



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 04:46 PM EDT

PDB ID : 3H44  
Title : Crystal Structure of Insulin Degrading Enzyme in Complex with macrophage inflammatory protein 1 alpha  
Authors : Ren, M.; Guo, Q.; Tang, W.J.  
Deposited on : 2009-04-17  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

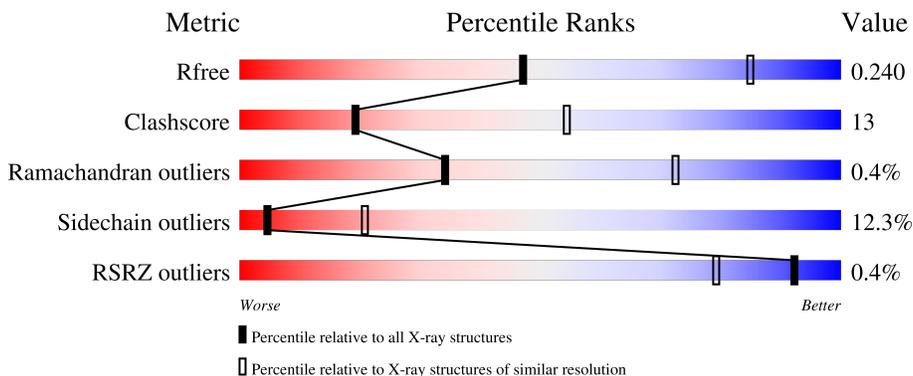
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	990	
1	B	990	
2	C	70	
2	D	70	

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	DIO	A	2001	-	-	-	X
3	DIO	B	2001	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15937 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	956	7821	5036	1314	1449	22	0	0	0
1	B	955	7815	5033	1313	1447	22	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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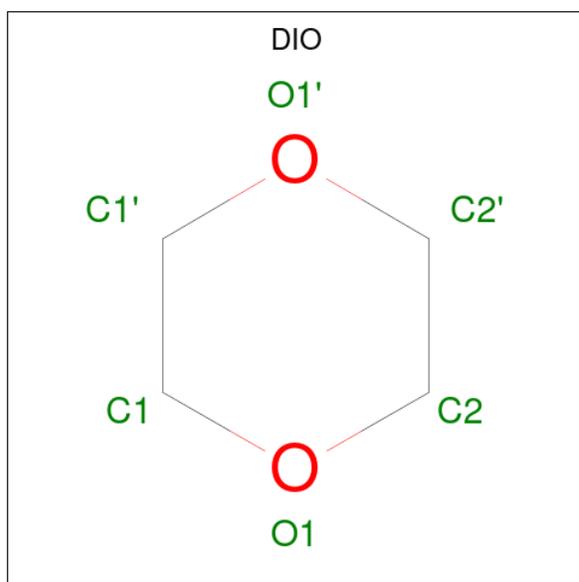
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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called C-C motif chemokine 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			75	44	18	13			
2	D	8	Total	C	N	O	0	0	0
			55	32	12	11			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	B	61	Total O 61 61	0	0
5	C	1	Total O 1 1	0	0
5	D	5	Total O 5 5	0	0





LYS  
TYR  
VAL  
SER  
ASP  
LEU  
GLU  
LEU  
SER  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.74Å 262.74Å 90.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-3.00) 99.7 (49.65-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0044	Depositor
R, $R_{free}$	0.183 , 0.237 0.192 , 0.240	Depositor DCC
$R_{free}$ test set	3612 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, 0.333 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: ZN, DIO

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	0.68	0/8016	0.79	8/10843 (0.1%)
1	B	0.66	2/8010 (0.0%)	0.78	7/10835 (0.1%)
2	C	1.06	0/73	1.10	0/93
2	D	0.88	0/53	1.90	1/68 (1.5%)
All	All	0.67	2/16152 (0.0%)	0.79	16/21839 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CG-CD	5.87	1.66	1.51
1	B	189	GLU	CG-CD	5.63	1.60	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	GLN	CB-CA-C	12.67	135.74	110.40
1	B	52	ASN	CB-CA-C	-7.28	95.84	110.40
1	B	53	HIS	N-CA-C	-7.28	91.35	111.00
1	B	52	ASN	N-CA-C	7.05	130.03	111.00
1	A	328	SER	CB-CA-C	-6.54	97.68	110.10

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	7821	0	7760	197	0
1	B	7815	0	7755	209	0
2	C	75	0	81	6	0
2	D	55	0	55	6	0
3	A	18	0	24	7	0
3	B	18	0	24	6	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	66	0	0	4	0
5	B	61	0	0	3	0
5	C	1	0	0	0	0
5	D	5	0	0	0	0
All	All	15937	0	15699	406	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 13.

The worst 5 of 406 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:B:855:PRO:HB2	1:B:857:HIS:CD2	1.69	1.25
1:A:329:ASN:O	1:A:329:ASN:ND2	1.82	1.10
1:B:427:LYS:NZ	3:B:2001:DIO:H22	1.78	0.98
1:B:855:PRO:CG	1:B:857:HIS:NE2	2.28	0.97
1:B:427:LYS:HZ1	3:B:2001:DIO:H22	1.28	0.95

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	952/990 (96%)	877 (92%)	69 (7%)	6 (1%)	25	64
1	B	951/990 (96%)	885 (93%)	64 (7%)	2 (0%)	47	82
2	C	6/70 (9%)	4 (67%)	2 (33%)	0	100	100
2	D	4/70 (6%)	2 (50%)	2 (50%)	0	100	100
All	All	1913/2120 (90%)	1768 (92%)	137 (7%)	8 (0%)	34	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	GLY
1	A	488	LYS
1	A	674	ARG
1	A	757	PRO
1	A	869	THR

### 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	852/879 (97%)	752 (88%)	100 (12%)	5	22
1	B	851/879 (97%)	743 (87%)	108 (13%)	4	19
2	C	7/62 (11%)	5 (71%)	2 (29%)	0	2
2	D	5/62 (8%)	4 (80%)	1 (20%)	1	7
All	All	1715/1882 (91%)	1504 (88%)	211 (12%)	4	21

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	SER
1	B	472	ARG
1	B	950	ARG
1	B	226	LEU
1	B	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	828	GLN
1	B	957	HIS
1	B	125	ASN
1	B	922	ASN
1	B	783	ASN

### 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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	DIO	A	2001	-	6,6,6	0.60	0	6,6,6	1.01	1 (16%)
3	DIO	A	2000	-	6,6,6	0.57	0	6,6,6	1.04	0
3	DIO	B	2000	-	6,6,6	0.52	0	6,6,6	0.99	0
3	DIO	A	2002	-	6,6,6	0.57	0	6,6,6	0.73	0
3	DIO	B	2001	-	6,6,6	0.54	0	6,6,6	0.78	0
3	DIO	B	2002	-	6,6,6	0.52	0	6,6,6	0.96	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	DIO	A	2001	-	-	-	0/1/1/1
3	DIO	A	2000	-	-	-	0/1/1/1
3	DIO	B	2000	-	-	-	0/1/1/1
3	DIO	A	2002	-	-	-	0/1/1/1
3	DIO	B	2001	-	-	-	0/1/1/1
3	DIO	B	2002	-	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	DIO	C2-O1-C1	2.04	116.71	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	DIO	3	0
3	A	2000	DIO	3	0
3	A	2002	DIO	1	0
3	B	2001	DIO	6	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, 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	956/990 (96%)	-0.51	1 (0%) 95 89	25, 45, 62, 80	0
1	B	955/990 (96%)	-0.42	4 (0%) 92 79	20, 54, 69, 85	0
2	C	10/70 (14%)	0.42	1 (10%) 7 2	40, 82, 86, 89	0
2	D	8/70 (11%)	0.54	1 (12%) 3 1	52, 59, 90, 92	0
All	All	1929/2120 (90%)	-0.45	7 (0%) 92 79	20, 49, 67, 92	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	857	HIS	3.2
2	D	21	VAL	2.6
1	A	965	SER	2.2
1	B	964	ASP	2.2
2	C	21	VAL	2.1

### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DIO	A	2001	6/6	0.44	1.07	155,155,155,155	0
3	DIO	B	2001	6/6	0.50	1.22	158,158,158,159	0
3	DIO	A	2000	6/6	0.81	0.35	98,99,99,99	0
4	ZN	C	42	1/1	0.88	0.19	2,2,2,2	0
3	DIO	A	2002	6/6	0.93	0.24	52,54,56,58	0
3	DIO	B	2000	6/6	0.93	0.32	93,93,94,94	0
4	ZN	B	1	1/1	0.95	0.24	2,2,2,2	0
3	DIO	B	2002	6/6	0.97	0.25	55,56,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.