



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1ON8  
Title : Crystal structure of mouse alpha-1,4-N-acetylhexosaminyltransferase (EXTL2) with UDP and GlcUAb(1-3)Galb(1-O)-naphthalenelmethanol an acceptor substrate analog  
Authors : Pedersen, L.C.; Dong, J.; Taniguchi, F.; Kitagawa, H.; Krahn, J.M.; Pedersen, L.G.; Sugahara, K.; Negishi, M.  
Deposited on : 2003-02-27  
Resolution : 2.70 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

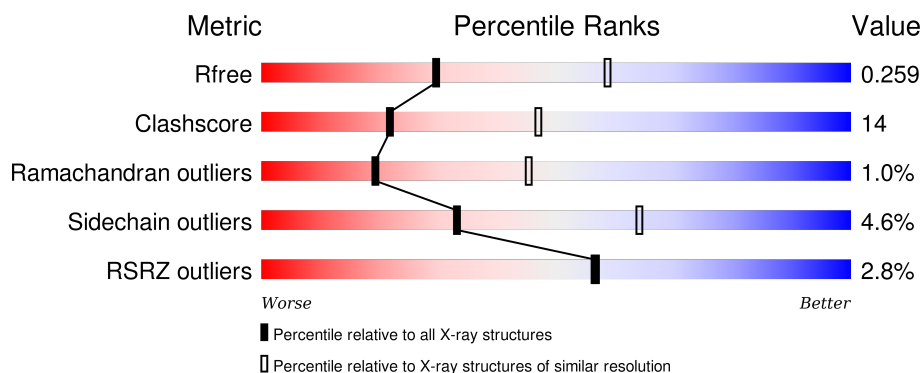
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	293	<div> <div>3%</div> <div>64%</div> <div>25%</div> <div>•</div> <div>10%</div> </div>
1	B	293	<div> <div>2%</div> <div>61%</div> <div>27%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4393 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 Alpha-1,4-N-acetylhexosaminyltransferase EXTL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2110	1362	354	383	11			
1	B	262	Total	C	N	O	S	0	0	0
			2078	1342	348	377	11			

- Molecule 2 is a polymer of unknown type called SUGAR (GCU-GAL).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			24	12	12		
2	B	2	Total	C	O	0	0
			24	12	12		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

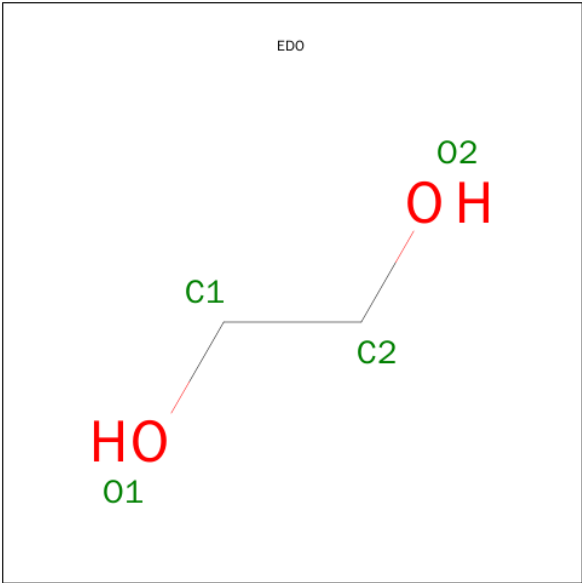
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total 53	O 53	0	0
6	B	44	Total 44	O 44	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.16 Å   125.16 Å   83.69 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.98-2.70) 96.8 (19.98-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.71 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.192   ,   0.254 0.195   ,   0.259	Depositor DCC
$R_{free}$ test set	888 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18472 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GAL, UDP, MN, EDO, BDP

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	0.38	0/2169	0.63	0/2949
1	B	0.36	0/2135	0.60	0/2906
All	All	0.37	0/4304	0.61	0/5855

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	2110	0	2051	57	0
1	B	2078	0	2015	63	0
2	A	24	0	17	0	0
2	B	24	0	17	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	53	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	0	4	0
All	All	4393	0	4134	118	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 14.

All (118) 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:288:GLU:O	1:A:292:GLN:HB2	1.75	0.86
1:B:71:MET:CE	1:B:80:LEU:HD12	2.19	0.72
1:A:318:GLN:HE22	1:B:205:ASN:HB3	1.56	0.71
1:B:238:ILE:HD12	1:B:245:ASP:HA	1.71	0.71
1:A:214:ILE:HG12	1:A:246:ASP:HB3	1.71	0.70
1:B:226:LEU:HD23	1:B:252:LEU:HD21	1.73	0.70
1:A:79:LEU:HD22	1:A:277:THR:HB	1.72	0.70
1:B:64:LEU:O	1:B:64:LEU:HD23	1.92	0.70
1:B:146:ALA:HB2	1:B:168:TRP:CZ3	2.27	0.69
1:B:71:MET:HE3	1:B:80:LEU:HD12	1.76	0.67
1:B:272:ASN:OD1	1:B:274:GLU:HB2	1.94	0.66
1:A:71:MET:CE	1:A:80:LEU:HD12	2.26	0.65
1:B:133:ARG:HG2	6:B:636:HOH:O	1.97	0.65
1:A:147:VAL:HG23	1:A:221:SER:HB3	1.77	0.65
1:B:133:ARG:HD3	1:B:239:ASP:OD1	1.96	0.64
1:B:64:LEU:HD12	1:B:145:ASN:ND2	2.13	0.64
1:A:199:GLN:HE21	1:A:200:THR:HG22	1.64	0.63
1:A:201:PRO:HG3	1:A:311:TYR:CE1	2.34	0.63
1:B:63:ALA:C	1:B:65:ASP:H	2.02	0.62
1:B:146:ALA:HB2	1:B:168:TRP:CH2	2.34	0.62
1:B:182:LYS:HD2	6:B:640:HOH:O	1.98	0.62
1:A:307:MET:HE1	1:A:309:LEU:HB2	1.81	0.61
1:B:90:VAL:HG21	1:B:161:LEU:HD12	1.82	0.61
1:A:238:ILE:HD12	1:A:245:ASP:HA	1.82	0.61
1:A:182:LYS:HG2	1:A:183:HIS:N	2.15	0.60
1:B:87:TYR:O	1:B:93:LEU:HD22	2.02	0.60
1:A:146:ALA:HB2	1:A:168:TRP:CH2	2.37	0.59
1:B:307:MET:HE1	1:B:309:LEU:HB2	1.84	0.59
1:A:95:LYS:HD3	1:A:123:ILE:HD12	1.85	0.58
1:B:243:ASN:O	1:B:244:CYS:HB2	2.03	0.58
1:B:197:GLU:H	1:B:197:GLU:CD	2.07	0.58
1:A:120:ILE:HD13	1:A:120:ILE:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HE2	1:A:201:PRO:HD3	1.88	0.56
1:A:146:ALA:HB2	1:A:168:TRP:CZ3	2.41	0.56
1:B:120:ILE:H	1:B:120:ILE:HD13	1.70	0.55
1:B:71:MET:HE2	1:B:80:LEU:HD12	1.88	0.55
1:A:91:PRO:O	1:A:92:SER:HB2	2.08	0.54
1:A:274:GLU:O	1:A:277:THR:HG22	2.09	0.53
1:B:292:GLN:O	1:B:295:TYR:HB3	2.09	0.53
1:A:306:GLY:O	1:A:308:PRO:HD3	2.09	0.53
1:B:133:ARG:NH1	1:B:235:HIS:HB3	2.24	0.53
1:A:168:TRP:HA	1:A:176:ILE:HG13	1.91	0.52
1:B:214:ILE:HG12	1:B:246:ASP:HB3	1.91	0.52
1:B:73:THR:HB	1:B:80:LEU:HD13	1.90	0.52
1:A:201:PRO:HG2	1:A:202:GLY:N	2.25	0.52
1:B:243:ASN:OD1	1:B:244:CYS:N	2.43	0.51
1:A:71:MET:HE3	1:A:80:LEU:HD12	1.92	0.51
1:B:230:GLN:NE2	1:B:304:TYR:OH	2.42	0.51
1:B:272:ASN:OD1	1:B:274:GLU:CB	2.59	0.51
1:B:284:TRP:HA	1:B:289:HIS:CG	2.46	0.51
1:A:137:GLN:HA	1:A:228:GLN:NE2	2.25	0.50
1:A:95:LYS:HD3	1:A:123:ILE:CD1	2.42	0.49
1:A:252:LEU:C	1:A:252:LEU:HD23	2.32	0.49
1:A:252:LEU:HD23	1:A:253:VAL:N	2.27	0.49
1:B:112:TRP:CZ2	1:B:122:VAL:HG21	2.48	0.49
1:A:243:ASN:OD1	1:A:244:CYS:N	2.38	0.49
1:B:79:LEU:HD22	1:B:277:THR:HB	1.94	0.49
1:B:63:ALA:C	1:B:65:ASP:N	2.64	0.48
1:A:171:PHE:N	1:A:172:PRO:HD3	2.27	0.48
1:B:194:GLY:HA3	1:B:198:LEU:HD12	1.95	0.48
1:B:318:GLN:HB3	1:B:321:PHE:HB3	1.95	0.48
1:B:191:TYR:CZ	1:B:307:MET:HG3	2.49	0.47
1:B:168:TRP:HA	1:B:176:ILE:HG13	1.97	0.47
1:A:86:HIS:CD2	1:A:155:LEU:HD13	2.48	0.47
1:B:243:ASN:O	1:B:244:CYS:CB	2.61	0.47
1:A:120:ILE:HD13	1:A:120:ILE:N	2.30	0.47
1:A:150:VAL:HA	1:A:215:GLY:O	2.14	0.47
1:B:64:LEU:HD12	1:B:145:ASN:HD22	1.79	0.47
1:B:150:VAL:HA	1:B:215:GLY:O	2.14	0.47
1:A:297:ILE:O	1:A:301:VAL:HG23	2.15	0.47
1:A:227:PHE:HA	1:A:252:LEU:CD1	2.45	0.46
1:A:163:PHE:CD1	1:A:318:GLN:HG3	2.51	0.46
1:B:180:PRO:HD3	1:B:264:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:O	1:A:188:SER:C	2.54	0.46
1:A:187:SER:HB3	1:A:190:ILE:HB	1.96	0.46
1:B:194:GLY:HA3	1:B:198:LEU:CD1	2.46	0.46
1:B:301:VAL:CG2	1:B:307:MET:HG2	2.46	0.46
1:A:110:GLU:HB3	6:A:647:HOH:O	2.16	0.46
1:B:149:MET:SD	1:B:214:ILE:HD12	2.56	0.46
1:B:297:ILE:O	1:B:301:VAL:HG23	2.16	0.46
1:A:201:PRO:CG	1:A:202:GLY:N	2.79	0.45
1:B:150:VAL:HG12	1:B:151:ASP:O	2.16	0.45
1:A:72:GLN:HA	1:A:99:VAL:HB	1.97	0.45
1:B:214:ILE:HA	1:B:217:SER:OG	2.17	0.45
1:B:125:LYS:HD3	1:B:139:PHE:CD2	2.51	0.45
1:A:272:ASN:OD1	1:A:274:GLU:HG3	2.17	0.44
1:A:125:LYS:HD3	1:A:139:PHE:CE2	2.53	0.44
1:B:222:LYS:HG3	6:B:621:HOH:O	2.18	0.43
1:A:134:ASN:O	1:A:137:GLN:HG3	2.18	0.43
1:B:171:PHE:N	1:B:172:PRO:HD3	2.34	0.43
1:B:162:VAL:HG13	6:B:616:HOH:O	2.17	0.43
1:A:149:MET:HB3	1:A:214:ILE:O	2.19	0.43
1:B:79:LEU:HD13	1:B:276:GLU:O	2.19	0.43
1:A:131:LYS:HB3	1:A:133:ARG:HG2	2.00	0.42
1:B:124:PHE:O	1:B:126:PRO:HD3	2.19	0.42
1:B:238:ILE:HD12	1:B:245:ASP:CA	2.47	0.42
1:B:252:LEU:HD23	1:B:252:LEU:C	2.40	0.42
1:A:182:LYS:CG	1:A:183:HIS:N	2.82	0.42
1:A:201:PRO:HG2	1:A:202:GLY:H	1.84	0.42
1:A:224:LEU:O	1:A:228:GLN:HG2	2.19	0.42
1:B:259:LYS:HB3	1:B:260:PRO:CD	2.50	0.42
1:B:120:ILE:HD13	1:B:120:ILE:N	2.33	0.42
1:A:251:PHE:O	1:A:255:ARG:HG3	2.19	0.42
1:A:228:GLN:HG3	6:A:617:HOH:O	2.19	0.42
1:A:133:ARG:HD2	1:A:239:ASP:OD1	2.20	0.42
1:A:155:LEU:HD12	1:A:155:LEU:C	2.40	0.41
1:A:201:PRO:CD	1:A:202:GLY:H	2.33	0.41
1:B:250:ASN:O	1:B:254:THR:HG22	2.20	0.41
1:A:73:THR:HG21	1:A:80:LEU:HD22	2.03	0.41
1:B:201:PRO:HG2	1:B:202:GLY:H	1.86	0.41
1:B:107:GLY:HA2	1:B:108:PRO:HD3	1.86	0.41
1:B:201:PRO:HG3	1:B:311:TYR:CE1	2.56	0.41
1:B:224:LEU:O	1:B:228:GLN:HG2	2.21	0.41
1:A:205:ASN:HB2	1:B:318:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ILE:HD12	1:B:263:ILE:HB	2.02	0.40
1:A:133:ARG:NH1	1:A:239:ASP:OD2	2.53	0.40
1:A:112:TRP:CZ2	1:A:122:VAL:HG21	2.55	0.40
1:A:201:PRO:CG	1:A:202:GLY:H	2.35	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	263/293 (90%)	243 (92%)	18 (7%)	2 (1%)	24	51
1	B	258/293 (88%)	234 (91%)	21 (8%)	3 (1%)	16	39
All	All	521/586 (89%)	477 (92%)	39 (8%)	5 (1%)	19	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	B	203	PRO
1	A	202	GLY
1	B	204	GLY
1	B	276	GLU

### 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	230/263 (88%)	218 (95%)	12 (5%)	29	58
1	B	227/263 (86%)	218 (96%)	9 (4%)	38	69
All	All	457/526 (87%)	436 (95%)	21 (5%)	33	64

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

Mol	Chain	Res	Type
1	A	84	LEU
1	A	120	ILE
1	A	143	GLU
1	A	155	LEU
1	A	182	LYS
1	A	186	THR
1	A	197	GLU
1	A	252	LEU
1	A	268	ILE
1	A	280	TYR
1	A	283	MET
1	A	288	GLU
1	B	84	LEU
1	B	120	ILE
1	B	182	LYS
1	B	186	THR
1	B	197	GLU
1	B	203	PRO
1	B	205	ASN
1	B	268	ILE
1	B	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	292	GLN
1	A	318	GLN
1	B	75	ASN
1	B	145	ASN
1	B	199	GLN
1	B	230	GLN
1	B	292	GLN

### 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 ⓘ

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$
2	BDP	A	509	2	10,13,13	4.03	6 (60%)	15,19,19	1.46	2 (13%)
2	GAL	A	510	2	11,11,12	1.41	2 (18%)	12,15,17	0.77	0
2	BDP	B	519	2	10,13,13	3.86	6 (60%)	15,19,19	1.44	4 (26%)
2	GAL	B	520	2	11,11,12	1.35	2 (18%)	12,15,17	0.72	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
2	BDP	A	509	2	-	0/0/24/24	0/1/1/1
2	GAL	A	510	2	-	0/2/18/22	0/1/1/1
2	BDP	B	519	2	-	0/0/24/24	0/1/1/1
2	GAL	B	520	2	-	0/2/18/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	509	BDP	O2-C2	-8.85	1.21	1.43
2	B	519	BDP	O2-C2	-8.35	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	519	BDP	C4-C5	-3.36	1.46	1.53
2	A	509	BDP	C4-C5	-3.23	1.46	1.53
2	B	519	BDP	C1-C2	2.02	1.56	1.52
2	A	509	BDP	C1-C2	2.06	1.56	1.52
2	A	509	BDP	O1-C1	2.13	1.47	1.39
2	A	510	GAL	C1-C2	2.14	1.54	1.52
2	B	519	BDP	O1-C1	2.28	1.47	1.39
2	B	520	GAL	C4-C5	2.48	1.56	1.52
2	B	520	GAL	C1-C2	2.65	1.54	1.52
2	A	510	GAL	C4-C5	3.01	1.57	1.52
2	A	509	BDP	O5-C1	4.66	1.51	1.43
2	B	519	BDP	O5-C1	4.85	1.52	1.43
2	B	519	BDP	O5-C5	5.74	1.51	1.43
2	A	509	BDP	O5-C5	6.45	1.52	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	519	BDP	C1-C2-C3	-2.11	107.30	110.43
2	A	509	BDP	C4-C3-C2	-2.09	106.89	110.79
2	B	519	BDP	O4-C4-C5	-2.07	106.52	110.42
2	B	519	BDP	C4-C3-C2	-2.04	106.99	110.79
2	B	519	BDP	C3-C4-C5	2.74	113.98	108.66
2	A	509	BDP	C3-C4-C5	2.96	114.40	108.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	351	3	18,26,26	1.77	3 (16%)	26,40,40	2.93	4 (15%)
5	EDO	A	401	-	3,3,3	2.07	2 (66%)	2,2,2	0.47	0
4	UDP	B	352	3	18,26,26	1.72	3 (16%)	26,40,40	2.88	6 (23%)
5	EDO	B	402	-	3,3,3	2.17	2 (66%)	2,2,2	0.46	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
4	UDP	A	351	3	-	0/12/32/32	0/2/2/2
5	EDO	A	401	-	-	0/1/1/1	0/0/0/0
4	UDP	B	352	3	-	0/12/32/32	0/2/2/2
5	EDO	B	402	-	-	0/1/1/1	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	EDO	O1-C1	2.14	1.53	1.42
5	B	402	EDO	O1-C1	2.17	1.53	1.42
5	A	401	EDO	O2-C2	2.74	1.56	1.42
5	B	402	EDO	O2-C2	2.94	1.57	1.42
4	A	351	UDP	PB-O1B	3.12	1.61	1.51
4	B	352	UDP	PB-O1B	3.22	1.61	1.51
4	A	351	UDP	C6-N1	3.34	1.40	1.35
4	B	352	UDP	C6-N1	3.42	1.40	1.35
4	B	352	UDP	C4-N3	4.54	1.41	1.33
4	A	351	UDP	C4-N3	4.77	1.42	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	351	UDP	C5-C4-N3	-2.91	115.66	123.12
4	B	352	UDP	C5-C4-N3	-2.89	115.70	123.12
4	B	352	UDP	O3A-PA-O5'	-2.27	96.92	102.94
4	B	352	UDP	C4'-O4'-C1'	2.15	112.08	109.72
4	A	351	UDP	O5'-C5'-C4'	2.56	118.55	109.12
4	B	352	UDP	O5'-C5'-C4'	2.75	119.25	109.12
4	B	352	UDP	O3B-PB-O1B	4.63	125.47	110.58
4	A	351	UDP	O3B-PB-O1B	4.77	125.95	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	B	352	UDP	C4-N3-C2	12.43	126.45	114.14
4	A	351	UDP	C4-N3-C2	12.77	126.79	114.14

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	265/293 (90%)	-0.49	8 (3%) 54 54	13, 25, 50, 63	0
1	B	262/293 (89%)	-0.34	7 (2%) 58 58	16, 32, 52, 69	0
All	All	527/586 (89%)	-0.42	15 (2%) 56 57	13, 28, 51, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	PRO	4.2
1	B	63	ALA	3.5
1	A	279	GLY	3.5
1	B	203	PRO	3.0
1	B	281	SER	3.0
1	B	188	SER	3.0
1	A	188	SER	2.8
1	B	64	LEU	2.8
1	A	64	LEU	2.4
1	A	202	GLY	2.4
1	A	280	TYR	2.4
1	B	189	GLY	2.3
1	A	128	THR	2.1
1	B	104	GLY	2.1
1	A	278	ASN	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

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(Å <sup>2</sup> )	Q<0.9
2	BDP	A	509	13/13	0.95	0.16	0.89	35,39,43,44	0
2	BDP	B	519	13/13	0.96	0.15	0.37	45,48,50,52	0
2	GAL	A	510	11/12	0.92	0.18	-	45,46,49,52	0
2	GAL	B	520	11/12	0.88	0.18	-	52,55,57,61	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	B	402	4/4	0.95	0.14	1.13	25,25,26,28	0
4	UDP	A	351	25/25	0.96	0.12	-0.76	25,28,32,35	0
5	EDO	A	401	4/4	0.98	0.10	-0.77	17,17,19,20	0
4	UDP	B	352	25/25	0.97	0.12	-0.83	27,33,35,36	0
3	MN	B	601	1/1	0.99	0.07	-1.92	41,41,41,41	0
3	MN	A	600	1/1	0.98	0.04	-2.75	37,37,37,37	0

### 6.5 Other polymers

There are no such residues in this entry.