



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:13 PM GMT

PDB ID : 1O0R
Title : Crystal structure of the catalytic domain of bovine beta1,4-galactosyltransferase complex with UDP-galactose
Authors : Ramakrishnan, B.; Balaji, P.V.; Qasba, P.K.
Deposited on : 2003-02-24
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
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 (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

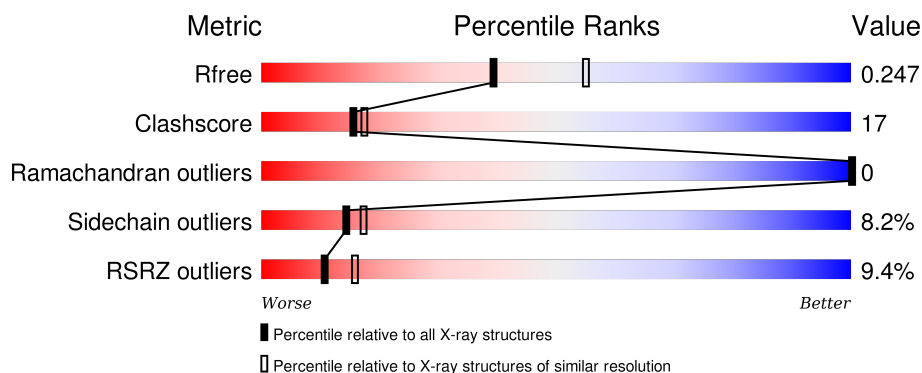
1 Overall quality at a glance

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 ≥ 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	286	<div> <div>5%</div> <div>68%</div> <div>23%</div> <div>• 5%</div> </div>
1	B	286	<div> <div>13%</div> <div>62%</div> <div>30%</div> <div>• 5%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4993 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2211	1419	381	398	13			
1	B	273	Total	C	N	O	S	0	0	0
			2225	1428	383	401	13			

There are 28 discrepancies between the modelled and reference sequences:

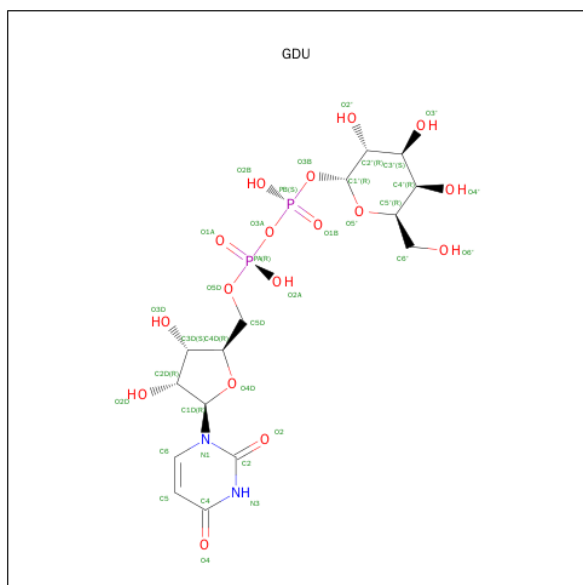
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ALA	-	SEE REMARK 999	UNP P08037
A	118	SER	-	SEE REMARK 999	UNP P08037
A	119	MET	-	SEE REMARK 999	UNP P08037
A	120	THR	-	SEE REMARK 999	UNP P08037
A	121	GLY	-	SEE REMARK 999	UNP P08037
A	122	GLY	-	SEE REMARK 999	UNP P08037
A	123	GLN	-	SEE REMARK 999	UNP P08037
A	124	GLN	-	SEE REMARK 999	UNP P08037
A	125	MET	-	SEE REMARK 999	UNP P08037
A	126	GLY	-	SEE REMARK 999	UNP P08037
A	127	ARG	-	SEE REMARK 999	UNP P08037
A	128	GLY	-	SEE REMARK 999	UNP P08037
A	129	SER	-	SEE REMARK 999	UNP P08037
A	342	THR	CYS	ENGINEERED	UNP P08037
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037

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Chain	Residue	Modelled	Actual	Comment	Reference
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
B	342	THR	CYS	ENGINEERED	UNP P08037

- Molecule 2 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

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

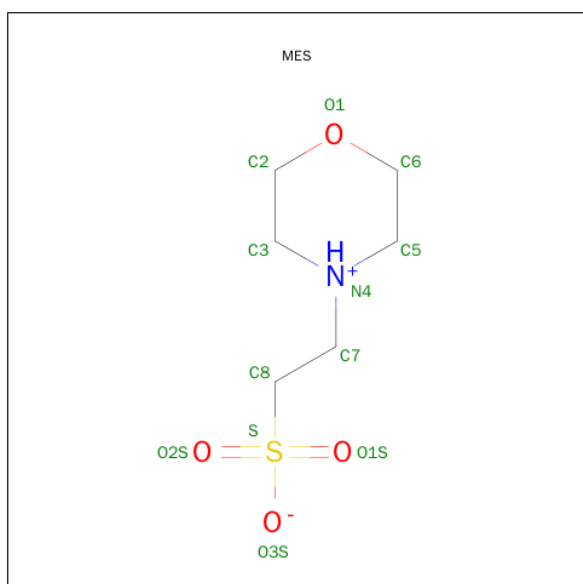
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



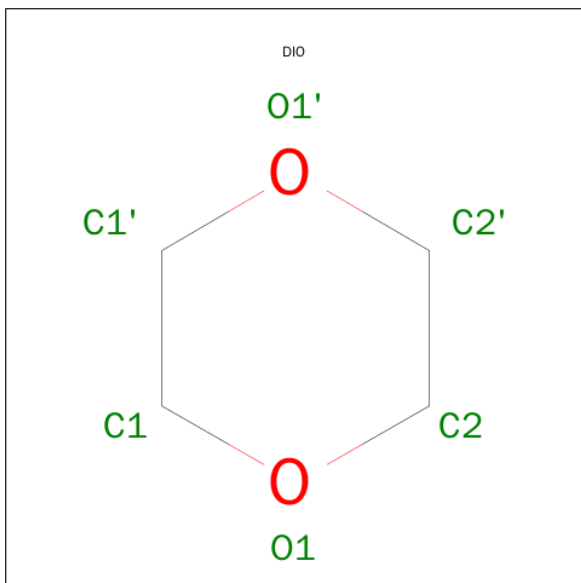
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		

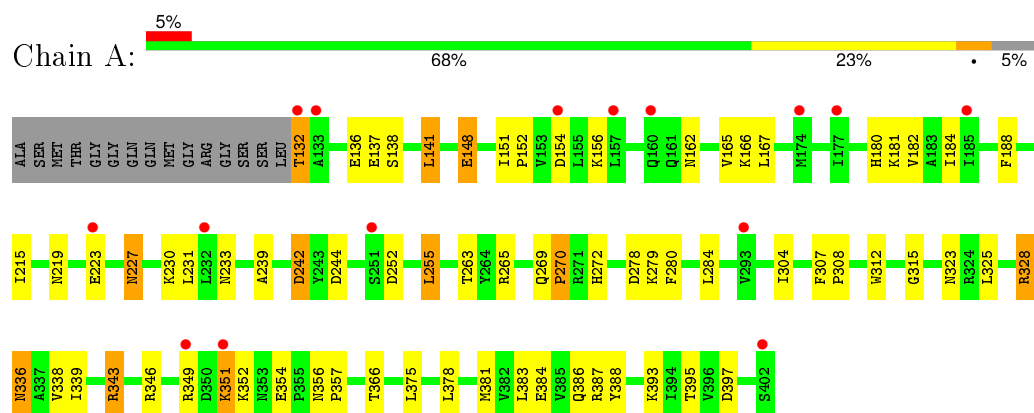
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	226	Total	O	0	0
			226	226		
7	B	213	Total	O	0	0
			213	213		

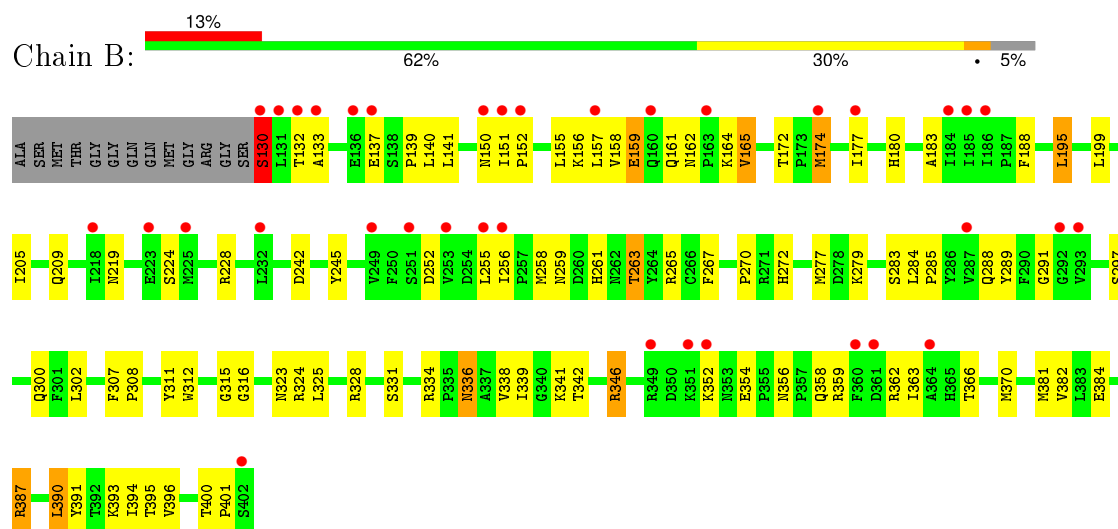
3 Residue-property plots [i](#)

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: beta-1,4-galactosyltransferase



- Molecule 1: beta-1,4-galactosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.36 Å 91.78 Å 142.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.53 – 2.30 37.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.53-2.30) 98.5 (37.52-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.251 0.198 , 0.247	Depositor DCC
R_{free} test set	2966 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29785 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4993	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, DIO, GDU, MES, 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	0.48	0/2271	0.71	1/3076 (0.0%)
1	B	0.50	1/2285 (0.0%)	0.76	3/3095 (0.1%)
All	All	0.49	1/4556 (0.0%)	0.74	4/6171 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	SER	CB-OG	5.09	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	SER	N-CA-C	-9.08	86.48	111.00
1	B	130	SER	CA-CB-OG	-5.72	95.75	111.20
1	A	315	GLY	N-CA-C	5.70	127.35	113.10
1	B	315	GLY	N-CA-C	5.18	126.06	113.10

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	2211	0	2176	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2225	0	2192	86	0
2	A	36	0	22	0	0
2	B	36	0	22	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	15	0	0	1	0
5	A	12	0	13	5	0
6	A	6	0	8	2	0
6	B	6	0	8	0	0
7	A	226	0	0	11	0
7	B	213	0	0	7	0
All	All	4993	0	4441	155	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 17.

All (155) 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:151:ILE:HD12	1:A:152:PRO:HD2	1.38	1.03
1:B:164:LYS:HG2	1:B:174:MET:HE1	1.48	0.93
1:A:132:THR:HA	7:A:1010:HOH:O	1.74	0.88
1:B:155:LEU:O	1:B:159:GLU:HG2	1.77	0.84
1:B:384:GLU:HB3	1:B:395:THR:CG2	2.07	0.84
1:B:130:SER:O	1:B:130:SER:OG	1.97	0.82
1:B:400:THR:HG23	1:B:401:PRO:HD2	1.64	0.80
1:B:352:LYS:HA	1:B:352:LYS:HE2	1.68	0.75
1:A:154:ASP:HA	7:A:1024:HOH:O	1.86	0.74
1:B:382:VAL:HA	1:B:396:VAL:HG12	1.68	0.74
1:A:346:ARG:NE	1:A:346:ARG:HA	2.04	0.73
1:B:387:ARG:HH11	1:B:387:ARG:HG2	1.56	0.71
1:B:336:ASN:HD22	1:B:336:ASN:C	1.94	0.70
1:A:167:LEU:CD1	1:A:387:ARG:HB3	2.20	0.70
1:B:258:MET:HE3	1:B:341:LYS:HB3	1.74	0.68
1:B:252:ASP:HB2	1:B:255:LEU:HD12	1.74	0.67
1:B:150:ASN:O	1:B:152:PRO:HD3	1.96	0.65
1:A:151:ILE:CD1	1:A:152:PRO:HD2	2.21	0.65
1:B:358:GLN:O	1:B:362:ARG:HG3	1.97	0.64
1:A:181:LYS:HD3	7:A:1171:HOH:O	1.97	0.64
1:A:384:GLU:HB3	1:A:395:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HH21	1:A:343:ARG:HG3	1.63	0.62
1:A:252:ASP:HB2	1:A:255:LEU:HD22	1.81	0.62
1:B:297:SER:OG	1:B:300:GLN:HG3	2.00	0.61
1:B:164:LYS:HG2	1:B:174:MET:CE	2.28	0.61
1:B:224:SER:HB2	7:B:1166:HOH:O	2.01	0.60
1:A:395:THR:HG21	5:A:900:MES:H62	1.83	0.60
1:A:233:ASN:HB3	1:A:378:LEU:HD22	1.82	0.60
1:A:227:ASN:HD22	1:A:227:ASN:C	2.06	0.60
1:B:258:MET:HE2	1:B:342:THR:N	2.17	0.59
1:A:167:LEU:HD11	1:A:387:ARG:HB3	1.83	0.59
1:A:191:ARG:HH21	1:A:194:HIS:HD2	1.51	0.59
1:B:156:LYS:HA	1:B:159:GLU:HG3	1.85	0.58
1:A:384:GLU:HB3	1:A:395:THR:HG21	1.84	0.58
1:A:383:LEU:HB2	1:A:395:THR:HG23	1.86	0.57
1:B:307:PHE:HB3	1:B:308:PRO:HD2	1.86	0.57
1:B:272:HIS:HB3	1:B:334:ARG:HG2	1.87	0.57
1:B:277:MET:HE2	1:B:279:LYS:HD3	1.85	0.57
1:B:346:ARG:HG2	1:B:346:ARG:HH21	1.70	0.56
1:B:164:LYS:HB2	7:B:1227:HOH:O	2.06	0.56
1:A:137:GLU:HG2	7:A:1309:HOH:O	2.05	0.56
1:B:205:ILE:O	1:B:209:GLN:HG3	2.06	0.56
1:B:285:PRO:HG2	1:B:289:TYR:CG	2.41	0.55
1:A:395:THR:HG21	5:A:900:MES:H21	1.89	0.55
1:B:174:MET:HB2	7:B:1242:HOH:O	2.06	0.55
1:A:162:ASN:HB3	1:A:165:VAL:CG1	2.37	0.55
1:B:133:ALA:HA	1:B:177:ILE:HG22	1.89	0.55
1:B:356:ASN:O	1:B:359:ARG:HG2	2.07	0.54
1:A:395:THR:CB	5:A:900:MES:H62	2.36	0.54
1:A:278:ASP:OD2	1:A:343:ARG:HD3	2.07	0.54
1:A:307:PHE:HB3	1:A:308:PRO:HD2	1.89	0.54
1:B:324:ARG:HG2	1:B:370:MET:HG2	1.88	0.54
1:A:154:ASP:OD1	1:A:156:LYS:HB2	2.07	0.54
1:B:336:ASN:ND2	1:B:339:ILE:H	2.04	0.53
1:A:395:THR:O	1:A:395:THR:HG23	2.08	0.53
1:B:336:ASN:HD21	1:B:339:ILE:H	1.56	0.53
1:A:270:PRO:HG2	1:A:325:LEU:HD22	1.89	0.53
1:B:151:ILE:O	1:B:151:ILE:HG13	2.08	0.53
1:A:351:LYS:HA	7:A:1183:HOH:O	2.09	0.52
1:A:269:GLN:HB3	1:A:331:SER:O	2.09	0.52
1:A:148:GLU:HG3	1:A:148:GLU:O	2.10	0.52
1:B:272:HIS:HD2	1:B:334:ARG:HD3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:O	1:A:352:LYS:HG3	2.10	0.52
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.92	0.51
1:A:136:GLU:HG2	7:A:1309:HOH:O	2.10	0.51
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.46	0.51
1:B:336:ASN:ND2	1:B:338:VAL:HG22	2.25	0.51
1:A:279:LYS:HE3	1:A:280:PHE:CZ	2.46	0.50
1:A:343:ARG:HH21	1:A:343:ARG:CG	2.25	0.50
1:A:278:ASP:OD2	1:A:343:ARG:HA	2.11	0.50
1:A:336:ASN:ND2	1:A:339:ILE:H	2.10	0.50
1:B:156:LYS:HA	1:B:159:GLU:CG	2.42	0.50
1:A:312:TRP:O	1:A:356:ASN:HB2	2.12	0.50
1:B:255:LEU:C	1:B:256:ILE:HD12	2.32	0.49
1:A:242:ASP:OD2	1:A:387:ARG:NH2	2.46	0.49
1:B:311:TYR:HE2	1:B:363:ILE:HD12	1.77	0.49
1:B:133:ALA:HA	1:B:177:ILE:CG2	2.41	0.49
1:A:351:LYS:O	1:A:354:GLU:OE1	2.30	0.49
1:B:390:LEU:HB2	7:B:1009:HOH:O	2.11	0.49
1:B:272:HIS:HE1	1:B:291:GLY:O	1.95	0.49
1:B:346:ARG:HG2	1:B:346:ARG:NH2	2.27	0.49
1:B:336:ASN:ND2	1:B:336:ASN:C	2.63	0.48
1:B:338:VAL:O	1:B:341:LYS:HG3	2.14	0.48
1:A:284:LEU:HD11	1:A:334:ARG:CZ	2.44	0.48
1:B:172:THR:O	1:B:174:MET:HE3	2.14	0.48
1:A:388:TYR:CD2	6:A:905:DIO:H12	2.49	0.48
1:B:272:HIS:CD2	1:B:334:ARG:HH21	2.31	0.48
1:B:258:MET:CE	1:B:341:LYS:HB3	2.44	0.47
1:B:164:LYS:CG	1:B:174:MET:HE1	2.33	0.47
1:B:256:ILE:N	1:B:256:ILE:HD12	2.30	0.47
1:B:177:ILE:O	1:B:177:ILE:HG23	2.13	0.47
1:A:167:LEU:HD13	1:A:387:ARG:HB3	1.96	0.47
1:B:195:LEU:HD22	1:B:199:LEU:HG	1.96	0.47
1:B:336:ASN:HD21	1:B:338:VAL:HG22	1.79	0.47
1:B:312:TRP:O	1:B:356:ASN:HB2	2.15	0.47
1:A:395:THR:CG2	5:A:900:MES:H62	2.45	0.46
1:A:162:ASN:HB3	1:A:165:VAL:HG13	1.97	0.46
1:A:162:ASN:O	1:A:165:VAL:HG13	2.16	0.46
1:B:209:GLN:NE2	1:B:263:THR:HA	2.30	0.46
1:B:159:GLU:OE1	1:B:390:LEU:HD22	2.15	0.46
1:A:384:GLU:HB3	1:A:395:THR:HG22	1.97	0.46
1:B:177:ILE:HG23	7:B:1123:HOH:O	2.17	0.45
1:A:304:ILE:HG22	1:A:328:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLU:OE1	5:A:900:MES:O1	2.34	0.45
1:A:181:LYS:NZ	1:A:244:ASP:OD2	2.47	0.45
1:B:270:PRO:HD2	1:B:331:SER:O	2.17	0.45
1:B:158:VAL:CG1	1:B:390:LEU:HD21	2.47	0.45
1:A:191:ARG:HD2	1:A:194:HIS:CD2	2.52	0.45
1:B:267:PHE:HA	4:B:902:SO4:O2	2.17	0.45
1:A:194:HIS:HE1	7:A:1028:HOH:O	2.00	0.44
1:B:277:MET:HE1	7:B:1231:HOH:O	2.17	0.44
1:A:184:ILE:HD12	1:A:215:ILE:HD11	2.00	0.44
1:B:311:TYR:HE2	1:B:363:ILE:CD1	2.31	0.44
1:B:336:ASN:ND2	1:B:338:VAL:H	2.16	0.44
1:B:312:TRP:CD2	1:B:401:PRO:HG3	2.53	0.43
1:A:384:GLU:N	1:A:395:THR:CG2	2.81	0.43
1:A:154:ASP:OD2	1:A:156:LYS:HE2	2.17	0.43
1:B:180:HIS:CE1	1:B:265:ARG:HD3	2.53	0.43
1:A:343:ARG:NH2	1:A:343:ARG:CG	2.80	0.43
1:B:316:GLY:HA3	1:B:363:ILE:HD11	2.01	0.43
1:B:183:ALA:HB2	1:B:245:TYR:CG	2.54	0.43
1:B:270:PRO:HG2	1:B:325:LEU:HD22	1.99	0.43
1:B:139:PRO:HG2	1:B:140:LEU:HD22	2.01	0.43
1:A:227:ASN:ND2	1:A:230:LYS:H	2.17	0.43
1:B:390:LEU:O	1:B:391:TYR:HB3	2.19	0.42
1:A:323:ASN:HB2	1:A:366:THR:HG21	2.02	0.42
1:B:387:ARG:NH1	1:B:387:ARG:HG2	2.31	0.42
1:B:132:THR:HG22	1:B:133:ALA:N	2.35	0.42
1:B:387:ARG:HH11	1:B:387:ARG:CG	2.26	0.42
1:A:278:ASP:OD1	1:A:279:LYS:N	2.52	0.42
1:B:132:THR:CG2	1:B:133:ALA:N	2.83	0.42
6:A:905:DIO:H11	7:A:1200:HOH:O	2.19	0.42
1:A:166:LYS:HE2	7:A:1296:HOH:O	2.19	0.42
1:B:162:ASN:HB3	1:B:165:VAL:HG13	2.01	0.42
1:B:188:PHE:O	1:B:219:ASN:HA	2.20	0.41
1:B:400:THR:HG23	1:B:401:PRO:CD	2.43	0.41
1:A:188:PHE:O	1:A:219:ASN:HA	2.20	0.41
1:B:272:HIS:CD2	1:B:334:ARG:HD3	2.55	0.41
1:A:393:LYS:HD2	7:A:1037:HOH:O	2.20	0.41
1:B:312:TRP:CG	1:B:401:PRO:HG3	2.55	0.41
1:B:284:LEU:HD21	1:B:334:ARG:CZ	2.51	0.41
1:A:336:ASN:ND2	1:A:338:VAL:HB	2.36	0.41
1:B:316:GLY:CA	1:B:363:ILE:HD11	2.50	0.41
1:B:391:TYR:HE1	1:B:393:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:HA	7:A:1146:HOH:O	2.21	0.41
1:A:239:ALA:O	1:A:242:ASP:HB2	2.20	0.41
1:A:356:ASN:HA	1:A:357:PRO:HD2	1.94	0.41
1:B:394:ILE:HG22	1:B:396:VAL:HG13	2.03	0.40
1:B:387:ARG:CG	1:B:387:ARG:NH1	2.84	0.40
1:A:395:THR:O	1:A:395:THR:CG2	2.69	0.40
1:B:323:ASN:HB2	1:B:366:THR:HG21	2.02	0.40
1:A:272:HIS:HB3	1:A:334:ARG:HG2	2.03	0.40
1:B:259:ASN:OD1	1:B:261:HIS:HB2	2.21	0.40
1:B:159:GLU:HG2	1:B:159:GLU:H	1.51	0.40
1:B:228:ARG:NH2	7:B:1340:HOH:O	2.52	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	269/286 (94%)	260 (97%)	9 (3%)	0	100	100
1	B	271/286 (95%)	264 (97%)	7 (3%)	0	100	100
All	All	540/572 (94%)	524 (97%)	16 (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	244/254 (96%)	225 (92%)	19 (8%)	16	19
1	B	246/254 (97%)	225 (92%)	21 (8%)	13	16
All	All	490/508 (96%)	450 (92%)	40 (8%)	14	17

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	THR
1	A	141	LEU
1	A	148	GLU
1	A	182	VAL
1	A	195	LEU
1	A	227	ASN
1	A	231	LEU
1	A	242	ASP
1	A	255	LEU
1	A	263	THR
1	A	270	PRO
1	A	328	ARG
1	A	336	ASN
1	A	343	ARG
1	A	349	ARG
1	A	351	LYS
1	A	375	LEU
1	A	381	MET
1	A	386	GLN
1	B	130	SER
1	B	137	GLU
1	B	141	LEU
1	B	157	LEU
1	B	159	GLU
1	B	161	GLN
1	B	165	VAL
1	B	174	MET
1	B	195	LEU
1	B	242	ASP
1	B	263	THR
1	B	283	SER
1	B	288	GLN
1	B	302	LEU
1	B	328	ARG
1	B	336	ASN

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Mol	Chain	Res	Type
1	B	346	ARG
1	B	354	GLU
1	B	381	MET
1	B	387	ARG
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	190	ASN
1	A	194	HIS
1	A	207	GLN
1	A	227	ASN
1	A	336	ASN
1	B	160	GLN
1	B	180	HIS
1	B	207	GLN
1	B	272	HIS
1	B	288	GLN
1	B	299	GLN
1	B	310	ASN
1	B	336	ASN
1	B	386	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
2	GDU	A	404	3	29,38,38	2.02	9 (31%)	43,58,58	3.09	12 (27%)
5	MES	A	900	-	11,12,12	1.33	2 (18%)	14,16,16	0.82	0
4	SO4	A	903	-	4,4,4	3.15	2 (50%)	6,6,6	0.98	0
6	DIO	A	905	-	6,6,6	0.77	0	6,6,6	1.44	1 (16%)
2	GDU	B	806	3	29,38,38	2.10	9 (31%)	43,58,58	3.02	12 (27%)
4	SO4	B	901	-	4,4,4	3.17	2 (50%)	6,6,6	1.03	0
4	SO4	B	902	-	4,4,4	3.33	2 (50%)	6,6,6	0.95	0
4	SO4	B	904	-	4,4,4	3.30	2 (50%)	6,6,6	0.98	0
6	DIO	B	906	-	6,6,6	0.86	0	6,6,6	1.57	2 (33%)

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	GDU	A	404	3	-	0/19/59/59	0/3/3/3
5	MES	A	900	-	-	0/6/14/14	0/1/1/1
4	SO4	A	903	-	-	0/0/0/0	0/0/0/0
6	DIO	A	905	-	-	0/0/6/6	0/1/1/1
2	GDU	B	806	3	-	0/19/59/59	0/3/3/3
4	SO4	B	901	-	-	0/0/0/0	0/0/0/0
4	SO4	B	902	-	-	0/0/0/0	0/0/0/0
4	SO4	B	904	-	-	0/0/0/0	0/0/0/0
6	DIO	B	906	-	-	0/0/6/6	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	SO4	O3-S	-4.80	1.30	1.47
2	B	806	GDU	PB-O3B	-4.67	1.47	1.60
4	B	902	SO4	O3-S	-4.53	1.31	1.47
4	B	901	SO4	O3-S	-4.43	1.31	1.47
4	A	903	SO4	O3-S	-4.32	1.31	1.47
2	A	404	GDU	PB-O3B	-3.85	1.50	1.60
2	B	806	GDU	C5D-C4D	-2.62	1.43	1.51
2	A	404	GDU	C6-C5	-2.43	1.32	1.38
2	A	404	GDU	C5D-C4D	-2.39	1.43	1.51
2	B	806	GDU	O5D-C5D	-2.32	1.35	1.44
2	A	404	GDU	O5D-C5D	-2.15	1.36	1.44
2	B	806	GDU	C6-C5	-2.11	1.33	1.38
2	A	404	GDU	PB-O1B	2.27	1.59	1.51
2	B	806	GDU	O5'-C1'	2.35	1.47	1.41
5	A	900	MES	C3-N4	2.37	1.53	1.46
2	A	404	GDU	O5'-C5'	2.48	1.50	1.44
2	A	404	GDU	O5'-C1'	2.59	1.48	1.41
5	A	900	MES	C5-N4	2.68	1.54	1.46
2	B	806	GDU	PB-O1B	2.98	1.62	1.51
2	B	806	GDU	O5'-C5'	2.98	1.51	1.44
2	A	404	GDU	C4-N3	3.75	1.40	1.33
4	B	904	SO4	O1-S	4.42	1.62	1.47
4	B	901	SO4	O1-S	4.46	1.62	1.47
4	A	903	SO4	O1-S	4.51	1.62	1.47
2	B	806	GDU	C4-N3	4.63	1.41	1.33
4	B	902	SO4	O1-S	4.74	1.63	1.47
2	B	806	GDU	C6-N1	4.80	1.42	1.35
2	A	404	GDU	C6-N1	5.94	1.44	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	GDU	C5D-C4D-C3D	-5.61	92.93	115.21
2	B	806	GDU	C5D-C4D-C3D	-5.37	93.88	115.21
2	A	404	GDU	O5'-C5'-C6'	-4.01	96.23	106.36
2	B	806	GDU	O5'-C5'-C6'	-3.98	96.29	106.36
2	B	806	GDU	C5-C4-N3	-3.52	114.09	123.12
2	A	404	GDU	O4D-C1D-N1	-3.41	100.90	108.08
2	A	404	GDU	C5-C4-N3	-3.24	114.81	123.12
2	B	806	GDU	O4D-C1D-N1	-3.12	101.51	108.08
2	A	404	GDU	O3'-C3'-C4'	-2.91	103.78	110.34
2	A	404	GDU	O4D-C4D-C3D	-2.72	99.66	105.15
2	B	806	GDU	O4D-C4D-C3D	-2.61	99.88	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	806	GDU	O3'-C3'-C4'	-2.10	105.62	110.34
2	A	404	GDU	PB-O3A-PA	-2.06	126.95	132.73
6	B	906	DIO	C2-O1-C1	2.20	117.28	109.89
2	B	806	GDU	C4D-O4D-C1D	2.45	112.41	109.72
6	A	905	DIO	C2'-O1'-C1'	2.53	118.43	109.89
2	A	404	GDU	C2D-C3D-C4D	2.55	107.85	102.61
6	B	906	DIO	C2'-O1'-C1'	2.66	118.85	109.89
2	B	806	GDU	C2D-C3D-C4D	2.73	108.22	102.61
2	A	404	GDU	O3A-PB-O3B	2.84	111.80	103.63
2	A	404	GDU	O3B-PB-O1B	3.05	121.44	109.46
2	B	806	GDU	O3A-PB-O3B	3.19	112.81	103.63
2	B	806	GDU	O3B-PB-O1B	3.24	122.22	109.46
2	B	806	GDU	O5D-C5D-C4D	8.15	139.16	109.12
2	A	404	GDU	O5D-C5D-C4D	8.23	139.47	109.12
2	B	806	GDU	C4-N3-C2	13.17	127.18	114.14
2	A	404	GDU	C4-N3-C2	13.71	127.72	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	MES	5	0
6	A	905	DIO	2	0
4	B	902	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, 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	271/286 (94%)	0.28	15 (5%) 29 37	24, 34, 52, 65	0
1	B	273/286 (95%)	0.58	36 (13%) 4 7	24, 35, 61, 70	0
All	All	544/572 (95%)	0.43	51 (9%) 11 16	24, 35, 57, 70	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	SER	7.9
1	A	402	SER	7.5
1	B	130	SER	4.9
1	B	352	LYS	4.2
1	B	131	LEU	3.9
1	B	152	PRO	3.7
1	A	157	LEU	3.5
1	A	132	THR	3.5
1	B	174	MET	3.5
1	B	136	GLU	3.4
1	B	184	ILE	3.4
1	B	151	ILE	3.1
1	B	351	LYS	3.1
1	B	157	LEU	3.0
1	B	150	ASN	3.0
1	B	186	ILE	3.0
1	B	163	PRO	2.8
1	B	251	SER	2.8
1	A	177	ILE	2.8
1	B	249	VAL	2.8
1	B	177	ILE	2.7
1	A	293	VAL	2.7
1	B	137	GLU	2.7
1	B	255	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	223	GLU	2.6
1	B	287	VAL	2.5
1	A	174	MET	2.5
1	B	132	THR	2.5
1	B	225	MET	2.5
1	A	351	LYS	2.4
1	B	360	PHE	2.4
1	A	133	ALA	2.4
1	A	349	ARG	2.4
1	B	292	GLY	2.3
1	B	256	ILE	2.3
1	B	133	ALA	2.3
1	B	293	VAL	2.3
1	A	223	GLU	2.2
1	A	160	GLN	2.2
1	B	185	ILE	2.2
1	B	160	GLN	2.2
1	B	349	ARG	2.1
1	A	185	ILE	2.1
1	B	218	ILE	2.1
1	A	154	ASP	2.1
1	B	232	LEU	2.1
1	B	253	VAL	2.1
1	A	232	LEU	2.0
1	B	361	ASP	2.0
1	A	251	SER	2.0
1	B	364	ALA	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
4	SO4	B	901	5/5	0.94	0.20	1.47	77,78,78,78	0
5	MES	A	900	12/12	0.80	0.23	1.06	75,77,81,81	0
2	GDU	B	806	36/36	0.97	0.13	-0.64	26,30,34,36	0
2	GDU	A	404	36/36	0.96	0.12	-0.65	25,28,32,34	0
3	MN	A	403	1/1	0.99	0.09	-1.14	29,29,29,29	0
3	MN	B	805	1/1	1.00	0.09	-2.38	31,31,31,31	0
4	SO4	B	904	5/5	0.91	0.14	-	85,85,85,86	0
4	SO4	B	902	5/5	0.91	0.16	-	77,77,78,79	0
6	DIO	A	905	6/6	0.73	0.21	-	73,74,74,74	0
6	DIO	B	906	6/6	0.80	0.18	-	67,68,69,69	0
4	SO4	A	903	5/5	0.93	0.19	-	76,76,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.