



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2017 – 10:56 AM EST

PDB ID : 5GVV
Title : Crystal structure of the glycosyltransferase GlyE in *Streptococcus pneumoniae* TIGR4
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Deposited on : 2016-09-07
Resolution : 1.95 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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-20028442
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-20028442

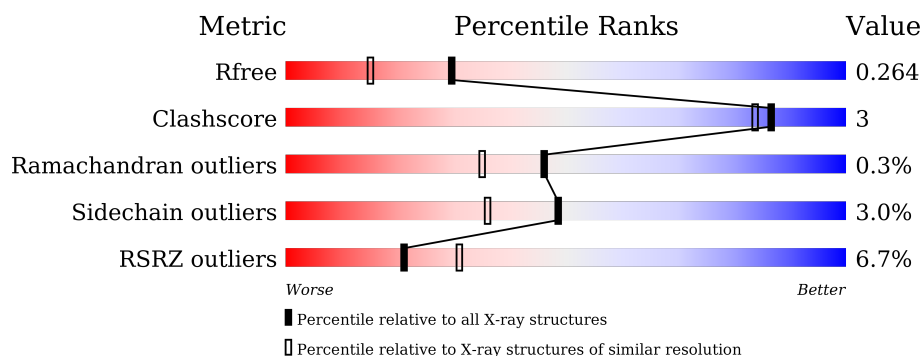
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 ≥ 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	406	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>• •</div> </div> </div>
1	F	406	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6995 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.

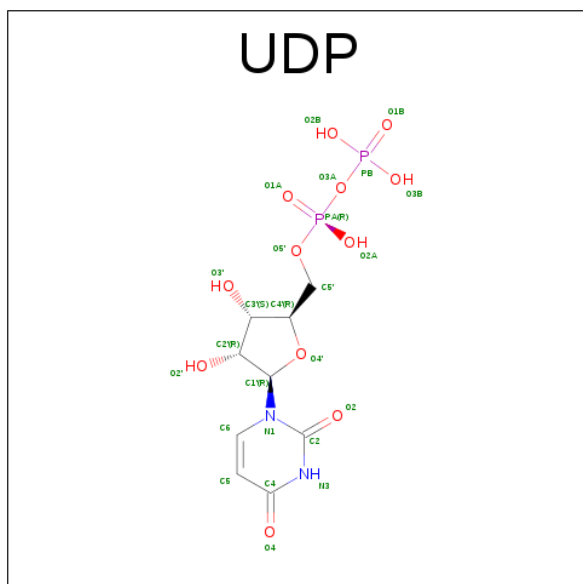
- Molecule 1 is a protein called Glycosyl transferase family 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	Se	0	0	0
			3222	2088	519	599	6	10			
1	F	385	Total	C	N	O	S	Se	0	0	0
			3168	2057	509	586	6	10			

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

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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

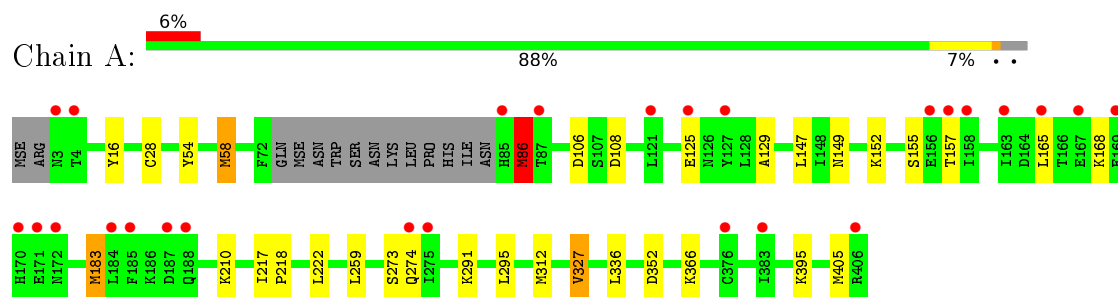
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	272	Total	O	0	0
			272	272		
4	F	281	Total	O	0	0
			281	281		

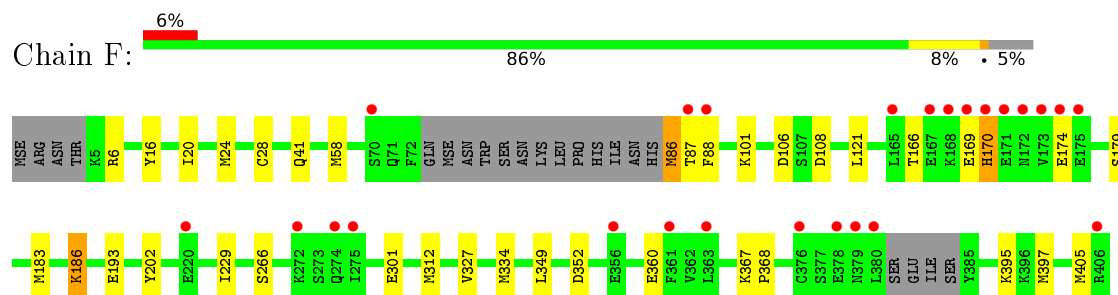
3 Residue-property plots [i](#)

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: Glycosyl transferase family 8



- Molecule 1: Glycosyl transferase family 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.17Å 88.21Å 128.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 1.95 48.81 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.81-1.95) 97.5 (48.81-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.257 0.212 , 0.264	Depositor DCC
R_{free} test set	3105 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	1.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6995	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 28.51 % 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 1.8190e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0/3293	0.51	3/4448 (0.1%)
1	F	0.33	0/3238	0.50	2/4373 (0.0%)
All	All	0.32	0/6531	0.51	5/8821 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	MSE	N-CA-C	8.07	132.78	111.00
1	F	86	MSE	CB-CA-C	-7.42	95.55	110.40
1	F	86	MSE	N-CA-CB	-5.86	100.05	110.60
1	A	58	MSE	CG-SE-CE	5.16	110.25	98.90
1	A	405	MSE	CB-CA-C	-5.03	100.33	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3222	0	3155	15	0
1	F	3168	0	3107	20	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	11	0	0
3	F	25	0	11	0	0
4	A	272	0	0	0	0
4	F	281	0	0	4	0
All	All	6995	0	6284	34	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 (34) 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:210:LYS:HD3	1:F:334:MSE:HE3	1.60	0.83
1:A:28:CYS:HB3	1:A:58:MSE:HE1	1.61	0.82
1:A:165:LEU:HD21	1:A:183:MSE:HG2	1.68	0.76
1:F:28:CYS:HB3	1:F:58:MSE:HE1	1.74	0.68
1:A:312:MSE:SE	1:A:327:VAL:HG13	2.48	0.63
1:F:193:GLU:OE2	4:F:601:HOH:O	2.17	0.57
1:F:20:ILE:O	1:F:24:MSE:HG3	2.07	0.55
1:F:101:LYS:NZ	1:F:121:LEU:O	2.43	0.50
1:F:28:CYS:CB	1:F:58:MSE:HE1	2.42	0.49
1:F:312:MSE:SE	1:F:327:VAL:HG13	2.62	0.49
1:F:41:GLN:NE2	4:F:605:HOH:O	2.30	0.47
1:A:28:CYS:CB	1:A:58:MSE:HE1	2.37	0.46
1:F:179:SER:O	1:F:183:MSE:HG3	2.16	0.46
1:A:395:LYS:HE2	1:A:395:LYS:H	1.81	0.45
1:A:149:ASN:ND2	1:A:152:LYS:HG3	2.31	0.45
1:F:186:LYS:HG3	1:F:186:LYS:H	1.53	0.45
1:A:106:ASP:HB3	1:A:108:ASP:OD1	2.17	0.45
1:A:129:ALA:HB3	1:A:147:LEU:HB3	2.00	0.44
1:F:202:TYR:HB2	1:F:229:ILE:HD11	2.00	0.43
1:F:352:ASP:OD1	4:F:602:HOH:O	2.21	0.43
1:F:367:LYS:HA	1:F:368:PRO:HD2	1.91	0.43
1:F:395:LYS:HB2	1:F:395:LYS:HE3	1.59	0.43
1:F:106:ASP:HB3	1:F:108:ASP:OD1	2.19	0.43
1:F:166:THR:O	1:F:170:HIS:HB3	2.19	0.42
1:A:217:ILE:HA	1:A:218:PRO:HD3	1.88	0.42
1:A:54:TYR:CD1	1:A:259:LEU:HD11	2.55	0.42
1:A:291:LYS:O	1:A:295:LEU:HG	2.19	0.41
1:F:6:ARG:N	1:F:6:ARG:HD3	2.35	0.41
1:F:86:MSE:O	1:F:88:PHE:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HE3	1:A:152:LYS:HB3	1.68	0.41
1:A:168:LYS:HB3	1:A:168:LYS:HE2	1.82	0.41
1:A:366:LYS:HE2	1:A:366:LYS:HB2	1.67	0.41
1:F:301:GLU:OE2	4:F:603:HOH:O	2.22	0.41
1:F:301:GLU:CG	1:F:405:MSE:HE1	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	388/406 (96%)	380 (98%)	7 (2%)	1 (0%)	46	35
1	F	379/406 (93%)	368 (97%)	10 (3%)	1 (0%)	46	35
All	All	767/812 (94%)	748 (98%)	17 (2%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	87	THR
1	A	86	MSE

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	355/357 (99%)	343 (97%)	12 (3%)	44	30
1	F	348/357 (98%)	339 (97%)	9 (3%)	54	43
All	All	703/714 (98%)	682 (97%)	21 (3%)	48	36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	86	MSE
1	A	125	GLU
1	A	155	SER
1	A	157	THR
1	A	183	MSE
1	A	222	LEU
1	A	273	SER
1	A	274	GLN
1	A	327	VAL
1	A	336	LEU
1	A	352	ASP
1	F	16	TYR
1	F	169	GLU
1	F	170	HIS
1	F	174	GLU
1	F	186	LYS
1	F	266	SER
1	F	349	LEU
1	F	360	GLU
1	F	397	MSE

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

Mol	Chain	Res	Type
1	F	379	ASN

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 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$
3	UDP	A	502	2	20,26,26	1.15	1 (5%)	24,40,40	1.36	1 (4%)
3	UDP	F	502	2	20,26,26	1.15	1 (5%)	24,40,40	1.33	1 (4%)

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	502	2	-	0/12/32/32	0/2/2/2
3	UDP	F	502	2	-	0/12/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	UDP	C4-N3	3.00	1.38	1.33
3	A	502	UDP	C4-N3	3.08	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	F	502	UDP	C4-N3-C2	5.03	119.51	114.21
3	A	502	UDP	C4-N3-C2	5.34	119.84	114.21

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

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, 95th 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 ²)	Q<0.9
1	A	382/406 (94%)	0.56	26 (6%) 20 30	10, 19, 41, 63	0
1	F	375/406 (92%)	0.59	25 (6%) 21 31	10, 20, 42, 61	0
All	All	757/812 (93%)	0.57	51 (6%) 21 31	10, 20, 42, 63	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	274	GLN	6.1
1	A	4	THR	4.9
1	F	363	LEU	4.1
1	A	163	ILE	4.0
1	F	378	GLU	3.8
1	A	87	THR	3.7
1	A	127	TYR	3.6
1	A	187	ASP	3.6
1	A	171	GLU	3.5
1	F	272	LYS	3.5
1	A	85	HIS	3.5
1	F	356	GLU	3.4
1	F	87	THR	3.3
1	A	184	LEU	3.3
1	A	156	GLU	3.2
1	F	70	SER	3.1
1	A	274	GLN	3.1
1	A	3	ASN	3.1
1	F	174	GLU	3.0
1	F	170	HIS	3.0
1	A	383	ILE	3.0
1	A	188	GLN	2.9
1	F	380	LEU	2.9
1	F	172	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	169	GLU	2.8
1	A	172	ASN	2.8
1	A	406	ARG	2.7
1	F	171	GLU	2.7
1	F	167	GLU	2.6
1	F	376	CYS	2.6
1	F	406	ARG	2.6
1	A	158	ILE	2.5
1	F	275	ILE	2.5
1	F	88	PHE	2.5
1	A	169	GLU	2.5
1	F	379	ASN	2.5
1	A	157	THR	2.3
1	F	165	LEU	2.3
1	A	167	GLU	2.3
1	F	220	GLU	2.3
1	A	185	PHE	2.3
1	A	275	ILE	2.3
1	A	125	GLU	2.3
1	A	170	HIS	2.3
1	F	168	LYS	2.2
1	F	175	GLU	2.2
1	F	173	VAL	2.1
1	F	361	PHE	2.1
1	A	121	LEU	2.1
1	A	165	LEU	2.1
1	A	376	CYS	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](#)

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, 95th 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(Å ²)	Q<0.9
3	UDP	A	502	25/25	0.93	0.15	-0.02	17,25,30,31	0
3	UDP	F	502	25/25	0.93	0.12	-0.29	16,24,28,30	0
2	MN	F	501	1/1	0.93	0.11	-0.87	29,29,29,29	0
2	MN	A	501	1/1	0.86	0.10	-	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.