



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 03:05 PM EDT

PDB ID : 3GV5
Title : Human DNA polymerase iota in complex with T template DNA and incoming ddADP
Authors : Kirouac, K.N.; Ling, H.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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-20030345

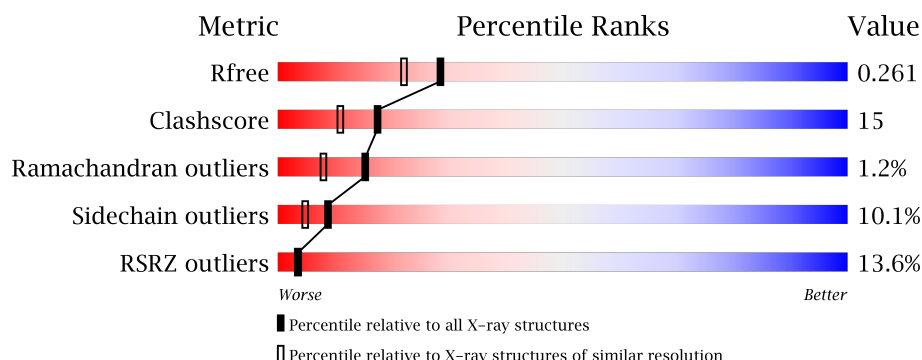
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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. 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	B	420	<div> <div>15%</div> <div> <div></div> <div>62%</div> <div>20%</div> <div>8%</div> <div>10%</div> </div> </div>
1	D	420	<div> <div>11%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>6%</div> <div>9%</div> </div> </div>
2	E	9	<div> <div></div> <div> <div>44%</div> <div>22%</div> <div>33%</div> </div> </div>
2	P	9	<div> <div></div> <div> <div>33%</div> <div>44%</div> <div>22%</div> </div> </div>
3	F	13	<div> <div></div> <div> <div>46%</div> <div>54%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	T	13	 62% 31% 8%

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
4	CA	B	421	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7703 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 DNA polymerase iota.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	379	Total	C	N	O	S	Se	0	0	0
			2990	1892	521	555	11	11			
1	D	383	Total	C	N	O	S	Se	0	1	0
			3020	1909	526	562	11	12			

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			
3	F	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Ca	0	0
			1	1		
4	B	3	Total	Ca	0	0
			3	3		
4	D	3	Total	Ca	0	0
			3	3		

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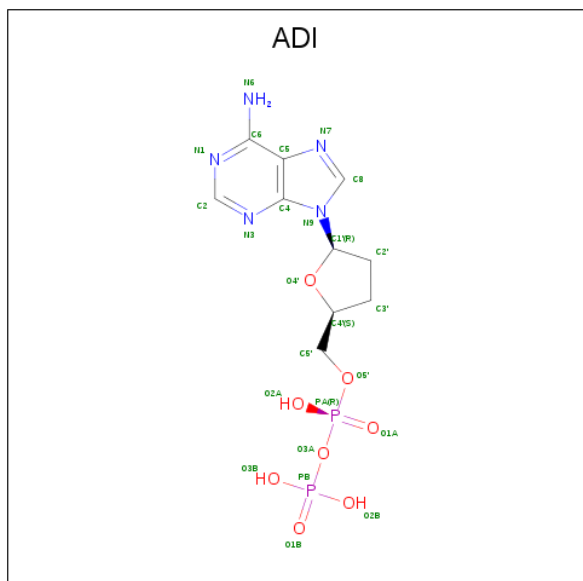
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: ADI) (formula: $C_{10}H_{15}N_5O_8P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			25	10	5	8	2		
6	D	1	Total	C	N	O	P	0	0
			25	10	5	8	2		

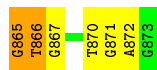
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	303	Total	O	0	0
			303	303		
7	P	32	Total	O	0	0
			32	32		
7	T	39	Total	O	0	0
			39	39		
7	D	306	Total	O	0	0
			306	306		
7	E	23	Total	O	0	0
			23	23		
7	F	34	Total	O	0	0
			34	34		



- Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'

Chain P:  33% 44% 22%



- Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'

Chain E:  44% 22% 33%



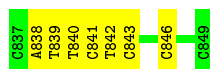
- Molecule 3: 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'

Chain T:  62% 31% 8%



- Molecule 3: 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'

Chain F:  46% 54%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.16Å 71.75Å 127.42Å 90.00° 112.53° 90.00°	Depositor
Resolution (Å)	51.57 – 2.00 51.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (51.57-2.00) 95.4 (51.54-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.253 0.216 , 0.261	Depositor DCC
R_{free} test set	1551 reflections (2.10%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: GOL, CA, ADI

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	B	0.59	1/3022 (0.0%)	0.81	7/4055 (0.2%)
1	D	0.95	8/3052 (0.3%)	0.91	16/4095 (0.4%)
2	E	1.07	0/213	1.90	8/329 (2.4%)
2	P	1.10	0/213	1.74	5/329 (1.5%)
3	F	1.11	0/285	1.84	12/435 (2.8%)
3	T	1.16	0/285	1.77	8/435 (1.8%)
All	All	0.85	9/7070 (0.1%)	1.07	56/9678 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	8
1	D	0	13
All	All	0	21

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	GLU	CG-CD	-27.52	1.10	1.51
1	D	358	GLU	CA-CB	-13.59	1.24	1.53
1	D	358	GLU	CD-OE1	12.00	1.38	1.25
1	D	358	GLU	CB-CG	11.19	1.73	1.52
1	D	358	GLU	CD-OE2	10.34	1.37	1.25

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	358	GLU	OE1-CD-OE2	-16.94	102.98	123.30
2	E	866	DT	O4'-C1'-N1	-10.12	100.92	108.00
1	D	318	LYS	N-CA-C	-9.64	84.97	111.00
2	P	866	DT	O4'-C1'-N1	-9.43	101.40	108.00
1	B	358	GLU	N-CA-C	8.86	134.92	111.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	LYS	Peptide
1	B	316	GLU	Peptide
1	B	317	ALA	Peptide
1	B	334	GLN	Peptide
1	B	357	ARG	Peptide

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	B	2990	0	3082	108	0
1	D	3020	0	3112	96	0
2	E	189	0	103	4	0
2	P	189	0	103	2	0
3	F	257	0	148	0	0
3	T	257	0	148	1	0
4	B	3	0	0	0	1
4	D	3	0	0	0	1
4	F	1	0	0	0	0
4	P	1	0	0	0	0
5	B	6	0	8	3	0
6	B	25	0	12	1	0
6	D	25	0	12	1	0
7	B	303	0	0	19	0
7	D	306	0	0	15	0
7	E	23	0	0	0	0
7	F	34	0	0	0	0
7	P	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	39	0	0	0	0
All	All	7703	0	6728	211	1

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 15.

The worst 5 of 211 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:47:ASN:HD21	1:B:49:GLU:HG2	1.16	1.08
1:D:172:ARG:HG3	1:D:172:ARG:HH11	0.93	1.07
1:D:35:LEU:HD21	1:D:187:MSE:HE1	1.38	1.02
1:D:172:ARG:HG3	1:D:172:ARG:NH1	1.46	1.01
1:D:87:LYS:HB2	7:D:645:HOH:O	1.59	1.00

All (1) 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)
4:B:421:CA:CA	4:D:423:CA:CA[1_565]	0.43	1.77

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	B	373/420 (89%)	363 (97%)	7 (2%)	3 (1%)	22	15
1	D	378/420 (90%)	359 (95%)	12 (3%)	7 (2%)	9	4
All	All	751/840 (89%)	722 (96%)	19 (2%)	10 (1%)	15	7

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	VAL
1	D	330	ASN
1	D	335	ASP
1	D	397	VAL
1	B	150	ALA

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	B	344/364 (94%)	309 (90%)	35 (10%)	8	4
1	D	348/364 (96%)	313 (90%)	35 (10%)	9	5
All	All	692/728 (95%)	622 (90%)	70 (10%)	9	5

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	396	ASN
1	D	87	LYS
1	D	314	GLU
1	B	404	THR
1	D	35	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	GLN
1	D	142	GLN
1	D	290	ASN
1	B	396	ASN
1	B	402	HIS

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z > 2$
5	GOL	B	422	-	5,5,5	0.55	0	5,5,5	0.30	0
6	ADI	B	425	4	23,27,27	1.18	2 (8%)	20,41,41	2.54	6 (30%)
6	ADI	D	424	4	23,27,27	1.14	2 (8%)	20,41,41	2.56	7 (35%)

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
5	GOL	B	422	-	-	0/4/4/4	0/0/0/0
6	ADI	B	425	4	-	0/12/25/25	0/3/3/3
6	ADI	D	424	4	-	0/12/25/25	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	425	ADI	PB-O3A	2.05	1.63	1.60
6	D	424	ADI	C2-N3	2.13	1.35	1.32
6	D	424	ADI	C5-C4	3.19	1.47	1.40
6	B	425	ADI	C5-C4	3.46	1.48	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	B	425	ADI	N3-C2-N1	-7.49	122.33	128.86
6	D	424	ADI	N3-C2-N1	-5.67	123.92	128.86
6	B	425	ADI	O4'-C1'-C2'	-3.50	102.88	106.67
6	B	425	ADI	C2'-C1'-N9	-3.19	106.40	112.47
6	D	424	ADI	O4'-C1'-C2'	-3.01	103.42	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	422	GOL	3	0
6	B	425	ADI	1	0
6	D	424	ADI	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	B	368/420 (87%)	1.29	62 (16%) 2 2	45, 56, 69, 80	0
1	D	372/420 (88%)	1.07	45 (12%) 5 5	17, 54, 66, 88	0
2	E	9/9 (100%)	-0.29	0 100 100	34, 37, 40, 41	0
2	P	9/9 (100%)	0.85	0 100 100	49, 51, 55, 57	0
3	F	13/13 (100%)	-0.08	0 100 100	31, 38, 52, 68	0
3	T	13/13 (100%)	0.71	0 100 100	45, 54, 68, 85	0
All	All	784/884 (88%)	1.13	107 (13%) 3 3	17, 55, 68, 88	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	SER	11.2
1	B	146	ASP	8.7
1	D	370	GLN	8.5
1	D	372	LEU	8.4
1	B	372	LEU	8.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	CA	B	421	1/1	1.00	0.30	2.54	35,35,35,35	0
4	CA	D	423	1/1	0.99	0.24	0.85	36,36,36,36	0
6	ADI	D	424	25/25	0.92	0.18	0.49	19,24,29,30	0
5	GOL	B	422	6/6	0.86	0.19	-0.38	32,34,34,35	0
4	CA	B	423	1/1	0.99	0.16	-1.16	28,28,28,28	0
4	CA	D	421	1/1	0.99	0.12	-1.35	14,14,14,14	0
4	CA	F	1	1/1	0.98	0.12	-1.53	19,19,19,19	0
6	ADI	B	425	25/25	0.93	0.14	-2.17	15,21,24,26	0
4	CA	B	424	1/1	0.99	0.10	-4.67	13,13,13,13	0
4	CA	D	422	1/1	0.91	0.21	-	43,43,43,43	0
4	CA	P	1	1/1	0.98	0.08	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.