



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:43 PM EDT

PDB ID : 2H1B
Title : ResA E80Q
Authors : Lewin, A.; Crow, A.; Oubrie, A.; Le Brun, N.E.
Deposited on : 2006-05-16
Resolution : 1.95 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

<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 : 2.23.2
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) : 2.23.2

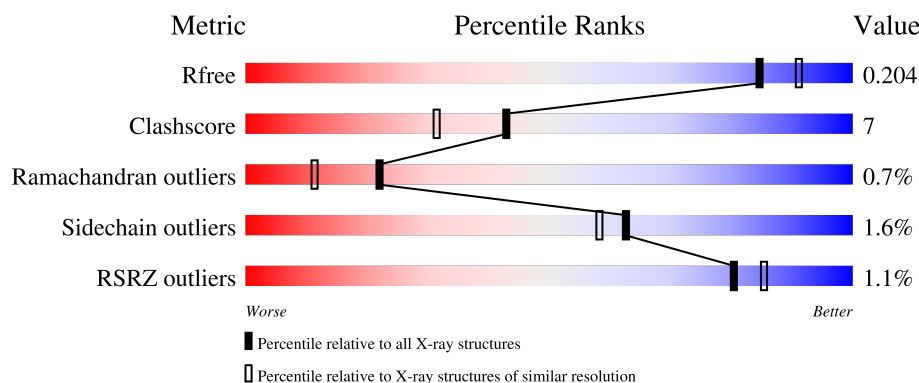
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of 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	143	
1	B	143	
1	C	143	
1	D	143	

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	A	703	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5082 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 Thiol-disulfide oxidoreductase resA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	7	0
			1124	725	180	211	8			
1	B	138	Total	C	N	O	S	0	5	0
			1132	729	190	206	7			
1	C	137	Total	C	N	O	S	0	6	0
			1110	716	181	206	7			
1	D	137	Total	C	N	O	S	0	5	0
			1107	716	181	203	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLN	GLU	engineered mutation	UNP P35160
B	80	GLN	GLU	engineered mutation	UNP P35160
C	80	GLN	GLU	engineered mutation	UNP P35160
D	80	GLN	GLU	engineered mutation	UNP P35160

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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		

Continued on next page...

Continued from previous page...

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


- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	110	Total O 110 110	0	0
4	C	155	Total O 155 155	0	0
4	D	113	Total O 113 113	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: Thiol-disulfide oxidoreductase resA

Chain A: 




- Molecule 1: Thiol-disulfide oxidoreductase resA

Chain B: 




- Molecule 1: Thiol-disulfide oxidoreductase resA

Chain C: 



- Molecule 1: Thiol-disulfide oxidoreductase resA

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.97Å 46.51Å 95.05Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 29.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.95) 99.9 (29.46-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.14 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.206 0.151 , 0.204	Depositor DCC
R_{free} test set	1993 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.75	0/1166	0.68	0/1579
1	B	0.61	0/1175	0.66	1/1589 (0.1%)
1	C	0.73	0/1149	0.68	0/1557
1	D	0.62	0/1143	0.64	0/1547
All	All	0.68	0/4633	0.67	1/6272 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	LEU	CA-CB-CG	-5.34	103.01	115.30

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	1124	0	1121	15	0
1	B	1132	0	1136	15	0
1	C	1110	0	1110	14	0
1	D	1107	0	1112	16	0
2	A	4	0	3	0	0
3	A	12	0	18	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	199	0	0	7	0
4	B	110	0	0	2	0
4	C	155	0	0	3	0
4	D	113	0	0	4	0
All	All	5082	0	4524	61	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 7.

All (61) 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:D:79[B]:LYS:HD3	4:D:742:HOH:O	1.59	1.02
1:A:128[B]:ASP:OD1	4:A:957:HOH:O	1.87	0.93
1:A:158:GLY:O	4:A:994:HOH:O	1.98	0.81
1:D:80:GLN:NE2	4:D:732:HOH:O	2.13	0.81
1:C:127:THR:HG22	4:C:709:HOH:O	1.83	0.78
1:C:128[B]:ASP:OD1	4:C:712:HOH:O	2.02	0.77
1:C:76:PRO:O	1:C:159[B]:THR:CG2	2.35	0.74
1:B:61:LYS:HE3	4:B:794:HOH:O	1.89	0.73
1:C:76:PRO:O	1:C:159[B]:THR:HG22	1.89	0.73
3:A:703:EDO:H12	4:A:872:HOH:O	1.90	0.70
1:A:107:LYS:HG2	1:A:125[A]:LEU:HD11	1.75	0.69
1:A:48[A]:GLU:OE1	4:A:982:HOH:O	2.11	0.68
1:A:74[B]:CYS:SG	1:A:141:PRO:HD3	2.33	0.68
1:C:133:ASP:OD1	4:C:819:HOH:O	2.14	0.66
1:A:63[B]:LYS:NZ	4:A:970:HOH:O	2.30	0.65
1:C:154:LYS:HG3	1:C:168:TYR:CE1	2.31	0.65
1:A:54:ARG:CB	3:A:703:EDO:H21	2.28	0.63
1:D:54:ARG:NH2	4:D:761:HOH:O	2.30	0.63
1:B:145:LEU:HD13	1:B:168:TYR:CD1	2.35	0.62
1:A:41:ASP:OD1	1:A:151:LYS:NZ	2.22	0.60
1:A:54:ARG:HB3	3:A:703:EDO:H21	1.83	0.60
1:B:54[C]:ARG:CG	1:B:54[C]:ARG:HH11	2.17	0.58
1:D:147:ASN:HD22	1:D:147:ASN:C	2.10	0.54
1:B:54[C]:ARG:NH1	1:B:54[C]:ARG:HG3	2.23	0.53
1:B:54[C]:ARG:HH11	1:B:54[C]:ARG:HG3	1.74	0.52
1:C:80:GLN:NE2	1:C:160:MET:H	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD12	1:D:137:VAL:HB	1.93	0.51
1:D:50:THR:O	1:D:107[B]:LYS:NZ	2.45	0.49
1:A:141:PRO:HG2	4:A:994:HOH:O	2.12	0.49
1:C:78:LYS:HG2	1:C:113:PHE:HZ	1.78	0.48
1:B:127:THR:HG22	4:B:774:HOH:O	2.13	0.48
1:A:128[B]:ASP:OD1	1:A:130:GLN:HG3	2.13	0.47
1:B:75:GLU:N	1:B:76:PRO:CD	2.78	0.47
1:B:77:CYS:O	1:B:81:PHE:HB2	2.15	0.47
1:D:55:ILE:HD12	1:D:124:VAL:CG1	2.45	0.46
1:B:54[C]:ARG:CG	1:B:54[C]:ARG:NH1	2.78	0.46
1:B:107[B]:LYS:HG2	1:B:125:LEU:HD13	1.96	0.46
1:C:76:PRO:O	1:C:159[B]:THR:HG23	2.12	0.45
1:D:158[B]:GLY:O	4:D:748:HOH:O	2.21	0.45
1:C:138:SER:CB	1:C:139:PRO:CD	2.95	0.44
1:D:49:ASP:HB3	1:D:55:ILE:HD11	1.98	0.44
1:C:154:LYS:HD3	1:C:155:VAL:N	2.33	0.43
1:B:50:THR:HB	1:B:111[B]:HIS:NE2	2.32	0.43
1:D:49:ASP:HB3	1:D:55:ILE:CD1	2.48	0.43
1:B:107[B]:LYS:HG2	1:B:125:LEU:CD1	2.48	0.43
1:A:54:ARG:HB2	3:A:703:EDO:H21	2.00	0.43
1:B:50:THR:HG21	1:B:114:MET:SD	2.58	0.43
1:B:41:ASP:OD1	1:B:151:LYS:NZ	2.39	0.42
1:B:138:SER:HB2	1:B:139:PRO:HD3	2.02	0.42
1:D:147:ASN:ND2	1:D:151:LYS:H	2.18	0.42
1:C:138:SER:HB3	1:C:139:PRO:CD	2.50	0.41
1:D:138:SER:HB3	1:D:139:PRO:HD3	2.02	0.41
1:C:78:LYS:HG2	1:C:113:PHE:CZ	2.56	0.41
1:A:138:SER:HB3	1:A:139:PRO:CD	2.51	0.41
1:D:87:GLN:OE1	1:D:166:HIS:HD2	2.03	0.40
1:D:132:LEU:CD1	1:D:137:VAL:HB	2.51	0.40
1:C:111:HIS:NE2	1:C:115[B]:LYS:HD2	2.37	0.40
1:A:38:GLU:HB2	1:A:40[B]:SER:H	1.86	0.40
1:A:74[B]:CYS:SG	4:A:983:HOH:O	2.22	0.40
1:D:79[B]:LYS:HD2	1:D:83:TYR:OH	2.22	0.40
1:D:108[B]:ILE:HD12	1:D:109:ALA:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	143/143 (100%)	142 (99%)	0	1 (1%)	22	11
1	B	142/143 (99%)	141 (99%)	0	1 (1%)	22	11
1	C	140/143 (98%)	139 (99%)	0	1 (1%)	22	11
1	D	140/143 (98%)	138 (99%)	1 (1%)	1 (1%)	22	11
All	All	565/572 (99%)	560 (99%)	1 (0%)	4 (1%)	22	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	C	138	SER
1	B	138	SER
1	D	138	SER

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	129/126 (102%)	127 (98%)	2 (2%)	62	58
1	B	128/126 (102%)	128 (100%)	0	100	100
1	C	126/126 (100%)	122 (97%)	4 (3%)	39	27
1	D	125/126 (99%)	121 (97%)	4 (3%)	39	27
All	All	508/504 (101%)	498 (98%)	10 (2%)	62	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	132	LEU
1	C	115[A]	LYS
1	C	115[B]	LYS
1	C	154	LYS
1	C	171	LEU
1	D	79[A]	LYS
1	D	79[B]	LYS
1	D	147	ASN
1	D	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	ASN
1	C	80	GLN
1	C	112	ASN
1	D	90	HIS
1	D	147	ASN
1	D	166	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A	701	-	3,3,3	0.56	0	2,2,2	0.22	0
3	EDO	B	704	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	B	705	-	3,3,3	0.54	0	2,2,2	0.41	0
3	EDO	A	703	-	3,3,3	0.33	0	2,2,2	0.62	0
2	ACT	A	801	-	1,3,3	1.13	0	0,3,3	-	-
3	EDO	A	707	-	3,3,3	0.37	0	2,2,2	0.53	0
3	EDO	C	702	-	3,3,3	0.53	0	2,2,2	0.24	0
3	EDO	D	706	-	3,3,3	0.58	0	2,2,2	0.47	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	A	701	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	D	706	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	EDO	4	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	138/143 (96%)	-0.66	0	100 100	2, 5, 12, 30	0
1	B	138/143 (96%)	-0.17	3 (2%)	62 70	5, 13, 25, 32	0
1	C	137/143 (95%)	-0.45	2 (1%)	73 81	3, 8, 16, 28	0
1	D	137/143 (95%)	-0.24	1 (0%)	87 92	4, 13, 22, 27	0
All	All	550/572 (96%)	-0.38	6 (1%)	80 85	2, 9, 22, 32	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	GLY	3.9
1	C	39	GLY	3.4
1	B	138	SER	3.1
1	B	159	THR	2.8
1	D	175	GLY	2.4
1	B	54[A]	ARG	2.2

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(Å ²)	Q<0.9
3	EDO	A	703	4/4	0.91	0.23	26,27,29,29	0
3	EDO	B	704	4/4	0.92	0.11	18,19,19,21	0
2	ACT	A	801	4/4	0.95	0.09	29,30,30,30	0
3	EDO	B	705	4/4	0.95	0.11	13,14,15,15	0
3	EDO	D	706	4/4	0.95	0.19	15,16,18,19	0
3	EDO	C	702	4/4	0.98	0.05	12,13,14,14	0
3	EDO	A	701	4/4	0.99	0.07	5,6,8,10	0
3	EDO	A	707	4/4	0.99	0.09	4,7,7,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.