Q8WZA1
B	668	GLN	-	expression tag	UNP Q8WZA1
B	669	GLY	-	expression tag	UNP Q8WZA1

- Molecule 2 is a protein called mannosyl-peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			58	38	9	11			
2	G	5	Total	C	N	O	0	0	0
			31	20	5	6			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).

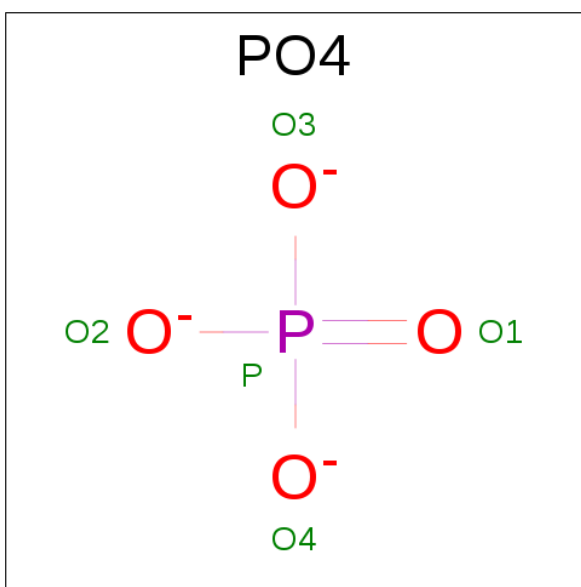


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

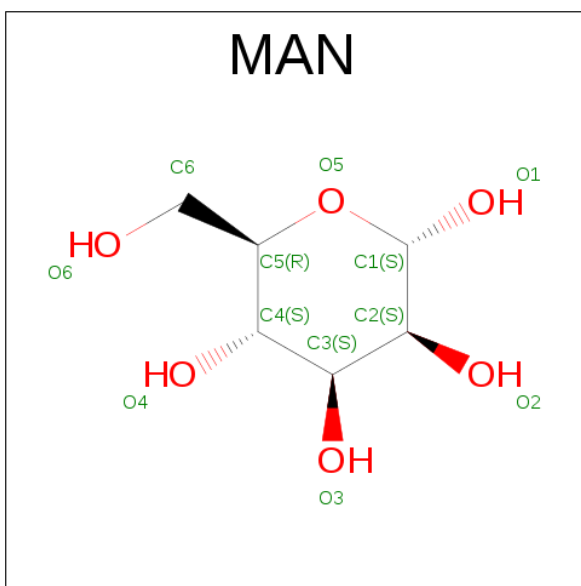
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



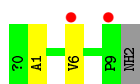
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is water.

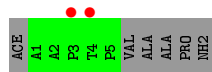
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total 51	O 51	0	0
7	B	48	Total 48	O 48	0	0
7	G	2	Total 2	O 2	0	0







- Molecule 2: mannosyl-peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.16Å 126.54Å 172.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.37 – 2.60 46.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.37-2.60) 95.0 (46.37-2.60)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.199 , 0.238 0.193 , 0.234	Depositor DCC
$R_{free}$ test set	2224 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: UDP, MN, PO4, ACE, MAN

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	0.28	0/3334	0.48	1/4533 (0.0%)
1	B	0.30	0/4587	0.50	1/6233 (0.0%)
2	F	0.28	0/58	0.51	0/83
2	G	0.21	0/32	0.42	0/45
All	All	0.30	0/8011	0.49	2/10894 (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	A	626	VAL	C-N-CD	-5.80	107.85	120.60
1	B	261	LEU	CA-CB-CG	-5.20	103.34	115.30

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	3231	0	3143	24	0
1	B	4446	0	4356	56	0
2	F	58	0	59	2	0
2	G	31	0	32	0	0
3	A	25	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	11	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
6	F	11	0	10	0	0
6	G	11	0	10	0	0
7	A	51	0	0	0	0
7	B	48	0	0	1	0
7	G	2	0	0	0	0
All	All	7946	0	7632	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 80 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:102:GLU:HG2	1:B:241:LYS:HE2	1.56	0.88
1:B:254:CYS:O	1:B:266:ARG:NH2	2.11	0.84
1:B:435:GLU:HG3	1:B:615:PHE:CG	2.16	0.81
1:B:122:ASP:OD1	1:B:127:GLN:NE2	2.16	0.76
1:A:337:ILE:HD12	1:A:345:MET:HE2	1.70	0.73

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	394/578 (68%)	378 (96%)	16 (4%)	0	100	100
1	B	555/578 (96%)	537 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	8/11 (73%)	8 (100%)	0	0	100	100
2	G	3/11 (27%)	3 (100%)	0	0	100	100
All	All	960/1178 (82%)	926 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	357/504 (71%)	352 (99%)	5 (1%)	74	90
1	B	487/504 (97%)	483 (99%)	4 (1%)	86	95
2	F	5/5 (100%)	5 (100%)	0	100	100
2	G	3/5 (60%)	3 (100%)	0	100	100
All	All	852/1018 (84%)	843 (99%)	9 (1%)	84	93

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	617	LYS
1	B	635	LYS
1	B	278	VAL
1	A	509[A]	ASN
1	B	123	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	GLN
1	B	326	GLN
1	B	408	GLN
1	B	608	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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$
3	UDP	A	701	4	20,26,26	1.16	1 (5%)	24,40,40	1.40	1 (4%)
5	PO4	A	703	-	4,4,4	0.70	0	6,6,6	0.23	0
3	UDP	B	701	4	20,26,26	1.15	1 (5%)	24,40,40	1.40	2 (8%)
6	MAN	F	101	2	11,11,12	0.61	0	15,15,17	1.57	3 (20%)
6	MAN	G	101	2	11,11,12	1.02	1 (9%)	15,15,17	0.84	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
3	UDP	A	701	4	-	0/12/32/32	0/2/2/2
5	PO4	A	703	-	-	0/0/0/0	0/0/0/0
3	UDP	B	701	4	-	0/12/32/32	0/2/2/2
6	MAN	F	101	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	G	101	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	101	MAN	O5-C1	-2.63	1.39	1.43
3	B	701	UDP	C4-N3	3.03	1.38	1.33
3	A	701	UDP	C4-N3	3.05	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	MAN	O2-C2-C3	-2.26	105.63	110.19
6	G	101	MAN	O2-C2-C3	-2.12	105.91	110.19
3	B	701	UDP	C4'-O4'-C1'	2.04	111.81	109.64
6	F	101	MAN	O5-C1-C2	2.60	115.05	110.89
6	F	101	MAN	C1-O5-C5	4.17	118.27	112.14

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	394/578 (68%)	-0.16	11 (2%) 56 49	32, 51, 98, 163	0
1	B	551/578 (95%)	-0.01	18 (3%) 50 43	33, 56, 97, 129	0
2	F	9/11 (81%)	1.29	2 (22%) 1 0	65, 77, 115, 121	0
2	G	5/11 (45%)	1.87	2 (40%) 0 0	102, 115, 140, 162	0
All	All	959/1178 (81%)	-0.05	33 (3%) 49 41	32, 54, 100, 163	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	TYR	5.2
2	F	9	PRO	5.2
1	A	254	CYS	4.9
1	A	255	HIS	4.7
1	A	281	CYS	3.4

### 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](#)

There are no carbohydrates in this entry.

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	A	703	5/5	0.71	0.40	9.38	151,151,152,153	0
3	UDP	A	701	25/25	0.82	0.32	3.12	84,112,145,155	0
6	MAN	G	101	11/12	0.75	0.33	2.00	104,115,119,120	0
3	UDP	B	701	25/25	0.84	0.24	1.67	105,124,174,174	0
6	MAN	F	101	11/12	0.90	0.18	-0.03	47,62,73,76	0
4	MN	B	702	1/1	0.32	0.23	-	176,176,176,176	0
4	MN	A	702	1/1	0.81	0.08	-	157,157,157,157	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.