



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:18 PM GMT

PDB ID : 4EE3  
Title : Crystal structure of human M340H-beta-1,4-galactosyltransferase-1 (M340H-B4GAL-T1) in complex with pentasaccharide  
Authors : Ramakrishnan, B.; Qasba, P.K.  
Deposited on : 2012-03-28  
Resolution : 2.30 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

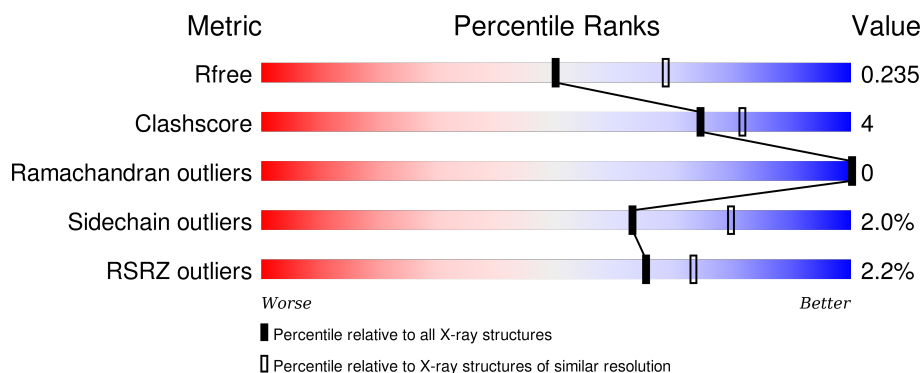
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


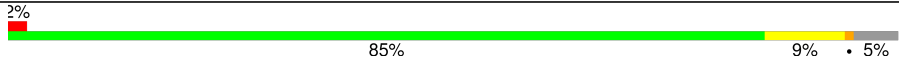

The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	287	 2% 83% 11% • 5%
1	B	287	 2% 85% 9% • 5%
1	C	287	 2% 84% 10% • 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	410	-	-	X	X
5	SO4	A	412	-	-	-	X
5	SO4	A	415	-	-	-	X
5	SO4	B	408	-	-	-	X
5	SO4	B	412	-	-	-	X
5	SO4	B	413	-	-	-	X
6	GOL	A	416	-	-	-	X
6	GOL	B	415	-	-	X	X
6	GOL	C	412	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7573 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 Beta-1,4-galactosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2218	1420	386	401	11			
1	B	273	Total	C	N	O	S	0	0	0
			2218	1420	386	401	11			
1	C	273	Total	C	N	O	S	0	0	0
			2218	1420	386	401	11			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	-	EXPRESSION TAG	UNP P15291
A	113	SER	-	EXPRESSION TAG	UNP P15291
A	114	MET	-	EXPRESSION TAG	UNP P15291
A	115	THR	-	EXPRESSION TAG	UNP P15291
A	116	GLY	-	EXPRESSION TAG	UNP P15291
A	117	GLY	-	EXPRESSION TAG	UNP P15291
A	118	GLN	-	EXPRESSION TAG	UNP P15291
A	119	GLN	-	EXPRESSION TAG	UNP P15291
A	120	MET	-	EXPRESSION TAG	UNP P15291
A	121	GLY	-	EXPRESSION TAG	UNP P15291
A	122	ARG	-	EXPRESSION TAG	UNP P15291
A	123	GLY	-	EXPRESSION TAG	UNP P15291
A	124	SER	-	EXPRESSION TAG	UNP P15291
A	125	ALA	-	EXPRESSION TAG	UNP P15291
A	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
A	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
A	340	HIS	MET	ENGINEERED MUTATION	UNP P15291
B	112	ALA	-	EXPRESSION TAG	UNP P15291
B	113	SER	-	EXPRESSION TAG	UNP P15291
B	114	MET	-	EXPRESSION TAG	UNP P15291
B	115	THR	-	EXPRESSION TAG	UNP P15291
B	116	GLY	-	EXPRESSION TAG	UNP P15291
B	117	GLY	-	EXPRESSION TAG	UNP P15291

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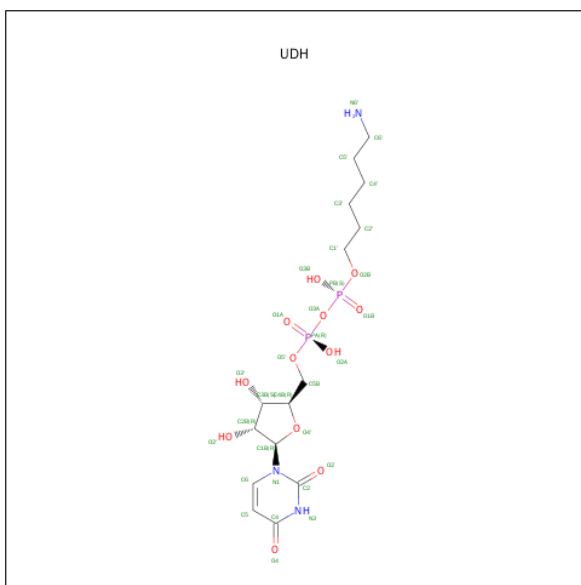
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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLN	-	EXPRESSION TAG	UNP P15291
B	119	GLN	-	EXPRESSION TAG	UNP P15291
B	120	MET	-	EXPRESSION TAG	UNP P15291
B	121	GLY	-	EXPRESSION TAG	UNP P15291
B	122	ARG	-	EXPRESSION TAG	UNP P15291
B	123	GLY	-	EXPRESSION TAG	UNP P15291
B	124	SER	-	EXPRESSION TAG	UNP P15291
B	125	ALA	-	EXPRESSION TAG	UNP P15291
B	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
B	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
B	340	HIS	MET	ENGINEERED MUTATION	UNP P15291
C	112	ALA	-	EXPRESSION TAG	UNP P15291
C	113	SER	-	EXPRESSION TAG	UNP P15291
C	114	MET	-	EXPRESSION TAG	UNP P15291
C	115	THR	-	EXPRESSION TAG	UNP P15291
C	116	GLY	-	EXPRESSION TAG	UNP P15291
C	117	GLY	-	EXPRESSION TAG	UNP P15291
C	118	GLN	-	EXPRESSION TAG	UNP P15291
C	119	GLN	-	EXPRESSION TAG	UNP P15291
C	120	MET	-	EXPRESSION TAG	UNP P15291
C	121	GLY	-	EXPRESSION TAG	UNP P15291
C	122	ARG	-	EXPRESSION TAG	UNP P15291
C	123	GLY	-	EXPRESSION TAG	UNP P15291
C	124	SER	-	EXPRESSION TAG	UNP P15291
C	125	ALA	-	EXPRESSION TAG	UNP P15291
C	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
C	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
C	340	HIS	MET	ENGINEERED MUTATION	UNP P15291

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			62	34	2	26		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		
2	C	5	Total	C	N	O	0	0
			62	34	2	26		

- Molecule 3 is 6-AMINOHEXYL-URIDINE-C1,5'-DIPHOSPHATE (three-letter code: UDH) (formula: C<sub>15</sub>H<sub>27</sub>N<sub>3</sub>O<sub>12</sub>P<sub>2</sub>).

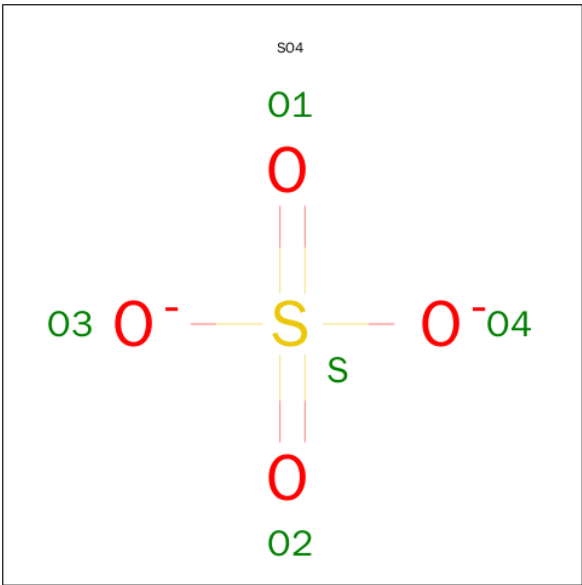


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 15	N 3	O 12	P 2	0	0
3	B	1	Total 32	C 15	N 3	O 12	P 2	0	0
3	C	1	Total 32	C 15	N 3	O 12	P 2	0	0

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



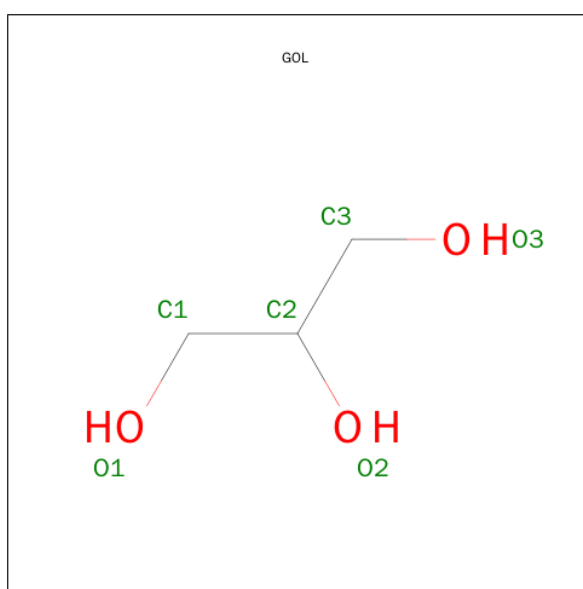
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	184	Total	O	0	0
			184	184		
7	B	186	Total	O	0	0
			186	186		

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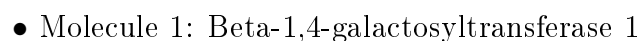
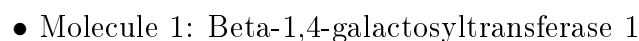


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	157	Total	O	0	0
			157	157		



- Molecule 1: Beta-1,4-galactosyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.61Å 195.16Å 143.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.31 – 2.30 36.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (36.31-2.30) 90.8 (36.31-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.187 , 0.240 0.182 , 0.235	Depositor DCC
$R_{free}$ test set	3388 reflections (5.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.9	EDS
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.009 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 60812 reflections	Xtriage
$F_o$ , $F_c$ correlation	0.95	EDS
Total number of atoms	7573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: GOL, BGC, NAG, MN, GAL, SO4, UDH

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	0.92	0/2280	0.90	4/3097 (0.1%)
1	B	0.94	0/2280	0.92	5/3097 (0.2%)
1	C	0.85	1/2280 (0.0%)	0.84	0/3097
All	All	0.90	1/6840 (0.0%)	0.89	9/9291 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	144	GLU	CG-CD	5.03	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	A	150	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	204	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	B	166	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	185	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	320	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	358	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	187	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	153	LEU	CB-CG-CD2	-5.06	102.39	111.00

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	2218	0	2162	21	0
1	B	2218	0	2162	15	0
1	C	2218	0	2162	17	0
2	A	62	0	54	2	0
2	B	61	0	52	1	0
2	C	62	0	54	1	0
3	A	32	0	25	0	0
3	B	32	0	25	0	0
3	C	32	0	25	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	40	0	0	3	0
5	B	30	0	0	1	0
5	C	20	0	0	2	0
6	A	6	0	8	1	0
6	B	6	0	8	4	0
6	C	6	0	8	0	0
7	A	184	0	0	1	0
7	B	186	0	0	3	0
7	C	157	0	0	0	0
All	All	7573	0	6745	55	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 4.

All (55) 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)
6:B:415:GOL:H31	7:B:668:HOH:O	1.85	0.76
1:B:266:PRO:HG3	1:B:321:LEU:HD22	1.74	0.68
1:A:264:SER:N	5:A:413:SO4:O3	2.27	0.66
1:A:273:MET:CE	1:A:275:LYS:HE2	2.26	0.66
1:A:312:GLY:HA2	2:A:403:NAG:H83	1.80	0.63
1:B:254:MET:HB3	7:B:652:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:TYR:N	5:A:410:SO4:O4	2.33	0.62
1:A:273:MET:HE1	1:A:275:LYS:HE2	1.80	0.62
1:A:357:ASP:HB3	7:A:618:HOH:O	2.02	0.60
1:B:254:MET:SD	1:B:339:ARG:HG3	2.42	0.60
1:A:303:PHE:HB3	1:A:304:PRO:HD2	1.84	0.59
1:A:136:LEU:HA	1:C:254:MET:HE1	1.84	0.59
1:B:139:GLY:HA2	1:B:257:HIS:HD2	1.70	0.57
1:C:266:PRO:HG3	1:C:321:LEU:HD22	1.90	0.54
1:A:225:ALA:HB2	1:A:313:GLU:HG3	1.90	0.54
1:A:306:ASN:HD22	1:A:306:ASN:H	1.55	0.52
2:A:403:NAG:O4	6:A:416:GOL:H2	2.08	0.52
1:A:313:GLU:O	1:A:317:ILE:HG13	2.10	0.51
1:B:310:TRP:CD1	6:B:415:GOL:H12	2.46	0.51
1:C:145:PHE:HB2	5:C:411:SO4:O1	2.10	0.51
1:A:167:TYR:HB3	1:A:209:TYR:CE2	2.49	0.48
1:B:141:MET:SD	7:B:664:HOH:O	2.60	0.48
1:C:131:PRO:HD2	1:C:206:GLN:HE22	1.80	0.47
1:A:376:TYR:O	5:A:410:SO4:O4	2.33	0.47
1:B:225:ALA:HB2	1:B:313:GLU:HG3	1.96	0.47
1:C:264:SER:N	5:C:409:SO4:O1	2.34	0.46
1:B:273:MET:CE	1:B:275:LYS:HE2	2.46	0.46
1:B:319:ASN:HB3	1:B:323:PHE:CE1	2.51	0.46
1:C:369:ASP:OD2	1:C:369:ASP:C	2.54	0.45
1:C:354:GLN:OE1	1:C:358:ARG:NH2	2.48	0.45
1:A:254:MET:SD	1:A:339:ARG:HG3	2.57	0.44
1:B:303:PHE:HB3	1:B:304:PRO:HD2	1.98	0.44
1:B:184:PHE:O	1:B:215:ASN:HA	2.18	0.44
1:C:254:MET:HE3	1:C:254:MET:HB3	1.69	0.43
1:A:308:TRP:O	1:A:352:ASN:HB2	2.18	0.43
1:A:347:LYS:O	1:A:348:LYS:HB2	2.18	0.43
1:B:271:VAL:HG22	1:B:336:GLY:HA3	2.00	0.43
1:B:306:ASN:HD22	1:B:306:ASN:H	1.67	0.43
1:C:225:ALA:HB2	1:C:313:GLU:HG3	2.01	0.42
1:C:300:ILE:HB	1:C:320:ARG:HB3	2.00	0.42
1:C:312:GLY:HA2	2:C:403:NAG:H83	2.00	0.42
1:C:352:ASN:HA	1:C:353:PRO:HD3	1.71	0.42
1:A:316:ASP:O	1:A:320:ARG:HG3	2.20	0.41
1:C:309:GLY:HA2	1:C:349:ASN:OD1	2.20	0.41
1:C:248:ASP:HB3	3:C:406:UDH:O3'	2.20	0.41
1:C:341:ILE:O	1:C:343:HIS:HD2	2.03	0.41
1:A:180:ILE:HG13	1:A:245:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HA	1:C:198:LEU:HD13	1.76	0.41
1:A:314:ASP:OD1	1:A:314:ASP:N	2.54	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD13	1.96	0.41
1:B:310:TRP:NE1	6:B:415:GOL:H12	2.37	0.40
1:A:266:PRO:CG	1:A:321:LEU:HD22	2.50	0.40
2:B:403:NAG:O4	6:B:415:GOL:H2	2.20	0.40
1:B:398:SER:HB2	5:B:410:SO4:O3	2.22	0.40
1:C:314:ASP:OD1	1:C:314:ASP:N	2.54	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	271/287 (94%)	261 (96%)	10 (4%)	0	100	100
1	B	271/287 (94%)	265 (98%)	6 (2%)	0	100	100
1	C	271/287 (94%)	265 (98%)	6 (2%)	0	100	100
All	All	813/861 (94%)	791 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	244/252 (97%)	241 (99%)	3 (1%)	78	89
1	B	244/252 (97%)	240 (98%)	4 (2%)	70	84
1	C	244/252 (97%)	236 (97%)	8 (3%)	45	61
All	All	732/756 (97%)	717 (98%)	15 (2%)	63	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	MET
1	A	306	ASN
1	A	364	GLU
1	B	127	LEU
1	B	147	MET
1	B	153	LEU
1	B	306	ASN
1	C	133	GLU
1	C	147	MET
1	C	254	MET
1	C	257	HIS
1	C	306	ASN
1	C	342	ARG
1	C	345	ARG
1	C	352	ASN

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	186	ASN
1	A	257	HIS
1	A	306	ASN
1	B	186	ASN
1	B	306	ASN
1	C	206	GLN
1	C	233	GLN
1	C	257	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 ⓘ

15 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	BGC	A	401	2	12,12,12	0.66	0	17,17,17	1.09	1 (5%)
2	GAL	A	402	2	11,11,12	0.45	0	14,15,17	1.47	2 (14%)
2	NAG	A	403	2	14,14,15	0.79	0	15,19,21	1.81	2 (13%)
2	NAG	A	404	2	14,14,15	0.57	0	15,19,21	1.20	1 (6%)
2	GAL	A	405	2	11,11,12	0.81	0	14,15,17	2.41	3 (21%)
2	BGC	B	401	2	12,12,12	0.65	0	17,17,17	0.78	0
2	GAL	B	402	2	11,11,12	0.80	0	14,15,17	1.35	2 (14%)
2	NAG	B	403	2	14,14,15	0.85	1 (7%)	15,19,21	1.92	3 (20%)
2	NAG	B	404	2	14,14,15	0.80	0	15,19,21	2.37	6 (40%)
2	GAL	B	405	2	10,10,12	0.72	0	12,13,17	1.45	2 (16%)
2	BGC	C	401	2	12,12,12	0.71	0	17,17,17	1.74	5 (29%)
2	GAL	C	402	2	11,11,12	0.69	0	14,15,17	1.02	1 (7%)
2	NAG	C	403	2	14,14,15	0.72	0	15,19,21	1.39	2 (13%)
2	NAG	C	404	2	14,14,15	0.54	0	15,19,21	1.38	1 (6%)
2	GAL	C	405	2	11,11,12	0.68	0	14,15,17	1.24	1 (7%)

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	BGC	A	401	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	A	402	2	-	0/2/19/22	0/1/1/1
2	NAG	A	403	2	-	0/6/23/26	0/1/1/1
2	NAG	A	404	2	-	0/6/23/26	0/1/1/1
2	GAL	A	405	2	-	0/2/19/22	0/1/1/1
2	BGC	B	401	2	-	0/2/22/22	0/1/1/1
2	GAL	B	402	2	-	0/2/19/22	0/1/1/1
2	NAG	B	403	2	-	0/6/23/26	0/1/1/1
2	NAG	B	404	2	-	0/6/23/26	0/1/1/1
2	GAL	B	405	2	-	0/2/15/22	0/1/1/1
2	BGC	C	401	2	-	0/2/22/22	0/1/1/1
2	GAL	C	402	2	-	0/2/19/22	0/1/1/1
2	NAG	C	403	2	-	0/6/23/26	0/1/1/1
2	NAG	C	404	2	-	0/6/23/26	0/1/1/1
2	GAL	C	405	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	NAG	O5-C1	-2.41	1.39	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	405	GAL	C1-O5-C5	-5.48	105.29	112.25
2	C	401	BGC	C1-C2-C3	-4.16	104.25	110.43
2	C	403	NAG	C2-N2-C7	-3.52	118.52	123.04
2	A	402	GAL	C2-C3-C4	-3.37	105.33	111.04
2	B	402	GAL	C2-C3-C4	-3.33	105.39	111.04
2	C	401	BGC	C1-O5-C5	-3.21	107.54	113.47
2	B	403	NAG	C2-N2-C7	-3.04	119.13	123.04
2	C	402	GAL	C2-C3-C4	-2.99	105.96	111.04
2	B	404	NAG	O7-C7-C8	-2.98	116.59	122.06
2	B	403	NAG	C3-C4-C5	-2.83	105.26	110.20
2	B	405	GAL	C4-C3-C2	-2.61	106.78	110.23
2	A	401	BGC	C1-O5-C5	-2.48	108.89	113.47
2	C	405	GAL	C2-C3-C4	-2.41	106.94	111.04
2	C	401	BGC	O5-C1-C2	-2.39	105.98	109.80
2	B	405	GAL	O5-C1-C2	-2.38	107.00	110.86
2	B	402	GAL	O5-C1-C2	-2.06	107.51	110.86
2	B	404	NAG	O3-C3-C2	2.12	113.31	109.11
2	A	402	GAL	C1-C2-C3	2.26	112.22	109.54
2	C	401	BGC	C3-C4-C5	2.28	114.18	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	BGC	O1-C1-C2	2.36	115.54	109.21
2	A	404	NAG	O5-C5-C6	2.37	112.49	107.35
2	A	403	NAG	C2-N2-C7	2.47	126.21	123.04
2	C	403	NAG	O4-C4-C5	2.50	115.87	109.24
2	B	404	NAG	O7-C7-N2	2.93	127.83	121.86
2	B	404	NAG	C1-O5-C5	2.98	116.03	112.25
2	B	404	NAG	C3-C4-C5	3.46	116.23	110.20
2	A	405	GAL	O5-C5-C6	3.50	114.92	107.35
2	C	404	NAG	C1-O5-C5	4.00	117.32	112.25
2	A	405	GAL	C6-C5-C4	4.57	124.28	113.02
2	B	403	NAG	C1-O5-C5	4.99	118.58	112.25
2	A	403	NAG	C1-O5-C5	5.05	118.65	112.25
2	B	404	NAG	C2-N2-C7	5.47	130.07	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	NAG	2	0
2	B	403	NAG	1	0
2	C	403	NAG	1	0

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	UDH	A	406	4	25,33,33	1.38	1 (4%)	33,47,47	1.94	4 (12%)
5	SO4	A	408	-	4,4,4	0.15	0	6,6,6	0.29	0
5	SO4	A	409	-	4,4,4	0.12	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	410	-	4,4,4	0.23	0	6,6,6	0.73	0
5	SO4	A	411	-	4,4,4	0.17	0	6,6,6	0.61	0
5	SO4	A	412	-	4,4,4	1.79	2 (50%)	6,6,6	1.32	1 (16%)
5	SO4	A	413	-	4,4,4	0.37	0	6,6,6	0.34	0
5	SO4	A	414	-	4,4,4	0.08	0	6,6,6	0.30	0
5	SO4	A	415	-	4,4,4	0.24	0	6,6,6	0.41	0
6	GOL	A	416	-	5,5,5	0.62	0	5,5,5	1.18	0
3	UDH	B	406	4	25,33,33	1.04	1 (4%)	33,47,47	1.76	4 (12%)
5	SO4	B	408	-	4,4,4	0.37	0	6,6,6	0.75	0
5	SO4	B	409	-	4,4,4	0.32	0	6,6,6	0.64	0
5	SO4	B	410	-	4,4,4	0.28	0	6,6,6	0.86	0
5	SO4	B	411	-	4,4,4	0.14	0	6,6,6	0.14	0
5	SO4	B	412	-	4,4,4	0.22	0	6,6,6	0.87	0
5	SO4	B	413	-	4,4,4	0.11	0	6,6,6	0.52	0
6	GOL	B	415	-	5,5,5	0.48	0	5,5,5	1.27	1 (20%)
3	UDH	C	406	4	25,33,33	1.01	1 (4%)	33,47,47	1.62	5 (15%)
5	SO4	C	408	-	4,4,4	0.30	0	6,6,6	0.45	0
5	SO4	C	409	-	4,4,4	0.58	0	6,6,6	0.28	0
5	SO4	C	410	-	4,4,4	0.21	0	6,6,6	0.31	0
5	SO4	C	411	-	4,4,4	0.21	0	6,6,6	0.58	0
6	GOL	C	412	-	5,5,5	0.31	0	5,5,5	0.55	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	UDH	A	406	4	-	0/21/41/41	0/2/2/2
5	SO4	A	408	-	-	0/0/0/0	0/0/0/0
5	SO4	A	409	-	-	0/0/0/0	0/0/0/0
5	SO4	A	410	-	-	0/0/0/0	0/0/0/0
5	SO4	A	411	-	-	0/0/0/0	0/0/0/0
5	SO4	A	412	-	-	0/0/0/0	0/0/0/0
5	SO4	A	413	-	-	0/0/0/0	0/0/0/0
5	SO4	A	414	-	-	0/0/0/0	0/0/0/0
5	SO4	A	415	-	-	0/0/0/0	0/0/0/0
6	GOL	A	416	-	-	0/4/4/4	0/0/0/0
3	UDH	B	406	4	-	0/21/41/41	0/2/2/2
5	SO4	B	408	-	-	0/0/0/0	0/0/0/0
5	SO4	B	409	-	-	0/0/0/0	0/0/0/0
5	SO4	B	410	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	411	-	-	0/0/0/0	0/0/0/0
5	SO4	B	412	-	-	0/0/0/0	0/0/0/0
5	SO4	B	413	-	-	0/0/0/0	0/0/0/0
6	GOL	B	415	-	-	0/4/4/4	0/0/0/0
3	UDH	C	406	4	-	0/21/41/41	0/2/2/2
5	SO4	C	408	-	-	0/0/0/0	0/0/0/0
5	SO4	C	409	-	-	0/0/0/0	0/0/0/0
5	SO4	C	410	-	-	0/0/0/0	0/0/0/0
5	SO4	C	411	-	-	0/0/0/0	0/0/0/0
6	GOL	C	412	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	412	SO4	O3-S	2.29	1.55	1.47
5	A	412	SO4	O1-S	2.50	1.55	1.47
3	B	406	UDH	C6-N1	3.21	1.40	1.35
3	C	406	UDH	C6-N1	3.85	1.41	1.35
3	A	406	UDH	C6-N1	5.56	1.43	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	406	UDH	PB-O3A-PA	-4.19	120.97	132.73
3	A	406	UDH	PB-O3A-PA	-3.94	121.67	132.73
3	B	406	UDH	PB-O3A-PA	-3.03	124.23	132.73
3	B	406	UDH	C6-N1-C2	-2.82	116.71	121.28
3	A	406	UDH	O2B-PB-O1B	-2.67	99.26	109.62
3	C	406	UDH	C6-N1-C2	-2.21	117.69	121.28
5	A	412	SO4	O3-S-O2	-2.13	90.41	110.19
3	C	406	UDH	O3A-PB-O2B	-2.12	97.30	102.94
6	B	415	GOL	O3-C3-C2	-2.11	99.95	110.18
3	A	406	UDH	O3B-PB-O1B	2.37	125.38	112.53
3	B	406	UDH	O3B-PB-O3A	2.47	116.30	105.09
3	C	406	UDH	O4'-C1B-N1	2.49	113.32	108.08
3	C	406	UDH	C4-N3-C2	5.94	120.03	114.14
3	B	406	UDH	C4-N3-C2	7.40	121.47	114.14
3	A	406	UDH	C4-N3-C2	8.50	122.56	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	410	SO4	2	0
5	A	413	SO4	1	0
6	A	416	GOL	1	0
5	B	410	SO4	1	0
6	B	415	GOL	4	0
3	C	406	UDH	1	0
5	C	409	SO4	1	0
5	C	411	SO4	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 ⓘ

### 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	273/287 (95%)	-0.19	6 (2%) 65 73	17, 27, 48, 59	0
1	B	273/287 (95%)	-0.17	5 (1%) 71 78	15, 24, 40, 54	0
1	C	273/287 (95%)	-0.12	7 (2%) 59 68	20, 33, 55, 66	0
All	All	819/861 (95%)	-0.16	18 (2%) 65 73	15, 28, 50, 66	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	LYS	4.6
1	C	126	SER	3.9
1	B	126	SER	3.8
1	C	398	SER	3.7
1	A	347	LYS	3.0
1	A	126	SER	2.9
1	C	219	ASP	2.8
1	A	353	PRO	2.8
1	A	350	GLU	2.4
1	B	182	ILE	2.3
1	A	219	ASP	2.2
1	C	396	THR	2.2
1	B	181	ILE	2.1
1	C	353	PRO	2.1
1	C	148	PRO	2.1
1	A	289	VAL	2.1
1	B	146	ASN	2.0
1	B	228	LEU	2.0

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	403	14/15	0.95	0.11	-0.24	38,43,45,46	0
2	NAG	B	403	14/15	0.96	0.10	-0.89	25,30,34,37	0
2	NAG	A	403	14/15	0.96	0.09	-0.94	34,37,40,40	0
2	BGC	C	401	12/12	0.92	0.24	-	68,71,74,77	0
2	NAG	C	404	14/15	0.86	0.30	-	78,81,86,93	0
2	BGC	A	401	12/12	0.87	0.19	-	49,54,58,61	0
2	GAL	A	402	11/12	0.95	0.17	-	38,49,55,60	0
2	GAL	A	405	11/12	0.69	0.54	-	91,95,97,97	0
2	GAL	B	405	10/12	0.84	0.64	-	85,90,93,95	0
2	GAL	C	405	11/12	0.61	0.58	-	99,103,106,107	0
2	GAL	C	402	11/12	0.91	0.24	-	55,66,70,72	0
2	NAG	A	404	14/15	0.90	0.27	-	67,70,75,84	0
2	GAL	B	402	11/12	0.96	0.17	-	39,44,51,52	0
2	NAG	B	404	14/15	0.90	0.31	-	55,60,65,76	0
2	BGC	B	401	12/12	0.91	0.22	-	49,54,58,58	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	SO4	B	412	5/5	0.89	0.30	8.62	77,77,80,80	0
5	SO4	A	412	5/5	0.73	0.24	4.59	36,39,51,56	0
5	SO4	A	410	5/5	0.93	0.20	3.64	73,75,76,76	0
5	SO4	B	408	5/5	0.95	0.23	3.62	49,52,55,58	0
5	SO4	A	415	5/5	0.83	0.19	3.34	90,92,94,95	0
6	GOL	A	416	6/6	0.93	0.21	3.01	41,49,51,52	0
6	GOL	C	412	6/6	0.88	0.21	2.62	58,63,64,68	0
5	SO4	B	413	5/5	0.88	0.27	2.54	89,89,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	415	6/6	0.90	0.22	2.17	32,42,44,46	0
5	SO4	C	410	5/5	0.80	0.32	1.53	98,99,99,100	0
5	SO4	B	410	5/5	0.85	0.20	1.45	66,69,71,75	0
5	SO4	C	411	5/5	0.90	0.21	1.39	86,86,87,89	0
5	SO4	A	409	5/5	0.94	0.13	0.39	59,61,62,66	0
5	SO4	C	408	5/5	0.98	0.10	-0.23	42,43,44,45	0
5	SO4	B	409	5/5	0.92	0.14	-0.23	77,80,81,82	0
3	UDH	B	406	32/32	0.98	0.13	-0.37	14,22,60,61	0
3	UDH	A	406	32/32	0.97	0.12	-0.46	22,27,58,64	0
3	UDH	C	406	32/32	0.97	0.12	-0.47	25,35,61,64	0
5	SO4	A	408	5/5	0.93	0.10	-1.49	82,83,84,85	0
4	MN	A	407	1/1	0.99	0.07	-2.09	31,31,31,31	0
4	MN	C	407	1/1	0.98	0.06	-5.02	36,36,36,36	0
5	SO4	A	413	5/5	0.79	0.33	-	93,93,95,95	0
5	SO4	C	409	5/5	0.69	0.43	-	80,83,84,85	0
5	SO4	B	411	5/5	0.95	0.27	-	81,82,83,84	0
4	MN	B	407	1/1	0.99	0.08	-	25,25,25,25	0
5	SO4	A	414	5/5	0.92	0.33	-	85,85,86,87	0
5	SO4	A	411	5/5	0.86	0.35	-	74,75,77,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.