



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:51 pm BST

PDB ID : 5FAW
Title : T502A mutant of choline TMA-lyase
Authors : Funk, M.A.; Drennan, C.L.
Deposited on : 2015-12-12
Resolution : 1.85 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 : 2.11
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) : 2.11

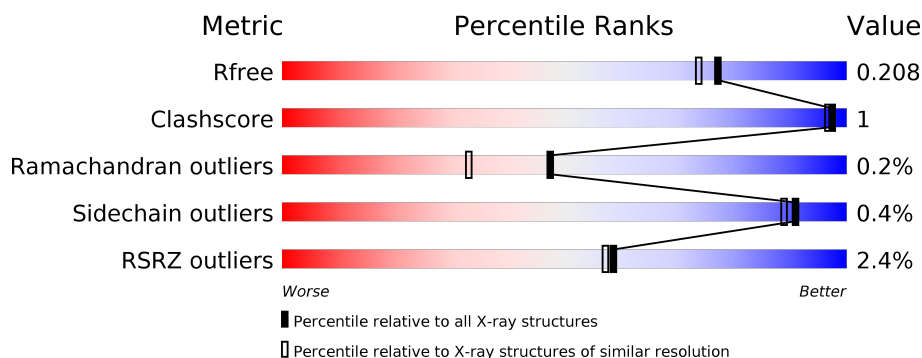
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	815	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 96%, yellow 96%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 96% .. </div> </div>
1	B	815	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 97%, yellow 97%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 4% 97% .. </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27642 atoms, of which 12501 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	803	Total	C	H	N	O	S	0	16	0
			12590	4026	6235	1082	1201	46			
1	B	806	Total	C	H	N	O	S	0	9	0
			12580	4025	6226	1082	1201	46			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP Q30W70
A	33	GLY	-	expression tag	UNP Q30W70
A	34	SER	-	expression tag	UNP Q30W70
A	35	SER	-	expression tag	UNP Q30W70
A	36	HIS	-	expression tag	UNP Q30W70
A	37	HIS	-	expression tag	UNP Q30W70
A	38	HIS	-	expression tag	UNP Q30W70
A	39	HIS	-	expression tag	UNP Q30W70
A	40	HIS	-	expression tag	UNP Q30W70
A	41	HIS	-	expression tag	UNP Q30W70
A	42	SER	-	expression tag	UNP Q30W70
A	43	SER	-	expression tag	UNP Q30W70
A	44	GLY	-	expression tag	UNP Q30W70
A	45	LEU	-	expression tag	UNP Q30W70
A	46	VAL	-	expression tag	UNP Q30W70
A	47	PRO	-	expression tag	UNP Q30W70
A	48	ARG	-	expression tag	UNP Q30W70
A	49	GLY	-	expression tag	UNP Q30W70
A	50	SER	-	expression tag	UNP Q30W70
A	51	HIS	-	expression tag	UNP Q30W70
A	52	MET	-	expression tag	UNP Q30W70
A	502	ALA	THR	engineered mutation	UNP Q30W70
B	32	MET	-	initiating methionine	UNP Q30W70
B	33	GLY	-	expression tag	UNP Q30W70
B	34	SER	-	expression tag	UNP Q30W70

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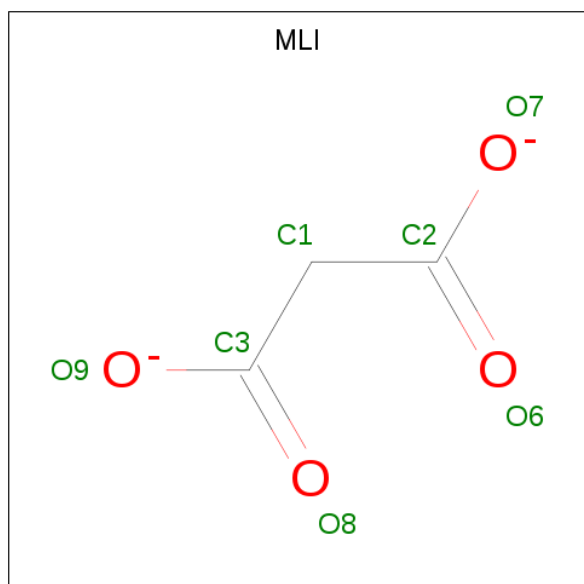
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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	SER	-	expression tag	UNP Q30W70
B	36	HIS	-	expression tag	UNP Q30W70
B	37	HIS	-	expression tag	UNP Q30W70
B	38	HIS	-	expression tag	UNP Q30W70
B	39	HIS	-	expression tag	UNP Q30W70
B	40	HIS	-	expression tag	UNP Q30W70
B	41	HIS	-	expression tag	UNP Q30W70
B	42	SER	-	expression tag	UNP Q30W70
B	43	SER	-	expression tag	UNP Q30W70
B	44	GLY	-	expression tag	UNP Q30W70
B	45	LEU	-	expression tag	UNP Q30W70
B	46	VAL	-	expression tag	UNP Q30W70
B	47	PRO	-	expression tag	UNP Q30W70
B	48	ARG	-	expression tag	UNP Q30W70
B	49	GLY	-	expression tag	UNP Q30W70
B	50	SER	-	expression tag	UNP Q30W70
B	51	HIS	-	expression tag	UNP Q30W70
B	52	MET	-	expression tag	UNP Q30W70
B	502	ALA	THR	engineered mutation	UNP Q30W70

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

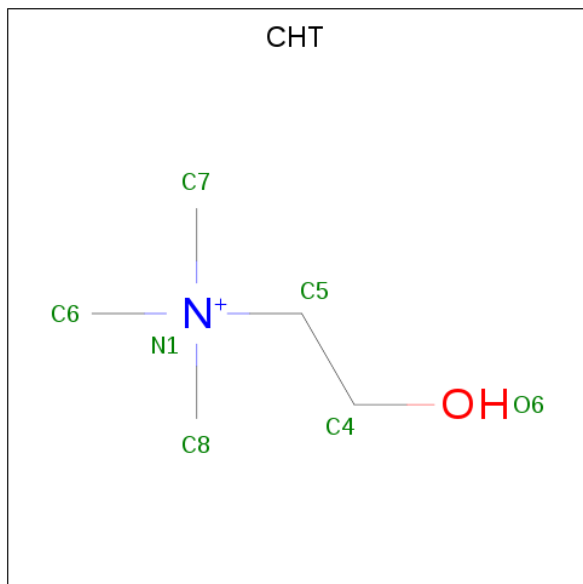
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	B	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: C₅H₁₄NO).

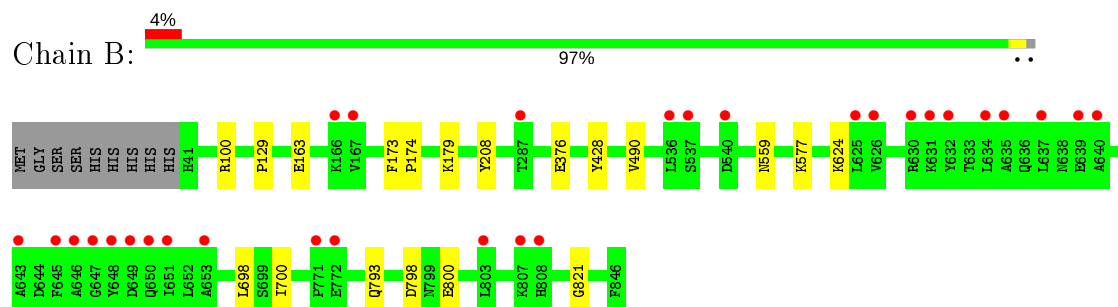


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			21	5	14	1	1		
4	B	1	Total	C	H	N	O	0	0
			21	5	14	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1245	Total	O	0	0
			1245	1245		
5	B	1129	Total	O	0	0
			1129	1129		

- Molecule 1: Choline trimethylamine-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	229.57 Å 229.57 Å 78.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 1.85 49.48 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.48-1.85) 98.1 (49.48-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.86 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.174 , 0.208 0.176 , 0.208	Depositor DCC
R_{free} test set	5327 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27642	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: NA, MLI, CHT

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	0.43	0/6538	0.53	0/8851
1	B	0.42	0/6515	0.53	1/8821 (0.0%)
All	All	0.43	0/13053	0.53	1/17672 (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	100	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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	6355	6235	6129	11	0
1	B	6354	6226	6169	8	1
2	A	2	0	0	0	0
3	A	35	10	10	0	0
3	B	7	2	2	0	0
4	A	7	14	14	1	0
4	B	7	14	14	0	0
5	A	1245	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1129	0	0	5	2
All	All	15141	12501	12338	20	4

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 1.

The worst 5 of 20 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:559:ASN:ND2	5:B:1003:HOH:O	2.17	0.77
1:A:266[B]:GLU:OE2	5:A:1001:HOH:O	2.05	0.75
1:A:178:ASN:OD1	5:A:1002:HOH:O	2.11	0.69
1:B:793:GLN:HE22	1:B:821:GLY:H	1.40	0.68
1:B:208:TYR:OH	5:B:1002:HOH:O	2.13	0.65

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:NZ	1:B:179:LYS:NZ[7_555]	1.81	0.39
5:A:1547:HOH:O	5:A:1584:HOH:O[1_556]	2.14	0.06
5:B:1244:HOH:O	5:B:1730:HOH:O[7_556]	2.19	0.01
5:B:1622:HOH:O	5:B:1788:HOH:O[7_556]	2.19	0.01

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	809/815 (99%)	790 (98%)	17 (2%)	2 (0%)	47 33
1	B	807/815 (99%)	784 (97%)	21 (3%)	2 (0%)	47 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1616/1630 (99%)	1574 (97%)	38 (2%)	4 (0%)	47 33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	700	ILE
1	B	700	ILE
1	B	490	VAL
1	A	490	VAL

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	682/686 (99%)	679 (100%)	3 (0%)	91 89
1	B	680/686 (99%)	677 (100%)	3 (0%)	91 89
All	All	1362/1372 (99%)	1356 (100%)	6 (0%)	91 89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	LEU
1	B	698	LEU
1	B	428	TYR
1	A	577	LYS
1	B	577	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
4	CHT	B	902	-	6,6,6	1.47	1 (16%)	8,8,8	0.71	0
3	MLI	A	905	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	904	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	B	901	-	0,6,6	0.00	-	0,7,7	0.00	-
4	CHT	A	908	-	6,6,6	1.37	0	8,8,8	0.44	0
3	MLI	A	902	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	906	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	903	-	0,6,6	0.00	-	0,7,7	0.00	-

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
4	CHT	B	902	-	-	0/4/4/4	-
3	MLI	A	905	-	-	0/0/4/4	-
3	MLI	A	904	-	-	0/0/4/4	-
3	MLI	B	901	-	-	0/0/4/4	-
4	CHT	A	908	-	-	0/4/4/4	-
3	MLI	A	902	-	-	0/0/4/4	-
3	MLI	A	906	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	A	903	-	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	CHT	C6-N1	-2.00	1.44	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	CHT	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	803/815 (98%)	-0.12	8 (0%) 82 82	11, 19, 32, 43	0
1	B	806/815 (98%)	0.06	30 (3%) 41 39	11, 20, 35, 48	0
All	All	1609/1630 (98%)	-0.03	38 (2%) 59 57	11, 20, 33, 48	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	630	ARG	4.2
1	B	632	TYR	3.4
1	A	285	ARG	3.1
1	A	808	HIS	3.0
1	B	648	TYR	3.0

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. 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	MLI	B	901	7/7	0.73	0.29	60,72,87,87	0
3	MLI	A	906	7/7	0.79	0.20	46,52,64,64	0
3	MLI	A	904	7/7	0.83	0.18	44,58,70,72	0
3	MLI	A	903	7/7	0.90	0.14	28,45,54,55	0
3	MLI	A	905	7/7	0.91	0.12	31,40,48,48	0
2	NA	A	907	1/1	0.91	0.21	57,57,57,57	0
4	CHT	A	908	7/7	0.93	0.24	23,27,32,32	0
4	CHT	B	902	7/7	0.94	0.27	20,34,44,44	0
3	MLI	A	902	7/7	0.94	0.14	27,44,53,54	0
2	NA	A	901	1/1	0.99	0.08	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.