



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:40 AM BST

PDB ID : 5NQA
Title : Crystal structure of GalNAc-T4 in complex with the monoglycopeptide 3
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Deposited on : 2017-04-19
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

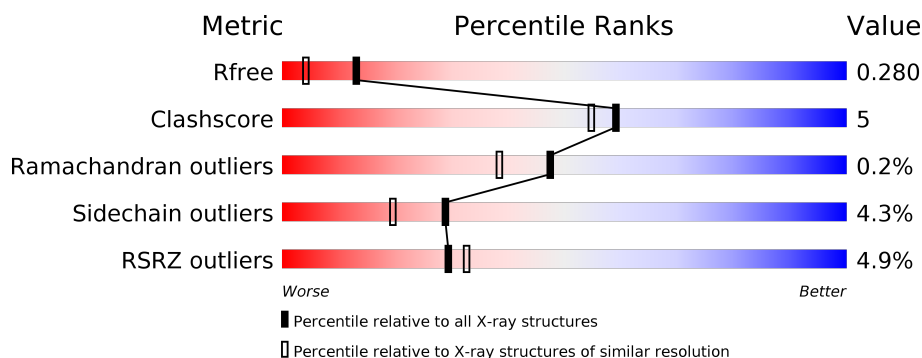
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 respectively. 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	578	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	578	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
2	G	16	<div> <div>6%</div> <div> <div></div> <div>94%</div> </div> </div>

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
3	EDO	B	626	-	-	-	X
5	NGA	G	101	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10430 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.

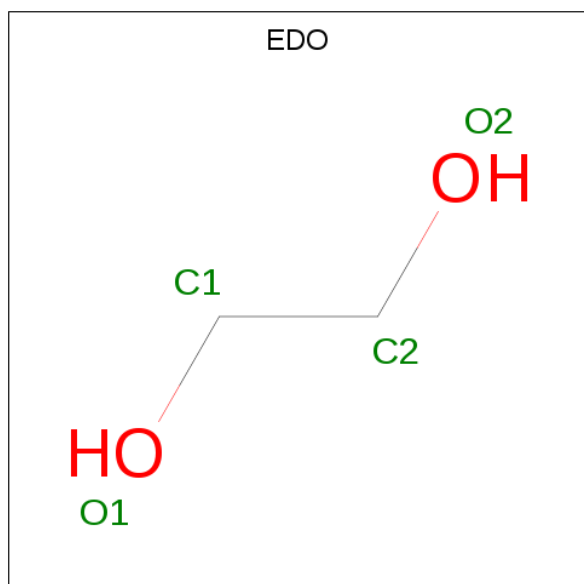
- Molecule 1 is a protein called Polypeptide N-acetylgalactosaminyltransferase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	4	0
			4215	2675	743	774	23			
1	B	514	Total	C	N	O	S	0	12	0
			4268	2709	753	783	23			

- Molecule 2 is a protein called Monoglycopeptide 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	1	Total	C	N	O	0	0	0
			7	4	1	2			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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[illegible]

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



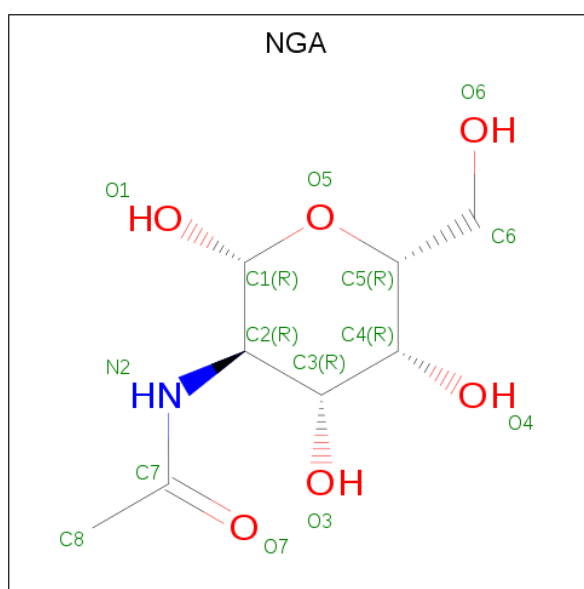
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	738	Total	O	0	0
			738	738		

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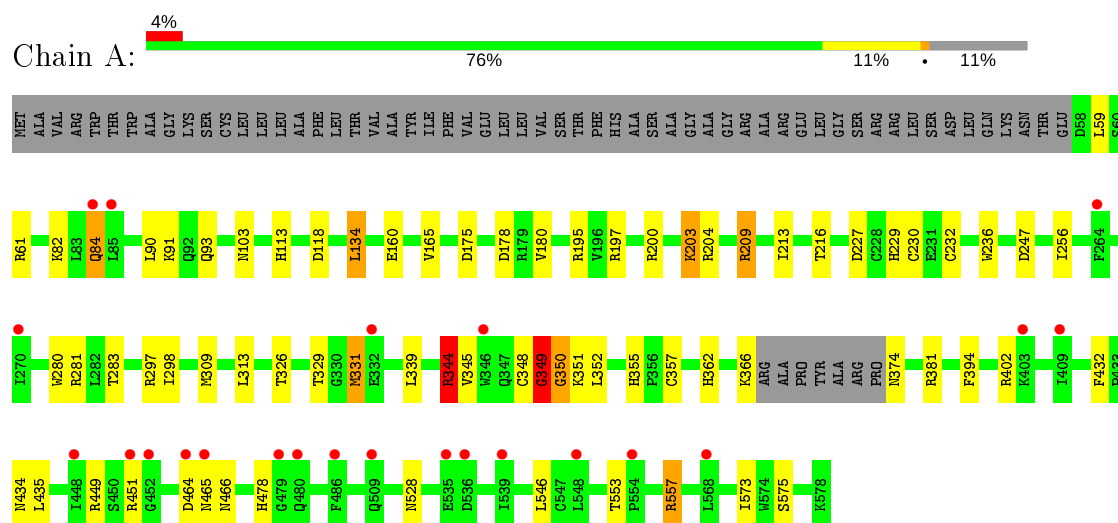
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	829	Total 829	O 829	0	0

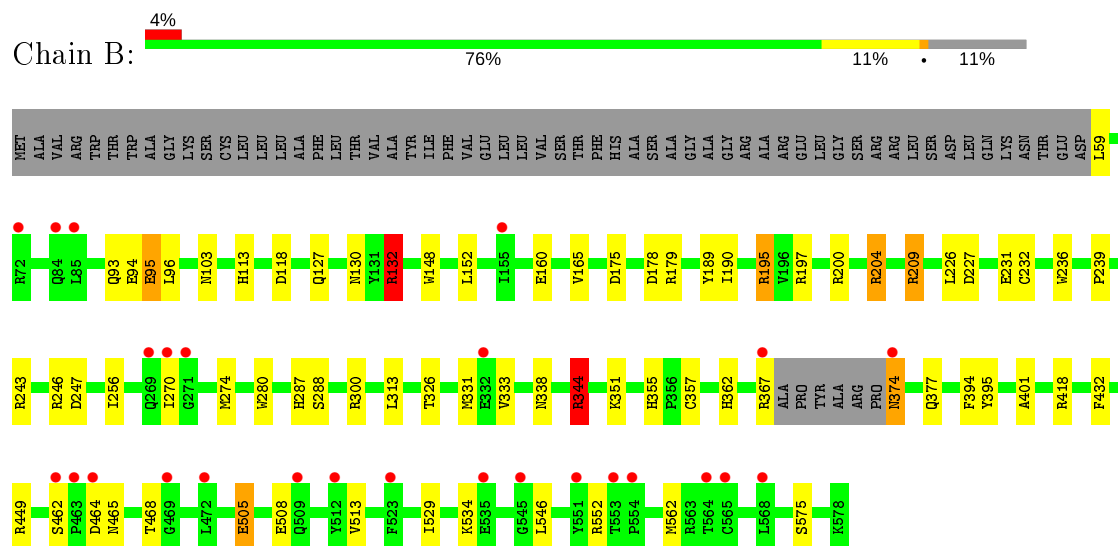
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Polypeptide N-acetylgalactosaminyltransferase 4



- Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 4



- Molecule 2: Monoglycopeptide 3



GLY
ALA
TS
GLY
ALA
GLY
ALA
GLY
ALA
GLY
THR
THR
PRO
GLY
PRO
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.45Å 79.88Å 88.61Å 116.47° 96.74° 104.72°	Depositor
Resolution (Å)	76.45 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (76.45-1.90) 97.6 (19.96-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.225 , 0.274 0.229 , 0.280	Depositor DCC
R_{free} test set	3182 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10430	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% 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: GOL, NGA, EDO

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	0.72	0/4336	0.91	15/5869 (0.3%)
1	B	0.75	1/4414 (0.0%)	0.90	12/5972 (0.2%)
2	G	0.90	0/6	0.91	0/7
All	All	0.73	1/8756 (0.0%)	0.90	27/11848 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	GLU	CD-OE1	5.85	1.32	1.25

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	GLY	N-CA-C	11.55	141.98	113.10
1	B	344	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	A	209	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	B	178	ASP	CB-CA-C	-7.68	95.03	110.40
1	A	344	ARG	NE-CZ-NH2	-6.90	116.85	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	CYS	Peptide
1	A	349	GLY	Mainchain,Peptide
1	B	464	ASP	Peptide

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	4215	0	4099	38	0
1	B	4268	0	4171	41	0
2	G	7	0	5	0	0
3	A	148	0	222	7	0
3	B	136	0	204	3	0
4	A	36	0	48	1	0
4	B	24	0	32	0	0
5	A	15	0	14	2	0
5	G	14	0	13	0	0
6	A	738	0	0	8	0
6	B	829	0	0	8	0
All	All	10430	0	8808	83	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.

The worst 5 of 83 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:434:ASN:O	1:A:435:LEU:CA	1.66	1.43
1:A:197[B]:ARG:NH1	1:A:197[B]:ARG:HG2	1.60	1.04
1:B:204[A]:ARG:HH11	1:B:204[A]:ARG:HG3	1.21	1.02
1:A:197[B]:ARG:HH11	1:A:197[B]:ARG:CG	1.74	1.00
1:A:197[B]:ARG:HH11	1:A:197[B]:ARG:HG2	0.81	0.95

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	512/578 (89%)	503 (98%)	7 (1%)	2 (0%)	34	24
1	B	522/578 (90%)	513 (98%)	9 (2%)	0	100	100
All	All	1034/1156 (89%)	1016 (98%)	16 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLY
1	A	350	GLY

5.3.2 Protein sidechains

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	460/507 (91%)	441 (96%)	19 (4%)	30	21
1	B	469/507 (92%)	447 (95%)	22 (5%)	26	16
2	G	1/5 (20%)	1 (100%)	0	100	100
All	All	930/1019 (91%)	889 (96%)	41 (4%)	29	19

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	SER
1	B	195	ARG
1	B	546	LEU

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Mol	Chain	Res	Type
1	B	95	GLU
1	B	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	ASN
1	A	541	HIS
1	B	517	ASN
1	A	528	ASN
1	B	93	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

83 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	$\# Z > 2$
3	EDO	B	630	-	3,3,3	0.58	0	2,2,2	0.11	0
3	EDO	B	629	-	3,3,3	0.49	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	638	-	5,5,5	0.33	0	5,5,5	0.36	0
3	EDO	B	623	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	B	606	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	B	607	-	3,3,3	0.39	0	2,2,2	0.45	0
3	EDO	B	602	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	B	625	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	A	630	-	3,3,3	0.50	0	2,2,2	0.06	0
3	EDO	A	632	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	A	634	-	3,3,3	0.51	0	2,2,2	0.15	0
5	NGA	G	101	2	14,14,15	0.39	0	17,19,21	1.29	1 (5%)
3	EDO	A	626	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	A	607	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	B	628	-	3,3,3	0.39	0	2,2,2	0.44	0
3	EDO	A	636	-	3,3,3	0.44	0	2,2,2	0.21	0
3	EDO	B	615	-	3,3,3	0.29	0	2,2,2	0.52	0
3	EDO	B	634	-	3,3,3	0.39	0	2,2,2	0.33	0
3	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	B	614	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	A	606	-	3,3,3	0.46	0	2,2,2	0.48	0
4	GOL	B	636	-	5,5,5	0.27	0	5,5,5	0.23	0
3	EDO	A	637	-	3,3,3	0.24	0	2,2,2	0.06	0
4	GOL	B	635	-	5,5,5	0.29	0	5,5,5	0.33	0
3	EDO	B	620	-	3,3,3	0.33	0	2,2,2	0.48	0
3	EDO	B	608	-	3,3,3	0.51	0	2,2,2	0.13	0
3	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.57	0
3	EDO	B	631	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	A	619	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	A	612	-	3,3,3	0.34	0	2,2,2	0.39	0
3	EDO	B	612	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	A	609	-	3,3,3	0.53	0	2,2,2	0.14	0
3	EDO	B	616	-	3,3,3	0.41	0	2,2,2	0.31	0
3	EDO	A	621	-	3,3,3	0.42	0	2,2,2	0.33	0
3	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.23	0
4	GOL	B	637	-	5,5,5	0.47	0	5,5,5	0.42	0
3	EDO	B	605	-	3,3,3	0.35	0	2,2,2	0.28	0
3	EDO	B	610	-	3,3,3	0.53	0	2,2,2	0.23	0
3	EDO	B	622	-	3,3,3	0.48	0	2,2,2	0.24	0
3	EDO	B	633	-	3,3,3	0.44	0	2,2,2	0.20	0
3	EDO	A	604	-	3,3,3	0.33	0	2,2,2	0.94	0
3	EDO	B	624	-	3,3,3	0.19	0	2,2,2	0.74	0
3	EDO	B	632	-	3,3,3	0.49	0	2,2,2	0.18	0
3	EDO	A	635	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	A	625	-	3,3,3	0.23	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	613	-	3,3,3	0.56	0	2,2,2	0.17	0
5	NGA	A	644	-	15,15,15	1.49	2 (13%)	21,21,21	3.50	5 (23%)
3	EDO	A	605	-	3,3,3	0.54	0	2,2,2	0.32	0
3	EDO	A	611	-	3,3,3	0.47	0	2,2,2	0.11	0
3	EDO	A	601	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	A	615	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	B	618	-	3,3,3	0.23	0	2,2,2	0.66	0
4	GOL	A	640	-	5,5,5	0.50	0	5,5,5	0.51	0
3	EDO	B	603	-	3,3,3	0.52	0	2,2,2	0.47	0
3	EDO	B	601	-	3,3,3	0.50	0	2,2,2	0.29	0
4	GOL	A	643	-	5,5,5	0.20	0	5,5,5	0.23	0
3	EDO	A	616	-	3,3,3	0.43	0	2,2,2	0.31	0
4	GOL	A	639	-	5,5,5	0.30	0	5,5,5	0.19	0
3	EDO	B	611	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	A	623	-	3,3,3	0.42	0	2,2,2	0.28	0
3	EDO	A	603	-	3,3,3	0.48	0	2,2,2	0.26	0
4	GOL	A	642	-	5,5,5	0.25	0	5,5,5	0.32	0
3	EDO	A	629	-	3,3,3	0.39	0	2,2,2	0.19	0
4	GOL	A	641	-	5,5,5	0.39	0	5,5,5	0.19	0
3	EDO	A	633	-	3,3,3	0.41	0	2,2,2	0.37	0
3	EDO	A	614	-	3,3,3	0.46	0	2,2,2	0.24	0
3	EDO	A	602	-	3,3,3	0.28	0	2,2,2	0.71	0
3	EDO	A	620	-	3,3,3	0.49	0	2,2,2	0.21	0
3	EDO	B	609	-	3,3,3	0.42	0	2,2,2	0.45	0
3	EDO	A	628	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	B	617	-	3,3,3	0.40	0	2,2,2	0.54	0
3	EDO	A	631	-	3,3,3	0.42	0	2,2,2	0.46	0
4	GOL	A	638	-	5,5,5	0.26	0	5,5,5	0.55	0
3	EDO	B	627	-	3,3,3	0.48	0	2,2,2	0.34	0
3	EDO	B	604	-	3,3,3	0.32	0	2,2,2	0.30	0
3	EDO	B	621	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	A	627	-	3,3,3	0.59	0	2,2,2	0.27	0
3	EDO	B	626	-	3,3,3	0.42	0	2,2,2	0.45	0
3	EDO	A	613	-	3,3,3	0.48	0	2,2,2	0.21	0
3	EDO	B	619	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	A	624	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	A	618	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.26	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	EDO	B	630	-	-	1/1/1/1	-
3	EDO	B	629	-	-	0/1/1/1	-
4	GOL	B	638	-	-	0/4/4/4	-
3	EDO	B	623	-	-	0/1/1/1	-
3	EDO	B	606	-	-	1/1/1/1	-
3	EDO	B	607	-	-	0/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	B	625	-	-	1/1/1/1	-
3	EDO	A	630	-	-	1/1/1/1	-
3	EDO	A	632	-	-	1/1/1/1	-
3	EDO	A	634	-	-	1/1/1/1	-
5	NGA	G	101	2	1/1/5/7	0/6/23/26	0/1/1/1
3	EDO	A	626	-	-	1/1/1/1	-
3	EDO	A	607	-	-	1/1/1/1	-
3	EDO	B	628	-	-	1/1/1/1	-
3	EDO	A	636	-	-	1/1/1/1	-
3	EDO	B	615	-	-	0/1/1/1	-
3	EDO	B	634	-	-	1/1/1/1	-
3	EDO	A	610	-	-	1/1/1/1	-
3	EDO	B	614	-	-	1/1/1/1	-
3	EDO	A	606	-	-	1/1/1/1	-
4	GOL	B	636	-	-	2/4/4/4	-
3	EDO	A	637	-	-	1/1/1/1	-
4	GOL	B	635	-	-	0/4/4/4	-
3	EDO	B	620	-	-	1/1/1/1	-
3	EDO	B	608	-	-	1/1/1/1	-
3	EDO	A	622	-	-	0/1/1/1	-
3	EDO	B	631	-	-	1/1/1/1	-
3	EDO	A	619	-	-	1/1/1/1	-
3	EDO	A	612	-	-	0/1/1/1	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	B	616	-	-	1/1/1/1	-
3	EDO	A	621	-	-	0/1/1/1	-
3	EDO	A	617	-	-	0/1/1/1	-
4	GOL	B	637	-	-	2/4/4/4	-
3	EDO	B	605	-	-	0/1/1/1	-
3	EDO	B	610	-	-	0/1/1/1	-
3	EDO	B	622	-	-	1/1/1/1	-
3	EDO	B	633	-	-	0/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
3	EDO	B	624	-	-	1/1/1/1	-
3	EDO	B	632	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	635	-	-	1/1/1/1	-
3	EDO	A	625	-	-	1/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
5	NGA	A	644	-	-	0/6/26/26	0/1/1/1
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	A	611	-	-	1/1/1/1	-
3	EDO	A	601	-	-	1/1/1/1	-
3	EDO	A	615	-	-	0/1/1/1	-
3	EDO	B	618	-	-	0/1/1/1	-
4	GOL	A	640	-	-	4/4/4/4	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
4	GOL	A	643	-	-	2/4/4/4	-
3	EDO	A	616	-	-	0/1/1/1	-
4	GOL	A	639	-	-	2/4/4/4	-
3	EDO	B	611	-	-	1/1/1/1	-
3	EDO	A	623	-	-	1/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
4	GOL	A	642	-	-	2/4/4/4	-
3	EDO	A	629	-	-	0/1/1/1	-
4	GOL	A	641	-	-	2/4/4/4	-
3	EDO	A	633	-	-	1/1/1/1	-
3	EDO	A	614	-	-	0/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	620	-	-	0/1/1/1	-
3	EDO	B	609	-	-	1/1/1/1	-
3	EDO	A	628	-	-	0/1/1/1	-
3	EDO	B	617	-	-	1/1/1/1	-
3	EDO	A	631	-	-	0/1/1/1	-
4	GOL	A	638	-	-	2/4/4/4	-
3	EDO	B	627	-	-	1/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-
3	EDO	B	621	-	-	0/1/1/1	-
3	EDO	A	627	-	-	1/1/1/1	-
3	EDO	B	626	-	-	1/1/1/1	-
3	EDO	A	613	-	-	1/1/1/1	-
3	EDO	B	619	-	-	1/1/1/1	-
3	EDO	A	624	-	-	0/1/1/1	-
3	EDO	A	618	-	-	1/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	644	NGA	C1-C2	-3.09	1.49	1.52
5	A	644	NGA	O1-C1	2.83	1.48	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	644	NGA	C1-C2-C3	-11.27	95.18	110.54
5	A	644	NGA	O1-C1-O5	6.62	130.26	110.38
5	A	644	NGA	C1-O5-C5	-5.92	102.48	113.66
5	A	644	NGA	O1-C1-C2	4.91	119.41	109.22
5	G	101	NGA	O5-C1-C2	-4.28	104.52	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	101	NGA	C1

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	640	GOL	C1-C2-C3-O3
4	A	642	GOL	C1-C2-C3-O3
4	A	639	GOL	C1-C2-C3-O3
4	A	639	GOL	O2-C2-C3-O3
4	B	637	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	EDO	1	0
3	A	606	EDO	1	0
3	A	637	EDO	1	0
3	A	622	EDO	1	0
3	A	604	EDO	1	0
5	A	644	NGA	2	0
3	A	611	EDO	2	0
3	B	618	EDO	1	0
3	A	603	EDO	1	0
3	B	617	EDO	1	0
4	A	638	GOL	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	514/578 (88%)	0.40	23 (4%) 33 36	17, 31, 53, 78	0
1	B	514/578 (88%)	0.39	26 (5%) 28 31	16, 30, 49, 68	0
2	G	1/16 (6%)	2.53	1 (100%) 0 0	56, 56, 56, 56	0
All	All	1029/1172 (87%)	0.40	50 (4%) 29 33	16, 31, 53, 78	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	LEU	6.5
1	A	464	ASP	4.9
1	A	554	PRO	4.8
1	B	270	ILE	4.7
1	B	535	GLU	4.0

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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
3	EDO	A	627	4/4	0.47	0.28	51,51,53,56	0
3	EDO	B	629	4/4	0.49	0.24	73,74,74,75	0
3	EDO	A	617	4/4	0.52	0.35	65,66,67,67	0
4	GOL	A	638	6/6	0.54	0.25	55,59,64,64	0
4	GOL	A	640	6/6	0.55	0.35	49,54,56,57	0
3	EDO	B	610	4/4	0.56	0.36	49,54,56,56	0
4	GOL	B	637	6/6	0.60	0.40	56,60,61,63	0
3	EDO	A	620	4/4	0.61	0.30	68,69,70,70	0
4	GOL	A	641	6/6	0.62	0.27	55,60,64,68	0
3	EDO	A	633	4/4	0.62	0.24	63,64,66,68	0
4	GOL	B	638	6/6	0.63	0.30	60,64,64,68	0
3	EDO	B	621	4/4	0.68	0.29	67,68,68,69	0
3	EDO	B	608	4/4	0.69	0.22	51,53,56,57	0
3	EDO	B	630	4/4	0.69	0.22	45,45,46,47	0
3	EDO	A	611	4/4	0.69	0.24	64,65,65,66	0
3	EDO	A	618	4/4	0.70	0.22	61,61,62,62	0
3	EDO	B	626	4/4	0.73	0.46	37,45,47,57	0
3	EDO	A	613	4/4	0.73	0.28	58,59,60,61	0
3	EDO	A	632	4/4	0.73	0.14	63,63,63,64	0
3	EDO	B	603	4/4	0.74	0.29	41,47,47,55	0
3	EDO	A	635	4/4	0.74	0.22	58,61,61,62	0
3	EDO	A	615	4/4	0.75	0.20	51,53,53,54	0
4	GOL	B	635	6/6	0.75	0.22	52,53,53,56	0
3	EDO	A	621	4/4	0.77	0.20	61,63,64,64	0
3	EDO	B	618	4/4	0.77	0.24	29,30,31,41	0
3	EDO	B	613	4/4	0.77	0.20	40,40,40,40	0
3	EDO	A	619	4/4	0.77	0.15	64,67,67,68	0
3	EDO	B	631	4/4	0.77	0.26	52,54,55,58	0
3	EDO	B	602	4/4	0.78	0.15	34,38,39,44	0
3	EDO	B	607	4/4	0.78	0.36	59,59,61,61	0
3	EDO	A	614	4/4	0.78	0.32	48,51,52,55	0
3	EDO	A	608	4/4	0.78	0.27	38,38,39,39	0
3	EDO	B	606	4/4	0.79	0.13	47,47,48,49	0
3	EDO	A	603	4/4	0.79	0.22	40,47,49,49	0
3	EDO	A	634	4/4	0.79	0.21	40,41,41,42	0
5	NGA	G	101	14/15	0.81	0.23	43,48,53,56	0
3	EDO	B	622	4/4	0.81	0.30	48,50,51,51	0
3	EDO	B	625	4/4	0.82	0.14	42,44,45,47	0
3	EDO	B	605	4/4	0.82	0.23	30,35,38,47	0
3	EDO	A	602	4/4	0.82	0.24	26,29,33,39	0
4	GOL	A	642	6/6	0.82	0.16	43,48,52,56	0
3	EDO	B	614	4/4	0.82	0.21	43,48,49,51	0
3	EDO	B	601	4/4	0.83	0.14	49,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	623	4/4	0.83	0.22	30,33,35,37	0
3	EDO	B	632	4/4	0.83	0.29	42,48,48,52	0
3	EDO	B	617	4/4	0.84	0.09	38,40,40,42	0
3	EDO	A	631	4/4	0.84	0.29	50,54,56,60	0
3	EDO	B	611	4/4	0.84	0.20	45,45,48,50	0
3	EDO	A	622	4/4	0.85	0.13	34,34,35,38	0
3	EDO	B	624	4/4	0.85	0.19	32,34,35,40	0
3	EDO	A	616	4/4	0.85	0.16	64,66,67,71	0
3	EDO	B	612	4/4	0.85	0.18	43,44,45,45	0
3	EDO	B	616	4/4	0.85	0.15	51,52,52,53	0
3	EDO	A	601	4/4	0.86	0.11	40,41,42,44	0
3	EDO	A	605	4/4	0.87	0.17	36,38,41,43	0
3	EDO	A	628	4/4	0.87	0.17	55,56,58,59	0
3	EDO	A	609	4/4	0.87	0.19	41,43,45,46	0
3	EDO	A	626	4/4	0.87	0.17	50,50,50,51	0
4	GOL	A	639	6/6	0.87	0.23	62,63,65,67	0
3	EDO	A	607	4/4	0.87	0.37	39,40,45,50	0
3	EDO	B	604	4/4	0.87	0.22	31,35,35,38	0
3	EDO	A	637	4/4	0.88	0.49	20,20,20,20	0
3	EDO	B	628	4/4	0.88	0.22	43,45,46,49	0
3	EDO	B	619	4/4	0.88	0.14	35,36,36,37	0
3	EDO	B	609	4/4	0.88	0.13	44,45,46,47	0
4	GOL	A	643	6/6	0.88	0.18	50,52,52,56	0
3	EDO	A	624	4/4	0.88	0.12	40,42,42,43	0
3	EDO	A	625	4/4	0.89	0.24	41,43,45,45	0
3	EDO	B	620	4/4	0.89	0.12	38,38,38,39	0
3	EDO	A	612	4/4	0.89	0.20	50,51,51,51	0
3	EDO	A	636	4/4	0.89	0.37	46,47,48,49	0
3	EDO	B	633	4/4	0.89	0.20	41,45,46,49	0
3	EDO	B	634	4/4	0.90	0.18	44,47,49,53	0
3	EDO	A	604	4/4	0.91	0.13	26,27,28,28	0
3	EDO	B	627	4/4	0.91	0.12	47,48,48,52	0
3	EDO	A	629	4/4	0.91	0.20	58,60,60,63	0
3	EDO	A	610	4/4	0.92	0.11	41,41,41,42	0
4	GOL	B	636	6/6	0.92	0.21	51,54,54,55	0
3	EDO	B	615	4/4	0.92	0.11	36,36,38,39	0
3	EDO	A	630	4/4	0.93	0.11	32,35,36,39	0
3	EDO	B	623	4/4	0.93	0.12	31,32,33,34	0
5	NGA	A	644	15/15	0.93	0.17	43,47,52,55	0
3	EDO	A	606	4/4	0.94	0.20	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.