



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2017 – 05:22 AM EDT

PDB ID : 4BXO  
Title : Architecture and DNA recognition elements of the Fanconi anemia FANCM-FAAP24 complex  
Authors : Coulthard, R.; Deans, A.; Swuec, P.; Bowles, M.; Purkiss, A.; Costa, A.; West, S.; McDonald, N.  
Deposited on : 2013-07-15  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
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)	:	rb-20029077

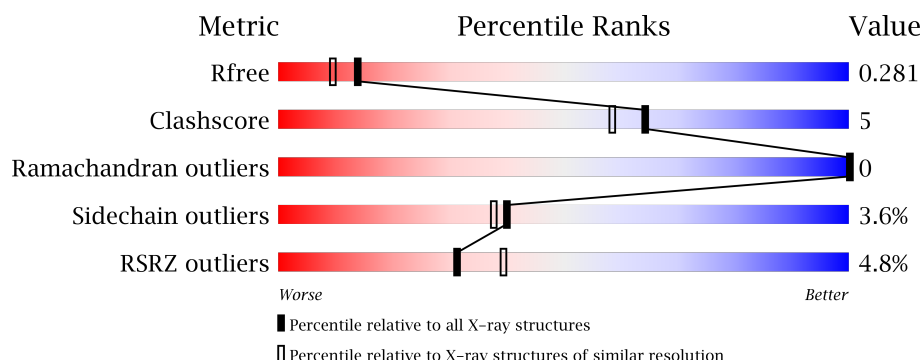
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	254	<div> <div>4%</div> <div>69%</div> <div>10%</div> <div>20%</div> </div>
2	B	217	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
3	H	11	<div> <div>27%</div> <div>45%</div> <div>55%</div> </div>
4	I	11	<div> <div>27%</div> <div>45%</div> <div>27%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3617 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 FANCONI ANEMIA GROUP M PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	1	0
			1574	1000	264	297	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1795	GLY	-	expression tag	UNP Q8IYD8
A	1796	SER	-	expression tag	UNP Q8IYD8
A	1797	GLY	-	expression tag	UNP Q8IYD8

- Molecule 2 is a protein called FANCONI ANEMIA-ASSOCIATED PROTEIN OF 24 KDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1494	960	252	275	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9BTP7
B	-1	SER	-	expression tag	UNP Q9BTP7
B	0	HIS	-	expression tag	UNP Q9BTP7
B	32	GLU	GLN	conflict	UNP Q9BTP7

- Molecule 3 is a DNA chain called 5'-D(\*TP\*CP\*AP\*GP\*CP\*AP\*TP\*CP\*AP\*TP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	11	Total	C	N	O	P	0	0	0
			227	109	44	64	10			

- Molecule 4 is a DNA chain called 5'-D(\*GP\*AP\*TP\*GP\*AP\*TP\*GP\*CP\*TP\*GP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	11	Total	C	N	O	P	0	0	0
			218	106	38	64	10			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	47	Total	O	0	0
			47	47		
6	H	4	Total	O	0	0
			4	4		
6	I	1	Total	O	0	0
			1	1		



● Molecule 1: FANCONI ANEMIA GROUP M PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.10 Å   125.10 Å   74.76 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	25.43 – 2.15 25.43 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.43-2.15) 98.6 (25.43-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.77 (at 2.15 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204   ,   0.255 0.223   ,   0.281	Depositor DCC
$R_{free}$ test set	1645 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CA

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	1.09	3/1598 (0.2%)	0.89	2/2156 (0.1%)
2	B	1.11	1/1519 (0.1%)	0.89	0/2064
3	H	1.84	4/255 (1.6%)	2.66	27/393 (6.9%)
4	I	1.63	1/243 (0.4%)	2.32	19/372 (5.1%)
All	All	1.21	9/3615 (0.2%)	1.28	48/4985 (1.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	DT	C1'-N1	7.24	1.58	1.49
1	A	1939	GLU	CG-CD	6.31	1.61	1.51
1	A	1991	CYS	CB-SG	-6.08	1.72	1.82
3	H	10	DG	C3'-O3'	-6.03	1.36	1.44
3	H	2	DA	N9-C4	5.81	1.41	1.37
3	H	5	DA	C6-N1	5.70	1.39	1.35
1	A	1853	CYS	CB-SG	-5.40	1.73	1.81
2	B	198	VAL	CB-CG2	5.30	1.64	1.52
4	I	9	DA	C3'-O3'	5.02	1.50	1.44

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	11	DA	O4'-C1'-N9	12.70	116.89	108.00
3	H	9	DT	O4'-C1'-N1	-11.94	99.64	108.00
3	H	9	DT	N3-C2-O2	-11.46	115.42	122.30
3	H	3	DT	O4'-C1'-N1	9.15	114.41	108.00
4	I	9	DA	P-O3'-C3'	8.65	130.08	119.70
3	H	7	DG	O4'-C1'-C2'	-8.62	99.00	105.90
3	H	2	DA	O4'-C1'-N9	8.44	113.91	108.00
3	H	7	DG	O4'-C4'-C3'	-8.13	101.12	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	DT	O4'-C1'-N1	8.11	113.68	108.00
3	H	1	DG	P-O3'-C3'	7.91	129.19	119.70
4	I	2	DC	P-O3'-C3'	7.74	128.99	119.70
4	I	1	DT	C1'-O4'-C4'	-7.67	102.43	110.10
3	H	6	DT	O4'-C4'-C3'	-7.43	101.53	104.50
3	H	8	DC	O4'-C1'-N1	7.19	113.03	108.00
3	H	9	DT	N1-C1'-C2'	7.01	125.91	112.60
3	H	3	DT	N3-C2-O2	-6.88	118.17	122.30
1	A	1871	MET	CG-SD-CE	6.87	111.20	100.20
3	H	9	DT	N1-C2-N3	6.68	118.61	114.60
4	I	1	DT	O3'-P-O5'	-6.66	91.35	104.00
3	H	9	DT	C6-N1-C2	-6.63	117.98	121.30
4	I	2	DC	N3-C4-N4	-6.62	113.36	118.00
3	H	8	DC	C4'-C3'-C2'	-6.44	97.31	103.10
4	I	6	DA	C2-N3-C4	-6.41	107.39	110.60
3	H	8	DC	P-O5'-C5'	-6.41	110.64	120.90
3	H	10	DG	N3-C4-C5	6.30	131.75	128.60
4	I	2	DC	N3-C2-O2	-6.24	117.53	121.90
4	I	2	DC	N1-C2-O2	6.20	122.62	118.90
3	H	6	DT	O4'-C1'-N1	-6.09	103.73	108.00
4	I	6	DA	N1-C6-N6	6.07	122.24	118.60
1	A	1866	ARG	NE-CZ-NH1	5.88	123.24	120.30
4	I	6	DA	C5-C6-N1	-5.81	114.80	117.70
4	I	2	DC	C5-C4-N4	5.78	124.25	120.20
4	I	1	DT	N3-C2-O2	-5.70	118.88	122.30
4	I	5	DC	N3-C4-N4	-5.58	114.09	118.00
4	I	3	DA	N1-C2-N3	-5.50	126.55	129.30
3	H	3	DT	C6-N1-C2	-5.50	118.55	121.30
3	H	3	DT	C6-C5-C7	-5.49	119.61	122.90
3	H	5	DA	C2-N3-C4	5.46	113.33	110.60
3	H	2	DA	C2-N3-C4	5.45	113.33	110.60
4	I	2	DC	C1'-O4'-C4'	-5.36	104.74	110.10
3	H	11	DA	C8-N9-C4	-5.29	103.68	105.80
4	I	9	DA	C4'-C3'-O3'	5.28	122.90	109.70
3	H	7	DG	C6-N1-C2	-5.23	121.96	125.10
4	I	1	DT	C4-C5-C7	5.19	122.11	119.00
4	I	10	DT	P-O5'-C5'	-5.10	112.73	120.90
3	H	7	DG	C3'-C2'-C1'	-5.10	96.38	102.50
3	H	1	DG	O4'-C1'-N9	5.06	111.54	108.00
3	H	4	DG	C3'-C2'-C1'	-5.02	96.47	102.50

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	1574	0	1565	10	0
2	B	1494	0	1513	16	0
3	H	227	0	126	5	0
4	I	218	0	126	3	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	48	0	0	2	0
6	B	47	0	0	1	0
6	H	4	0	0	0	0
6	I	1	0	0	0	0
All	All	3617	0	3330	33	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 5.

All (33) 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)
2:B:54:ASN:H	2:B:54:ASN:ND2	1.73	0.87
2:B:54:ASN:H	2:B:54:ASN:HD22	1.22	0.84
2:B:180:LYS:HD2	2:B:198:VAL:HG22	1.61	0.80
3:H:3:DT:H2'	3:H:4:DG:C8	2.27	0.69
4:I:3:DA:H1'	4:I:4:DG:H5'	1.73	0.69
3:H:6:DT:H2''	3:H:7:DG:O5'	1.94	0.68
2:B:139:GLU:O	2:B:142:LYS:HG2	1.97	0.65
2:B:19:ILE:HD12	2:B:38:ILE:HG21	1.80	0.64
2:B:21:ALA:HB2	2:B:40:LEU:HD21	1.81	0.62
2:B:29:GLN:OE1	6:B:2005:HOH:O	2.17	0.58
2:B:54:ASN:ND2	2:B:54:ASN:N	2.48	0.57
2:B:35:GLN:HG2	2:B:40:LEU:HB2	1.86	0.57
2:B:31:ALA:O	2:B:35:GLN:HG3	2.04	0.57
2:B:21:ALA:HB2	2:B:40:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LEU:HD23	2:B:104:LEU:C	2.29	0.53
1:A:1956:ASN:OD1	6:A:3036:HOH:O	2.19	0.52
3:H:2:DA:H2'	3:H:3:DT:C6	2.45	0.51
1:A:1889:SER:O	1:A:1981:ASN:HB3	2.11	0.50
1:A:1827:ILE:HD11	1:A:1847:VAL:HG11	1.93	0.50
1:A:1875:VAL:HG23	6:A:3019:HOH:O	2.11	0.49
1:A:1969:LYS:HE3	1:A:1972:ALA:HB2	1.96	0.48
3:H:3:DT:H2''	3:H:4:DG:O4'	2.15	0.47
3:H:9:DT:C2	4:I:4:DG:N2	2.85	0.44
1:A:1820:ILE:HD12	1:A:1843:LEU:HD21	2.00	0.43
4:I:9:DA:H4'	4:I:10:DT:OP1	2.19	0.42
1:A:1980:PRO:HD3	1:A:2025:TYR:CZ	2.54	0.42
2:B:19:ILE:HD11	2:B:133:VAL:HG21	2.02	0.41
1:A:1858:SER:HB3	1:A:1952:GLU:HB3	2.03	0.41
1:A:1884:ILE:HG21	1:A:1930:ILE:HD13	2.03	0.41
1:A:1867:SER:O	1:A:1871:MET:HG2	2.21	0.41
2:B:142:LYS:H	2:B:142:LYS:HG2	1.67	0.41
2:B:47:THR:HB	2:B:48:PRO:HD3	2.02	0.41
2:B:137:THR:HG22	2:B:137:THR:O	2.20	0.40

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	197/254 (78%)	193 (98%)	4 (2%)	0	100	100
2	B	192/217 (88%)	188 (98%)	4 (2%)	0	100	100
All	All	389/471 (83%)	381 (98%)	8 (2%)	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	175/231 (76%)	168 (96%)	7 (4%)	36	33
2	B	162/189 (86%)	157 (97%)	5 (3%)	45	44
All	All	337/420 (80%)	325 (96%)	12 (4%)	40	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1901	ASP
1	A	1950	LEU
1	A	1969	LYS
1	A	1982	ILE
1	A	2005	LEU
1	A	2006	GLN
1	A	2026	ILE
2	B	52	LEU
2	B	54	ASN
2	B	83	ASN
2	B	140	PRO
2	B	141	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1873	ASN
1	A	1876	ASN
1	A	1956	ASN
1	A	1993	GLN
2	B	54	ASN
2	B	70	ASN
2	B	134	GLN

### 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

### 5.7 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	202/254 (79%)	0.35	9 (4%) 34 42	23, 36, 53, 62	0
2	B	196/217 (90%)	0.11	8 (4%) 38 45	21, 32, 53, 71	0
3	H	11/11 (100%)	1.43	3 (27%) 1 1	46, 63, 106, 130	0
4	I	11/11 (100%)	0.60	0 100 100	43, 64, 87, 103	0
All	All	420/493 (85%)	0.27	20 (4%) 31 39	21, 35, 58, 130	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	1	DG	6.2
1	A	1875	VAL	4.3
1	A	1901	ASP	3.6
1	A	2034	MET	3.4
3	H	2	DA	3.3
2	B	140	PRO	3.2
2	B	141	SER	3.2
2	B	84	ASN	3.0
2	B	139	GLU	3.0
1	A	2032	ILE	2.6
1	A	2035	LEU	2.3
2	B	90	VAL	2.3
1	A	1873	ASN	2.3
1	A	1902	ARG	2.3
1	A	1960	HIS	2.2
2	B	83	ASN	2.1
1	A	1932	ILE	2.1
2	B	117	LEU	2.1
3	H	3	DT	2.0
2	B	129	VAL	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
5	CA	B	1217	1/1	0.93	0.05	-2.86	35,35,35,35	0
5	CA	B	1216	1/1	0.97	0.07	-5.20	32,32,32,32	0
5	CA	B	1215	1/1	0.95	0.05	-	34,34,34,34	0
5	CA	A	2050	1/1	0.96	0.07	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.