



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:49 am GMT

PDB ID : 4FKZ
Title : Crystal structure of Bacillus subtilis UDP-GlcNAc 2-epimerase in complex with UDP-GlcNAc and UDP
Authors : Yang, C.S.; Chen, S.C.; Kuan, S.M.; Chen, Y.R.; Liu, Y.H.; Chen, Y.
Deposited on : 2012-06-14
Resolution : 1.69 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

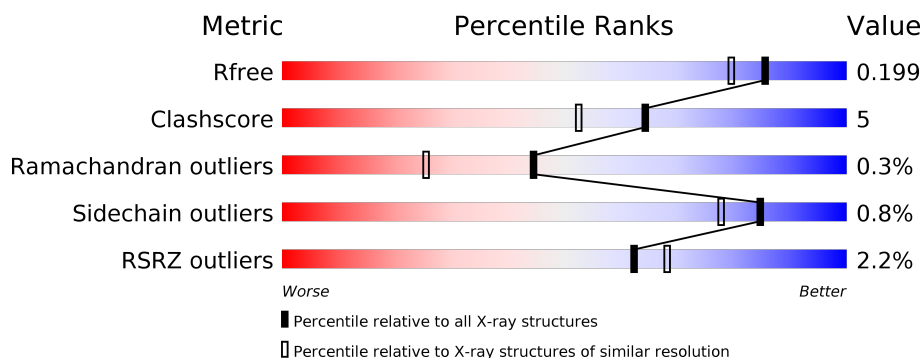
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	388	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	B	388	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7153 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.

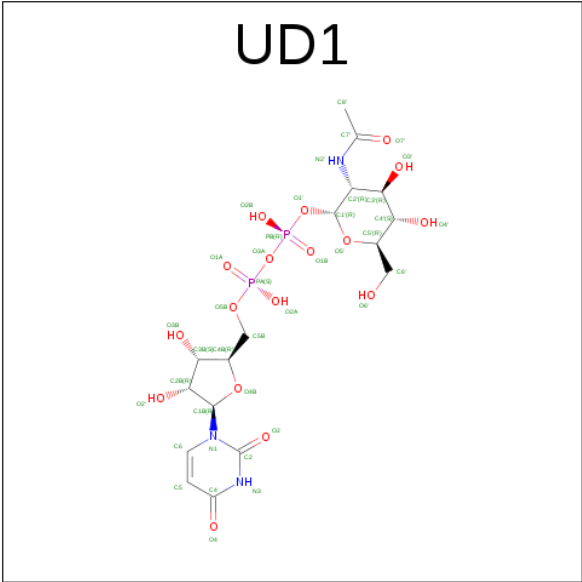
- Molecule 1 is a protein called UDP-N-acetylglucosamine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3042	1925	528	580	9			
1	B	376	Total	C	N	O	S	0	0	0
			2975	1884	513	569	9			

There are 16 discrepancies between the modelled and reference sequences:

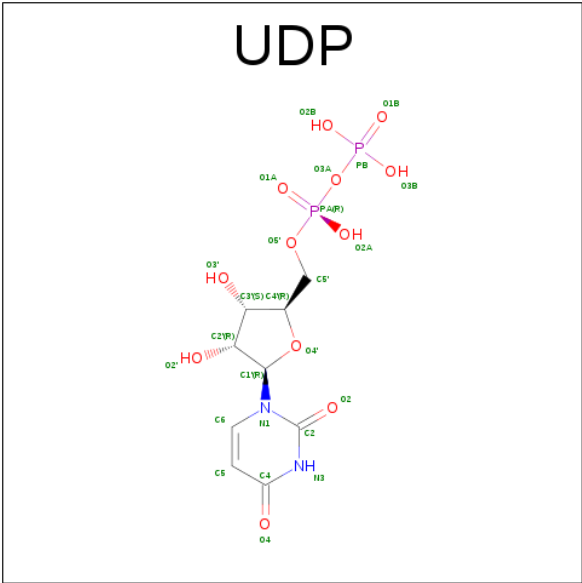
Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LEU	-	EXPRESSION TAG	UNP P39131
A	382	GLU	-	EXPRESSION TAG	UNP P39131
A	383	HIS	-	EXPRESSION TAG	UNP P39131
A	384	HIS	-	EXPRESSION TAG	UNP P39131
A	385	HIS	-	EXPRESSION TAG	UNP P39131
A	386	HIS	-	EXPRESSION TAG	UNP P39131
A	387	HIS	-	EXPRESSION TAG	UNP P39131
A	388	HIS	-	EXPRESSION TAG	UNP P39131
B	381	LEU	-	EXPRESSION TAG	UNP P39131
B	382	GLU	-	EXPRESSION TAG	UNP P39131
B	383	HIS	-	EXPRESSION TAG	UNP P39131
B	384	HIS	-	EXPRESSION TAG	UNP P39131
B	385	HIS	-	EXPRESSION TAG	UNP P39131
B	386	HIS	-	EXPRESSION TAG	UNP P39131
B	387	HIS	-	EXPRESSION TAG	UNP P39131
B	388	HIS	-	EXPRESSION TAG	UNP P39131

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	546	Total 546	O 546	0	0
4	B	462	Total 462	O 462	0	0

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- Molecule 1: UDP-N-acetylglucosamine 2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.29Å 209.34Å 46.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 1.69 32.29 – 1.69	Depositor EDS
% Data completeness (in resolution range)	98.0 (32.29-1.69) 98.0 (32.29-1.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.199 0.170 , 0.199	Depositor DCC
R_{free} test set	4989 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7153	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, UD1

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	0.47	0/3106	0.58	0/4205
1	B	0.45	0/3036	0.57	0/4111
All	All	0.46	0/6142	0.58	0/8316

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

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	3042	0	3014	34	0
1	B	2975	0	2953	24	0
2	A	39	0	25	2	0
2	B	39	0	25	1	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
4	A	546	0	0	15	0
4	B	462	0	0	11	0
All	All	7153	0	6039	58	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 (58) 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:380:LYS:HD2	1:A:381:LEU:H	1.25	1.01
1:B:185:ARG:H	1:B:272:ASN:HD21	1.15	0.94
1:A:190:HIS:HD2	1:A:192:VAL:H	1.23	0.86
1:B:154:GLN:HG2	4:B:922:HOH:O	1.79	0.82
1:A:354:GLU:OE1	1:A:357:ARG:CZ	2.32	0.77
1:B:89:LYS:HB3	4:B:923:HOH:O	1.85	0.76
1:A:70:LEU:HA	4:A:1040:HOH:O	1.91	0.69
1:A:380:LYS:CD	1:A:381:LEU:H	2.04	0.69
1:B:190:HIS:HD2	1:B:192:VAL:H	1.42	0.67
1:A:234:GLN:OE1	1:A:260:HIS:HE1	1.80	0.65
1:A:19:MET:HB3	4:A:1041:HOH:O	1.97	0.65
1:A:190:HIS:CD2	1:A:192:VAL:H	2.10	0.65
1:A:23:VAL:HG23	4:A:1041:HOH:O	1.97	0.62
1:B:185:ARG:N	1:B:272:ASN:HD21	1.93	0.62
1:A:383:HIS:O	1:A:384:HIS:HB2	2.00	0.61
1:A:148:HIS:HD2	4:A:509:HOH:O	1.82	0.60
1:A:366:HIS:HE1	4:A:553:HOH:O	1.84	0.59
1:B:82:ASP:OD1	1:B:112:HIS:HE1	1.86	0.59
1:A:73:ILE:HD12	4:A:1040:HOH:O	2.02	0.59
1:A:185:ARG:H	1:A:272:ASN:HD21	1.50	0.58
1:A:136:LEU:HD13	4:B:947:HOH:O	2.05	0.57
1:B:190:HIS:CD2	1:B:192:VAL:H	2.22	0.56
1:A:89:LYS:HG3	4:A:1009:HOH:O	2.07	0.55
1:A:151:PRO:HG2	4:A:573:HOH:O	2.06	0.54
1:A:88:ILE:HB	4:A:944:HOH:O	2.07	0.54
1:B:114:ILE:HD11	4:B:916:HOH:O	2.07	0.54
1:A:379:GLY:HA3	1:A:380:LYS:HE3	1.89	0.53
1:A:380:LYS:O	1:A:383:HIS:O	2.27	0.53
1:A:114:ILE:HD11	4:A:1009:HOH:O	2.08	0.52
1:B:185:ARG:H	1:B:272:ASN:ND2	1.96	0.52
1:B:234:GLN:OE1	1:B:260:HIS:HE1	1.93	0.51
1:A:383:HIS:O	1:A:384:HIS:CB	2.58	0.51
1:B:148:HIS:HD2	4:B:506:HOH:O	1.93	0.51
1:A:82:ASP:OD1	1:A:112:HIS:HE1	1.94	0.51
1:A:190:HIS:HE1	4:A:798:HOH:O	1.94	0.50
1:B:81:LEU:HD13	1:B:105:GLY:HA2	1.94	0.50
1:B:223:ILE:HD11	1:B:281:LEU:HD13	1.95	0.49
1:B:88:ILE:HB	4:B:682:HOH:O	2.12	0.49
1:B:266:GLU:HG2	4:B:569:HOH:O	2.13	0.48
1:B:207:HIS:HD2	4:B:520:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:HG3	1:A:309:GLU:OE2	2.13	0.47
1:A:81:LEU:HD13	1:A:105:GLY:HA2	1.96	0.47
1:B:195:GLN:HE21	1:B:260:HIS:CD2	2.33	0.46
1:A:148:HIS:HE1	4:A:578:HOH:O	2.00	0.45
1:B:18:LYS:HE2	1:B:176:ALA:HB2	1.99	0.45
1:A:207:HIS:HD2	4:A:517:HOH:O	2.00	0.45
1:A:354:GLU:OE1	1:A:357:ARG:NH2	2.50	0.45
1:B:148:HIS:HE1	4:B:603:HOH:O	2.01	0.44
1:B:154:GLN:HG3	4:B:696:HOH:O	2.18	0.43
1:A:100:THR:OG1	2:A:401:UD1:H8'1	2.18	0.43
1:B:361:GLU:OE1	1:B:374:PRO:HB3	2.20	0.42
1:A:234:GLN:OE1	1:A:260:HIS:CE1	2.67	0.42
1:A:73:ILE:HB	4:A:1040:HOH:O	2.19	0.41
1:B:10:PHE:O	1:B:38:VAL:HA	2.20	0.41
1:A:207:HIS:CD2	4:A:517:HOH:O	2.72	0.41
1:B:167:ASP:HB2	4:B:616:HOH:O	2.20	0.41
1:B:42:HIS:CD2	2:B:401:UD1:H5	2.55	0.41
1:A:207:HIS:HE1	2:A:401:UD1:O4'	2.05	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	382/388 (98%)	374 (98%)	6 (2%)	2 (0%)	32	15
1	B	374/388 (96%)	369 (99%)	5 (1%)	0	100	100
All	All	756/776 (97%)	743 (98%)	11 (2%)	2 (0%)	44	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	LYS
1	A	384	HIS

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	330/334 (99%)	328 (99%)	2 (1%)	89	84
1	B	323/334 (97%)	320 (99%)	3 (1%)	82	74
All	All	653/668 (98%)	648 (99%)	5 (1%)	85	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	GLU
1	A	380	LYS
1	B	167	ASP
1	B	306	GLU
1	B	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	112	HIS
1	A	139	GLN
1	A	148	HIS
1	A	190	HIS
1	A	207	HIS
1	A	260	HIS
1	A	272	ASN
1	A	348	ASN
1	A	366	HIS
1	B	48	GLN
1	B	112	HIS

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Mol	Chain	Res	Type
1	B	148	HIS
1	B	190	HIS
1	B	195	GLN
1	B	207	HIS
1	B	252	HIS
1	B	260	HIS
1	B	272	ASN
1	B	348	ASN
1	B	366	HIS

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	UD1	A	401	-	34,41,41	0.70	0	43,62,62	1.45	1 (2%)
3	UDP	A	402	-	21,26,26	0.96	1 (4%)	22,40,40	1.76	1 (4%)
2	UD1	B	401	-	34,41,41	0.69	0	43,62,62	1.42	1 (2%)
3	UDP	B	402	-	21,26,26	0.95	1 (4%)	22,40,40	1.94	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
2	UD1	A	401	-	-	0/22/63/63	0/3/3/3
3	UDP	A	402	-	-	0/12/32/32	0/2/2/2
2	UD1	B	401	-	-	0/22/63/63	0/3/3/3
3	UDP	B	402	-	-	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	B	402	UDP	O4'-C1'	2.08	1.44	1.41
3	A	402	UDP	O4'-C1'	2.69	1.45	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	UDP	C4-N3-C2	7.08	120.21	114.13
2	B	401	UD1	C4-N3-C2	7.61	120.67	114.13
3	B	402	UDP	C4-N3-C2	8.02	121.02	114.13
2	A	401	UD1	C4-N3-C2	8.03	121.03	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UD1	2	0
2	B	401	UD1	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 [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, 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	384/388 (98%)	-0.12	7 (1%) 69 74	10, 16, 29, 50	0
1	B	376/388 (96%)	0.01	10 (2%) 55 60	11, 18, 36, 52	0
All	All	760/776 (97%)	-0.06	17 (2%) 62 68	10, 17, 34, 52	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ASP	4.7
1	B	255	ASP	4.6
1	A	383	HIS	3.9
1	B	372	GLU	3.1
1	A	384	HIS	3.1
1	B	198	GLU	3.0
1	B	257	ASP	3.0
1	B	371	LYS	2.9
1	B	195	GLN	2.5
1	A	380	LYS	2.5
1	B	231	GLU	2.5
1	A	187	GLY	2.4
1	B	338	ASP	2.4
1	A	382	GLU	2.2
1	A	195	GLN	2.1
1	B	214	GLU	2.1
1	B	2	LYS	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(\AA^2)	Q<0.9
3	UDP	A	402	25/25	0.98	0.09	-0.09	12,13,14,14	0
3	UDP	B	402	25/25	0.98	0.08	-0.70	13,14,15,16	0
2	UD1	B	401	39/39	0.98	0.07	-0.99	11,12,15,15	0
2	UD1	A	401	39/39	0.99	0.06	-1.05	10,11,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.