



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:25 am GMT

PDB ID : 4UMB  
Title : Structural analysis of substrate-mimicking inhibitors in complex with *Neisseria meningitidis* 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase - the importance of accommodating the active site water  
Authors : Heyes, L.C.; Reichau, S.; Cross, P.J.; Parker, E.J.  
Deposited on : 2014-05-16  
Resolution : 2.17 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)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

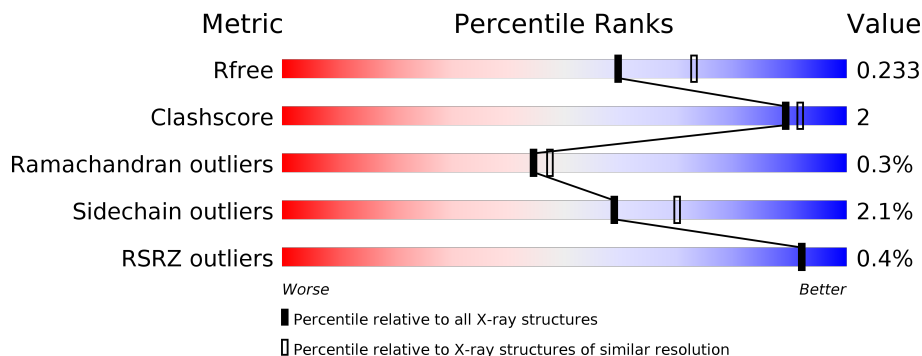
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	351	
1	B	351	
1	C	351	
1	D	351	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1352	-	-	-	X
3	PO4	C	1352	-	-	-	X
3	PO4	D	1352	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10942 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.

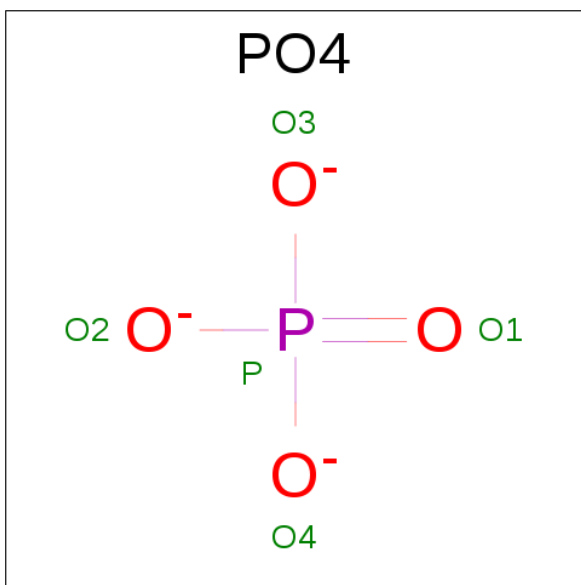
- Molecule 1 is a protein called PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2584	1615	468	486	15			
1	B	333	Total	C	N	O	S	0	1	0
			2558	1597	460	487	14			
1	C	333	Total	C	N	O	S	0	2	0
			2554	1596	460	483	15			
1	D	333	Total	C	N	O	S	0	2	0
			2548	1593	456	484	15			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

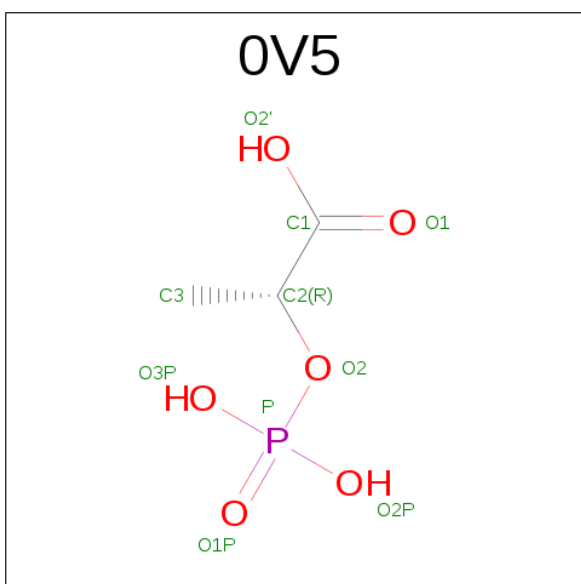
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is (2R)-2-(PHOSPHONOOXY)PROPANOIC ACID (three-letter code: 0V5) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	0
			10	3	6	1		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	1
			198	198		
5	B	139	Total	O	0	0
			139	139		
5	C	164	Total	O	0	0
			164	164		
5	D	133	Total	O	0	0
			133	133		

### 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: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:  91% 5%



- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain B:  91% 5%



- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain C:  91% 5%



- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain D:  91% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.44Å 133.73Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.99 – 2.17 48.32 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.99-2.17) 99.9 (48.32-2.17)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.201 , 0.227 0.208 , 0.233	Depositor DCC
$R_{free}$ test set	4166 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: PO4, MN, OV5

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	0.58	0/2632	0.71	3/3561 (0.1%)
1	B	0.54	0/2606	0.70	2/3529 (0.1%)
1	C	0.54	0/2602	0.69	1/3524 (0.0%)
1	D	0.55	0/2596	0.69	2/3517 (0.1%)
All	All	0.55	0/10436	0.70	8/14131 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	311	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	C	274	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	94	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	294	ASP	CB-CG-OD1	5.53	123.28	118.30

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	2584	0	2555	18	0
1	B	2558	0	2518	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2554	0	2512	16	0
1	D	2548	0	2499	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	10	0	6	0	0
4	B	10	0	6	0	0
4	C	10	0	6	0	0
4	D	10	0	6	0	0
5	A	198	0	0	6	0
5	B	139	0	0	4	0
5	C	164	0	0	5	0
5	D	133	0	0	1	0
All	All	10942	0	10108	44	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 2.

The worst 5 of 44 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:148[A]:ASP:OD1	5:B:2070:HOH:O	1.79	1.00
1:A:219:HIS:CD2	1:B:219:HIS:NE2	2.33	0.97
1:C:219:HIS:NE2	1:D:219:HIS:CD2	2.46	0.83
1:A:219:HIS:NE2	1:B:219:HIS:CD2	2.46	0.83
1:C:302[A]:MET:HG2	5:C:2050:HOH:O	1.77	0.83

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	336/351 (96%)	330 (98%)	5 (2%)	1 (0%)	44	47
1	B	332/351 (95%)	326 (98%)	5 (2%)	1 (0%)	44	47
1	C	333/351 (95%)	328 (98%)	4 (1%)	1 (0%)	44	47
1	D	333/351 (95%)	327 (98%)	5 (2%)	1 (0%)	44	47
All	All	1334/1404 (95%)	1311 (98%)	19 (1%)	4 (0%)	44	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	B	294	ASP
1	C	294	ASP
1	D	294	ASP

### 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	270/289 (93%)	265 (98%)	5 (2%)	62	73
1	B	269/289 (93%)	263 (98%)	6 (2%)	57	68
1	C	267/289 (92%)	260 (97%)	7 (3%)	51	61
1	D	266/289 (92%)	262 (98%)	4 (2%)	70	80
All	All	1072/1156 (93%)	1050 (98%)	22 (2%)	59	70

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250	GLU
1	C	219	HIS
1	D	236	ARG
1	B	306	HIS

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Mol	Chain	Res	Type
1	C	189	ASN

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 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$
3	PO4	A	1352	-	4,4,4	0.54	0	6,6,6	0.97	1 (16%)
4	0V5	A	1353	2	6,9,9	1.74	2 (33%)	7,13,13	2.82	2 (28%)
4	0V5	B	1351	2	6,9,9	1.46	1 (16%)	7,13,13	1.62	3 (42%)
3	PO4	B	1352	-	4,4,4	0.69	0	6,6,6	0.90	0
4	0V5	C	1351	2	6,9,9	2.11	2 (33%)	7,13,13	1.36	1 (14%)
3	PO4	C	1352	-	4,4,4	0.60	0	6,6,6	0.81	0
4	0V5	D	1351	2	6,9,9	1.79	2 (33%)	7,13,13	1.68	2 (28%)
3	PO4	D	1352	-	4,4,4	0.64	0	6,6,6	1.49	2 (33%)

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	PO4	A	1352	-	-	0/0/0/0	0/0/0/0
4	OV5	A	1353	2	-	0/5/9/9	0/0/0/0
4	OV5	B	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	B	1352	-	-	0/0/0/0	0/0/0/0
4	OV5	C	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	C	1352	-	-	0/0/0/0	0/0/0/0
4	OV5	D	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	D	1352	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1353	OV5	P-O2	2.20	1.63	1.59
4	D	1351	OV5	P-O2	2.40	1.63	1.59
4	A	1353	OV5	P-O1P	2.63	1.59	1.50
4	D	1351	OV5	P-O1P	2.68	1.59	1.50
4	C	1351	OV5	P-O2	2.79	1.64	1.59

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1353	OV5	C3-C2-C1	-6.33	105.28	113.35
4	D	1351	OV5	C3-C2-C1	-2.85	109.72	113.35
3	D	1352	PO4	O3-P-O1	-2.55	100.12	110.97
4	D	1351	OV5	O2P-P-O1P	-2.31	101.47	110.50
4	B	1351	OV5	C3-C2-C1	-2.15	110.61	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	335/351 (95%)	-0.33	0 <b>100</b> <b>100</b>	15, 22, 30, 47	0
1	B	333/351 (94%)	-0.19	4 (1%) 79 79	17, 24, 37, 50	0
1	C	333/351 (94%)	-0.22	0 <b>100</b> <b>100</b>	17, 24, 34, 49	0
1	D	333/351 (94%)	-0.16	1 (0%) 93 93	18, 24, 37, 48	0
All	All	1334/1404 (95%)	-0.23	5 (0%) 92 92	15, 24, 36, 50	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	GLU	2.9
1	B	348	ALA	2.2
1	B	293	GLN	2.1
1	D	292	GLU	2.1
1	B	349	ARG	2.0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	1352	5/5	0.94	0.16	6.13	51,52,55,57	0
3	PO4	A	1352	5/5	0.93	0.19	6.13	41,45,50,50	0
3	PO4	D	1352	5/5	0.94	0.18	2.63	43,45,48,48	0
3	PO4	B	1352	5/5	0.93	0.17	1.92	35,36,40,40	0
4	OV5	C	1351	10/10	0.97	0.09	-0.89	20,25,26,27	0
4	OV5	B	1351	10/10	0.98	0.09	-0.91	18,20,21,21	0
2	MN	B	1350	1/1	0.99	0.08	-0.92	20,20,20,20	0
4	OV5	A	1353	10/10	0.98	0.08	-1.06	18,20,21,22	0
4	OV5	D	1351	10/10	0.98	0.11	-1.08	22,24,25,26	0
2	MN	A	1351	1/1	0.99	0.06	-1.61	18,18,18,18	0
2	MN	D	1350	1/1	0.99	0.07	-2.10	20,20,20,20	0
2	MN	C	1350	1/1	0.99	0.05	-2.65	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.