

# wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 05:40 am BST

PDB ID : 1R8H

Title: Comparison of the structure and DNA binding properties of the E2 proteins

from an oncogenic and a non-oncogenic human papillomavirus

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Deposited on : 2003-10-24

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 (i) symbol.

The following versions of software and data (see references (1)) 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)

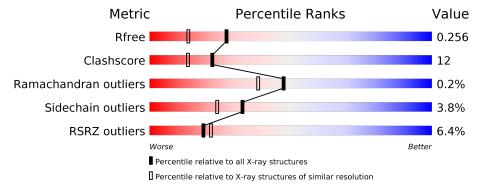
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance (i)

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	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 <=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	87	79%	16%	5%
1	В	87	86%	11%	<del>.</del>
1	С	87	61% 32%		5%
1	D	87	85%	14%	
1	Е	87	78%	18%	<del>-</del>
1	F	87	55% 36%	5%	6 5%



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
2	PO4	Ε	505	_	_	X	-



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5125 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 Regulatory protein E2.

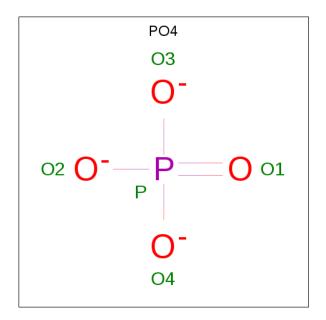
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	87	Total	С	N	О	S	30	4	0
1	A	01	748	480	139	125	4	30	4	0
1	В	87	Total	С	N	О	S	20	4	0
1	Ъ	01	748	480	139	125	4	20	4	
1	$^{\rm C}$	83	Total	С	N	О	S	14	21	0
1		0.0	866	551	164	145	6		21	
1	D	87	Total	С	N	О	S	26	0	0
1	ש	01	722	463	134	121	4	20	0	
1	Е	87	Total	С	N	О	S	23	0	0
1	12	01	722	463	134	121	4	20	0	
1	F	83	Total	С	N	О	S	14	21	0
1	1'	00	866	551	164	145	6	14	<u> </u>	$\begin{vmatrix} 0 \end{vmatrix}$

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	MET	LEU	SEE REMARK 999	UNP Q84294
В	363	MET	LEU	SEE REMARK 999	UNP Q84294
С	363	MET	LEU	SEE REMARK 999	UNP Q84294
D	363	MET	LEU	SEE REMARK 999	UNP Q84294
Е	363	MET	LEU	SEE REMARK 999	UNP Q84294
F	363	MET	LEU	SEE REMARK 999	UNP Q84294

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	В	1	Total O P 5 4 1	0	0
2	В	1	Total O P 5 4 1	0	0
2	С	1	Total O P 5 4 1	0	0
2	С	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	Е	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	Е	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0



### • Molecule 3 is water.

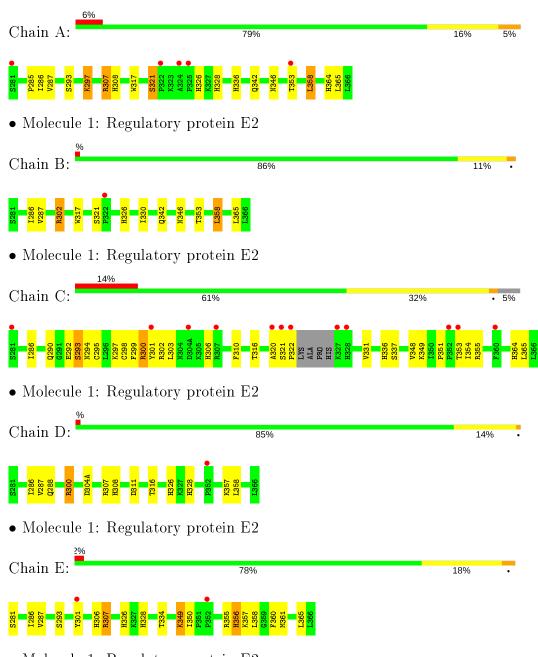
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	В	69	Total O 69 69	0	0
3	С	48	Total O 48 48	0	0
3	D	68	Total O 68 68	0	0
3	Е	75	Total O 75 75	0	0
3	F	49	Total O 49 49	0	0



# 3 Residue-property plots (i)

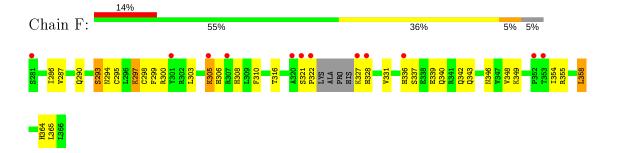
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Regulatory protein E2



• Molecule 1: Regulatory protein E2







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	$71.66 ext{Å}$ $71.66 ext{Å}$ $195.00 ext{Å}$	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 1.90	Depositor
Resolution (A)	19.71 - 1.90	EDS
% Data completeness	93.4 (20.00-1.90)	Depositor
(in resolution range)	93.4 (19.71-1.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.08 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
υ .	0.191 , 0.258	Depositor
$R, R_{free}$	0.201 , $0.256$	DCC
$R_{free}$ test set	2143 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , 45.8	EDS
L-test for twinning <sup>2</sup>	$< L >=0.53, < L^2>=0.37$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



 $<sup>^{1}</sup>$ Intensities estimated from amplitudes.

# 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: PO4

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	Bo	nd lengths	Bond angles		
MIGI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.93	$1/779 \ (0.1\%)$	1.45	4/1055~(0.4%)	
1	В	1.03	$2/779 \ (0.3\%)$	0.91	2/1055~(0.2%)	
1	С	0.93	2/901 (0.2%)	0.86	1/1211 (0.1%)	
1	D	1.11	$2/745 \ (0.3\%)$	1.08	6/1007~(0.6%)	
1	E	1.03	$2/745 \ (0.3\%)$	0.95	1/1007 (0.1%)	
1	F	0.95	3/901 (0.3%)	0.89	2/1211 (0.2%)	
All	All	1.00	$12/4850 \ (0.2\%)$	1.04	$16/6546 \ (0.2\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
1	D	0	1
1	E	0	1
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	D	300	ARG	CD-NE	-19.52	1.13	1.46
1	В	302	ARG	CD-NE	-15.84	1.19	1.46
1	Е	307	ARG	CD-NE	-14.71	1.21	1.46
1	A	307	ARG	NE-CZ	-12.12	1.17	1.33
1	F	349	LYS	CG-CD	-11.24	1.14	1.52

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



Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mid \mathbf{Ideal}(^o) \mid$
1	Α	307	ARG	NE-CZ-NH1	-23.87	108.36	120.30
1	A	307	ARG	NE-CZ-NH2	22.21	131.41	120.30
1	A	307	ARG	CD-NE-CZ	19.25	150.55	123.60
1	D	300	ARG	CD-NE-CZ	-13.39	104.85	123.60
1	E	307	ARG	CG-CD-NE	13.09	139.29	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	ARG	Sidechain
1	В	302	ARG	Sidechain
1	D	300	ARG	Sidechain
1	E	307	ARG	Sidechain

#### 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	748	0	738	13	0
1	В	748	0	738	7	0
1	С	866	0	844	44	0
1	D	722	0	713	8	0
1	E	722	0	715	13	0
1	F	866	0	845	42	0
2	A	10	0	0	0	0
2	В	10	0	0	0	0
2	С	10	0	0	1	0
2	D	15	0	0	1	0
2	E	15	0	0	2	0
2	F	10	0	0	0	0
3	A	74	0	0	3	0
3	В	69	0	0	1	0
3	С	48	0	0	6	0
3	D	68	0	0	1	0
3	Е	75	0	0	3	0
3	F	49	0	0	4	0
All	All	5125	0	4593	105	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 12.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:C:301[B]:TYR:HE1	1:F:294[B]:ASN:ND2	1.07	1.42
1:C:301[B]:TYR:CE1	1:F:294[B]:ASN:ND2	1.89	1.37
1:C:321:SER:OG	1:C:322:PRO:HD2	1.15	1.33
1:F:321:SER:OG	1:F:322:PRO:HD2	1.16	1.31
1:C:321:SER:OG	1:C:322:PRO:CD	1.94	1.15

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	89/87 (102%)	87 (98%)	1 (1%)	1 (1%)	14 5
1	В	89/87 (102%)	87 (98%)	2 (2%)	0	100 100
1	С	100/87 (115%)	94 (94%)	6 (6%)	0	100 100
1	D	85/87 (98%)	83 (98%)	2 (2%)	0	100 100
1	E	85/87 (98%)	83 (98%)	2 (2%)	0	100 100
1	F	100/87 (115%)	92 (92%)	8 (8%)	0	100 100
All	All	$548/522 \ (105\%)$	526 (96%)	21 (4%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

$\mathbf{Mol}$	Chain	${ m Res}$	Type
1	A	321	SER



#### 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	Perce	$\operatorname{ntiles}$
1	A	85/81 (105%)	80 (94%)	5 (6%)	19	10
1	В	85/81 (105%)	82 (96%)	3 (4%)	36	27
1	С	98/81 (121%)	93 (95%)	5 (5%)	24	14
1	D	81/81 (100%)	81 (100%)	0	100	100
1	Е	81/81 (100%)	76 (94%)	5 (6%)	18	9
1	F	98/81 (121%)	91 (93%)	7 (7%)	14	6
All	All	528/486 (109%)	503 (95%)	25 (5%)	33	16

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	300[B]	ARG
1	Е	281	SER
1	F	305[B]	LYS
1	С	353	THR
1	Е	293	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	290	GLN
1	D	326	HIS
1	E	326	HIS
1	D	288	GLN
1	E	346	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 carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

14 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).

N / L 1	TD.	C1 '	D	Link	В	ond leng	$\operatorname{gths}$	В	ond ang	gles
Mol	Type	Chain	Res	Res Lillk	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	PO4	С	514	_	4,4,4	0.75	0	6,6,6	0.67	0
2	PO4	В	511	-	4,4,4	0.83	0	6,6,6	1.00	0
2	PO4	A	510	-	4,4,4	0.81	0	6,6,6	1.06	0
2	PO4	E	506	-	4,4,4	0.85	0	6,6,6	0.52	0
2	PO4	D	504	-	4,4,4	0.99	0	6,6,6	0.67	0
2	PO4	D	503	-	4,4,4	0.78	0	6,6,6	0.68	0
2	PO4	A	508	-	4,4,4	0.98	0	6,6,6	0.76	0
2	PO4	F	507	-	4,4,4	0.90	0	6,6,6	0.58	0
2	PO4	E	505	-	4,4,4	0.81	0	6,6,6	1.01	0
2	PO4	Е	502	_	4,4,4	1.01	0	6,6,6	1.30	1 (16%)
2	PO4	F	513	-	4,4,4	0.80	0	6,6,6	0.74	0
2	PO4	В	509	-	4,4,4	0.77	0	6,6,6	0.60	0
2	PO4	С	512	_	4,4,4	1.02	0	6,6,6	1.14	1 (16%)
2	PO4	D	501	_	4,4,4	0.86	0	6,6,6	0.88	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	512	PO4	O4-P-O2	2.37	115.57	107.97
2	Ε	502	PO4	O4-P-O2	2.29	115.33	107.97



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	514	PO4	1	0
2	D	504	PO4	1	0
2	Ε	505	PO4	2	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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	87/87 (100%)	-0.13	5 (5%) 23 26	23, 33, 52, 55	14 (16%)
1	В	87/87 (100%)	-0.18	1 (1%) 80 82	23, 33, 52, 56	14 (16%)
1	С	83/87 (95%)	0.83	12 (14%) 2 2	23, 35, 52, 57	7 (8%)
1	D	87/87 (100%)	-0.30	1 (1%) 80 82	24, 35, 49, 54	7 (8%)
1	E	87/87 (100%)	-0.28	2 (2%) 60 63	24, 35, 48, 54	6 (6%)
1	F	83/87 (95%)	0.87	12 (14%) 2 2	24, 35, 51, 57	7 (8%)
All	All	514/522 (98%)	0.12	33 (6%) 19 22	23, 34, 52, 57	55 (10%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	321	SER	19.4
1	С	281	SER	18.9
1	F	281	SER	18.8
1	F	322	PRO	17.1
1	С	322	PRO	16.5

### 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,  $95^{th}$  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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	PO4	F	513	5/5	0.89	0.25	70,72,73,74	0
2	PO4	С	512	5/5	0.89	0.12	44,56,58,59	0
2	PO4	A	510	5/5	0.90	0.14	48,58,59,60	0
2	PO4	F	507	5/5	0.90	0.12	47,57,58,59	0
2	PO4	D	504	5/5	0.92	0.17	51,58,60,60	0
2	PO4	С	514	5/5	0.92	0.20	68,68,69,70	0
2	PO4	В	509	5/5	0.93	0.14	51,60,60,61	0
2	PO4	В	511	5/5	0.93	0.14	58,61,61,63	0
2	PO4	Ε	505	5/5	0.94	0.20	65,66,68,68	0
2	PO4	D	503	5/5	0.94	0.19	64,64,67,68	0
2	PO4	A	508	5/5	0.95	0.14	66,66,67,68	0
2	PO4	E	506	5/5	0.95	0.11	48,55,55,55	0
2	PO4	D	501	5/5	0.96	0.11	45,46,49,51	0
2	PO4	E	502	5/5	0.98	0.07	43,43,45,45	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

