



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 10:39 pm BST

PDB ID : 3UR2
Title : Crystal Structure of PTE mutant H254G/H257W/L303T/K185R/I274N/A80V
Authors : Tsai, P.; Fox, N.G.; Li, Y.; Barondeau, D.P.; Raushel, F.M.
Deposited on : 2011-11-21
Resolution : 2.00 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

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

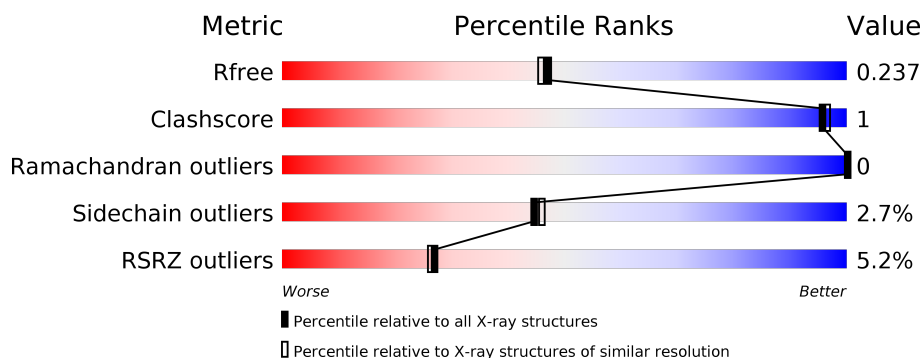
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

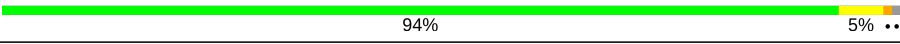
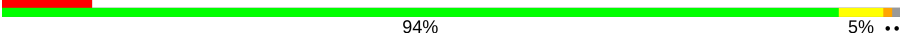
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	329	
1	B	329	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5408 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2502	1581	444	470	7			
1	B	325	Total	C	N	O	S	0	0	0
			2493	1576	445	465	7			

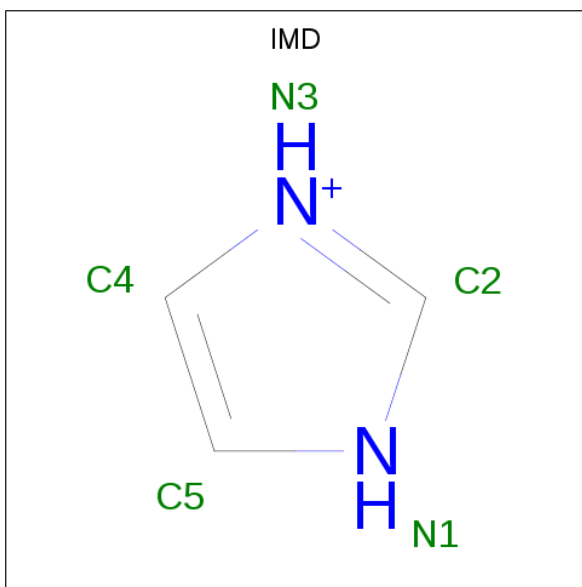
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	VAL	ALA	engineered mutation	UNP P0A434
A	185	ARG	LYS	engineered mutation	UNP P0A434
A	254	GLY	HIS	engineered mutation	UNP P0A434
A	257	TRP	HIS	engineered mutation	UNP P0A434
A	274	ASN	ILE	engineered mutation	UNP P0A434
A	303	THR	LEU	engineered mutation	UNP P0A434
B	80	VAL	ALA	engineered mutation	UNP P0A434
B	185	ARG	LYS	engineered mutation	UNP P0A434
B	254	GLY	HIS	engineered mutation	UNP P0A434
B	257	TRP	HIS	engineered mutation	UNP P0A434
B	274	ASN	ILE	engineered mutation	UNP P0A434
B	303	THR	LEU	engineered mutation	UNP P0A434

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

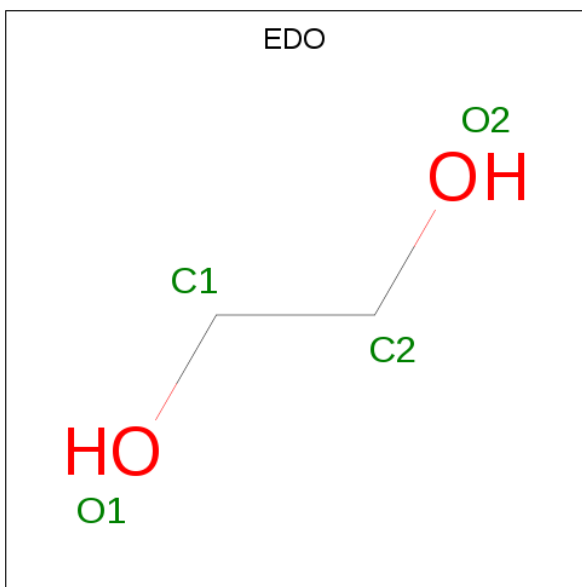
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Co	0	0
			2	2		
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	268	Total	O	0	0
			268	268		
5	B	110	Total	O	0	0
			110	110		

3 Residue-property plots [i](#)

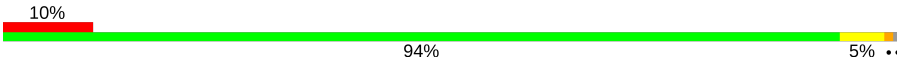
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

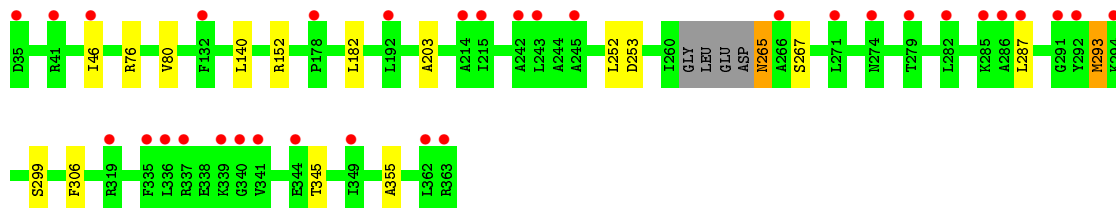
- Molecule 1: Parathion hydrolase

Chain A:  94% 5% ..



- Molecule 1: Parathion hydrolase

Chain B:  10% 94% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.06Å 85.24Å 87.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 38.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.00) 99.7 (38.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.246 0.205 , 0.237	Depositor DCC
R_{free} test set	2196 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k 0.019 for -l,-k,-h 0.017 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5408	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: EDO, CO, KCX, IMD

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	0.62	0/2537	0.77	4/3447 (0.1%)
1	B	0.61	0/2527	0.76	3/3430 (0.1%)
All	All	0.62	0/5064	0.76	7/6877 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	N-CA-C	-6.48	93.50	111.00
1	A	182	LEU	CA-CB-CG	5.89	128.86	115.30
1	B	203	ALA	N-CA-C	-5.61	95.85	111.00
1	A	184	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	253	ASP	N-CA-C	5.25	125.18	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2502	0	2510	6	0
1	B	2493	0	2509	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	10	1	0
3	B	5	0	5	0	0
4	A	16	0	24	1	0
5	A	268	0	0	0	0
5	B	110	0	0	0	0
All	All	5408	0	5058	11	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 1.

The worst 5 of 11 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:163:ILE:HD11	4:A:906:EDO:H12	1.59	0.84
1:A:36:ARG:HH21	1:A:45:THR:HG23	1.60	0.66
1:B:265:ASN:HD22	1:B:265:ASN:N	2.05	0.54
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.93	0.50
1:A:233:ASP:OD1	3:A:900:IMD:H5	2.14	0.47

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	324/329 (98%)	312 (96%)	12 (4%)	0	100	100
1	B	320/329 (97%)	306 (96%)	14 (4%)	0	100	100
All	All	644/658 (98%)	618 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	262/264 (99%)	255 (97%)	7 (3%)	44	46
1	B	261/264 (99%)	254 (97%)	7 (3%)	44	46
All	All	523/528 (99%)	509 (97%)	14 (3%)	44	46

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	GLU
1	B	140	LEU
1	B	293	MET
1	A	306	PHE
1	B	267	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	38	ASN
1	B	212	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	169	1,2	7,11,12	0.54	0	4,12,14	0.55	0
1	KCX	B	169	1,2	7,11,12	0.50	0	4,12,14	0.67	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
1	KCX	A	169	1,2	-	0/7/10/12	-
1	KCX	B	169	1,2	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	IMD	A	902	-	3,5,5	0.24	0	4,5,5	0.84	0
4	EDO	A	905	-	3,3,3	0.50	0	2,2,2	0.26	0
4	EDO	A	904	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	A	903	-	3,3,3	0.48	0	2,2,2	0.27	0
3	IMD	B	901	-	3,5,5	0.21	0	4,5,5	0.81	0
3	IMD	A	900	-	3,5,5	0.22	0	4,5,5	0.80	0
4	EDO	A	906	-	3,3,3	0.48	0	2,2,2	0.32	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	IMD	A	902	-	-	-	0/1/1/1
4	EDO	A	905	-	-	0/1/1/1	-
4	EDO	A	904	-	-	0/1/1/1	-
4	EDO	A	903	-	-	0/1/1/1	-
3	IMD	B	901	-	-	-	0/1/1/1
3	IMD	A	900	-	-	-	0/1/1/1
4	EDO	A	906	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	IMD	1	0
4	A	906	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	326/329 (99%)	-0.04	1 (0%) 94 93	19, 27, 41, 57	0
1	B	324/329 (98%)	0.75	33 (10%) 6 6	26, 47, 68, 80	0
All	All	650/658 (98%)	0.35	34 (5%) 27 26	19, 35, 64, 80	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	GLY	5.1
1	B	362	LEU	4.6
1	B	282	LEU	4.1
1	B	363	ARG	4.0
1	B	243	LEU	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	B	169	12/13	0.91	0.15	36,38,40,41	0
1	KCX	A	169	12/13	0.95	0.12	18,21,24,24	0

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(Å ²)	Q<0.9
4	EDO	A	905	4/4	0.79	0.21	40,40,41,42	0
4	EDO	A	903	4/4	0.80	0.23	45,47,48,50	0
4	EDO	A	904	4/4	0.80	0.22	58,58,58,58	0
3	IMD	B	901	5/5	0.83	0.17	55,56,56,56	0
4	EDO	A	906	4/4	0.84	0.22	56,57,57,57	0
3	IMD	A	902	5/5	0.86	0.34	49,50,51,51	0
3	IMD	A	900	5/5	0.96	0.10	26,26,26,27	0
2	CO	B	804	1/1	0.98	0.08	49,49,49,49	0
2	CO	B	803	1/1	0.99	0.09	39,39,39,39	0
2	CO	A	802	1/1	1.00	0.09	23,23,23,23	0
2	CO	A	801	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.