



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2017 – 03:43 AM EDT

PDB ID : 5MLO
Title : Crystal structure of human PCNA in complex with ZRANB3 PIP box peptide
Authors : Ariza, A.
Deposited on : 2016-12-07
Resolution : 1.96 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

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
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

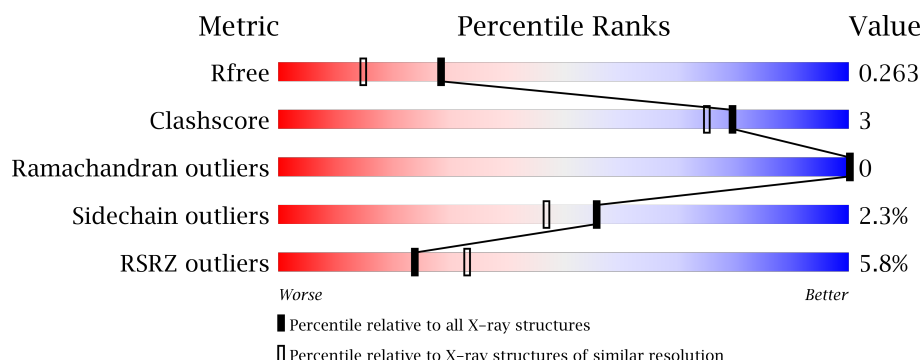
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	A	261	<div> <div>3%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	C	261	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	E	261	<div> <div>7%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
2	B	15	<div> <div>13%</div> <div>67%</div> <div>33%</div> </div>
2	D	15	<div> <div>33%</div> <div>67%</div> <div>7%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	15	<div><div></div><div>7%</div><div>47%</div><div>27%</div><div>27%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6705 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	4	0
			1987	1248	323	400	16			
1	C	255	Total	C	N	O	S	0	10	0
			2023	1270	334	402	17			
1	E	255	Total	C	N	O	S	0	9	0
			2015	1265	332	401	17			

- Molecule 2 is a protein called ZRANB3 PIP box peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			90	59	17	14			
2	D	11	Total	C	N	O	0	0	0
			99	64	18	17			
2	F	11	Total	C	N	O	0	0	0
			97	64	18	15			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	2
			126	126		

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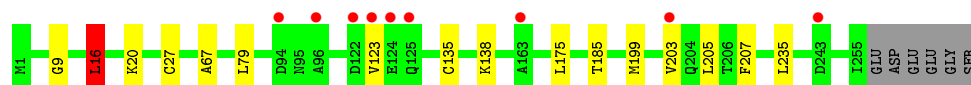
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	O 2	0	0
4	C	145	Total 146	O 146	0	1
4	E	112	Total 114	O 114	0	2
4	F	2	Total 2	O 2	0	0

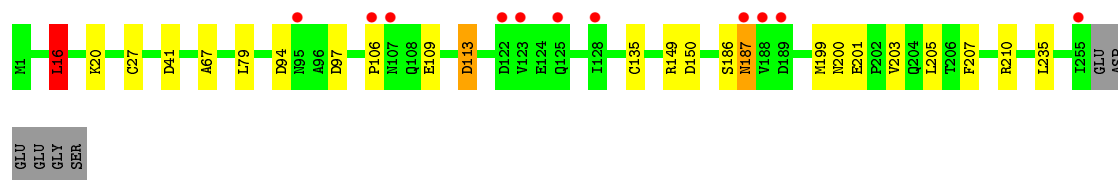
3 Residue-property plots [i](#)

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.

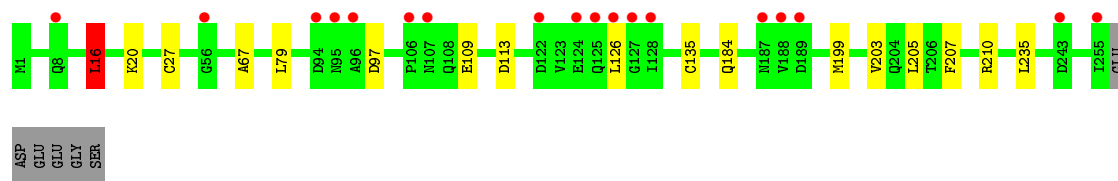
- Molecule 1: Proliferating cell nuclear antigen



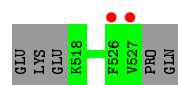
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen

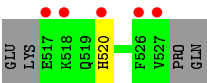


- Molecule 2: ZRANB3 PIP box peptide

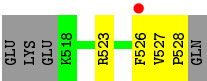


- Molecule 2: ZRANB3 PIP box peptide





● Molecule 2: ZRANB3 PIP box peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.14Å 86.80Å 156.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.34 – 1.96 78.34 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.34-1.96) 100.0 (78.34-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.211 , 0.259 0.217 , 0.263	Depositor DCC
R_{free} test set	3325 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.54	0/2024	0.68	1/2735 (0.0%)
1	C	0.61	0/2076	0.72	1/2803 (0.0%)
1	E	0.53	0/2065	0.69	1/2788 (0.0%)
2	B	0.35	0/92	0.41	0/121
2	D	0.34	0/101	0.39	0/133
2	F	0.40	0/100	0.60	0/133
All	All	0.55	0/6458	0.69	3/8713 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	LEU	CA-CB-CG	-7.92	97.08	115.30
1	E	16	LEU	CA-CB-CG	-7.75	97.48	115.30
1	A	16	LEU	CA-CB-CG	-7.40	98.27	115.30

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	1987	0	1995	9	0
1	C	2023	0	2049	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2015	0	2040	10	0
2	B	90	0	87	0	0
2	D	99	0	93	0	0
2	F	97	0	94	5	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	126	0	0	2	0
4	B	2	0	0	0	0
4	C	146	0	0	4	0
4	E	114	0	0	0	0
4	F	2	0	0	0	0
All	All	6705	0	6358	40	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 3.

All (40) 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:C:149[B]:ARG:HG2	1:C:149[B]:ARG:HH11	1.04	1.18
1:C:210[A]:ARG:HB2	1:C:210[A]:ARG:NH1	1.78	0.98
1:C:113[A]:ASP:OD1	4:C:401:HOH:O	1.83	0.95
1:C:149[B]:ARG:HG2	1:C:149[B]:ARG:NH1	1.73	0.90
1:C:210[A]:ARG:HB2	1:C:210[A]:ARG:HH11	1.39	0.86
1:C:149[B]:ARG:CG	1:C:149[B]:ARG:HH11	1.88	0.80
1:E:126:LEU:HG	2:F:526:PHE:CE2	2.19	0.77
1:E:210[A]:ARG:O	1:E:210[A]:ARG:NE	2.30	0.64
1:C:210[A]:ARG:HH11	1:C:210[A]:ARG:CB	2.09	0.64
1:A:135:CYS:SG	1:A:199:MET:HG3	2.38	0.63
1:C:135:CYS:SG	1:C:199:MET:HG3	2.40	0.62
1:E:135:CYS:SG	1:E:199:MET:HG3	2.41	0.60
1:E:16:LEU:HD13	1:E:79:LEU:CD1	2.37	0.55
1:C:210[A]:ARG:HB2	1:C:210[A]:ARG:CZ	2.37	0.54
1:C:16:LEU:HD13	1:C:79:LEU:CD1	2.38	0.54
1:C:149[B]:ARG:NH1	1:C:150:ASP:OD1	2.42	0.53
1:A:16:LEU:HD13	1:A:79:LEU:CD1	2.39	0.52
1:C:109:GLU:HA	4:C:515:HOH:O	2.08	0.51
1:C:187:ASN:OD1	1:C:187:ASN:C	2.50	0.50
1:A:203:VAL:HG12	1:A:205:LEU:HG	1.95	0.49
1:A:185:THR:HB	1:E:109:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LEU:HG	2:F:526:PHE:CD2	2.48	0.48
1:A:27:CYS:SG	1:A:67:ALA:HB1	2.54	0.48
1:E:27[A]:CYS:SG	1:E:67:ALA:HB1	2.53	0.48
1:C:200[B]:ASN:OD1	1:C:201[B]:GLU:OE1	2.32	0.47
1:C:149[B]:ARG:CG	1:C:149[B]:ARG:NH1	2.54	0.47
2:F:527:VAL:HG22	2:F:528:PRO:HD2	1.97	0.46
1:E:203:VAL:HG12	1:E:205:LEU:HG	1.98	0.46
1:C:106:PRO:HD2	4:C:502[B]:HOH:O	2.15	0.46
2:F:523:ARG:HA	2:F:526:PHE:CD2	2.50	0.46
1:E:126:LEU:HB3	2:F:526:PHE:CG	2.52	0.45
1:C:27[A]:CYS:SG	1:C:67:ALA:HB1	2.56	0.45
1:C:203:VAL:HG12	1:C:205:LEU:HG	1.98	0.45
1:C:94:ASP:HA	4:C:419:HOH:O	2.18	0.44
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.53	0.43
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.54	0.43
1:E:207:PHE:CZ	1:E:235:LEU:HB2	2.54	0.41
1:A:9:GLY:N	4:A:409:HOH:O	2.53	0.41
1:A:175:LEU:HD12	1:A:175:LEU:C	2.41	0.40
1:A:138:LYS:HE2	4:A:493:HOH:O	2.22	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	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
1	C	263/261 (101%)	259 (98%)	4 (2%)	0	100	100
1	E	262/261 (100%)	258 (98%)	4 (2%)	0	100	100
2	B	8/15 (53%)	8 (100%)	0	0	100	100
2	D	9/15 (60%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
All	All	808/828 (98%)	794 (98%)	14 (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	227/228 (100%)	224 (99%)	3 (1%)	73	69
1	C	233/228 (102%)	225 (97%)	8 (3%)	42	29
1	E	232/228 (102%)	226 (97%)	6 (3%)	51	40
2	B	10/15 (67%)	10 (100%)	0	100	100
2	D	11/15 (73%)	10 (91%)	1 (9%)	11	3
2	F	11/15 (73%)	11 (100%)	0	100	100
All	All	724/729 (99%)	706 (98%)	18 (2%)	56	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	20	LYS
1	A	123	VAL
1	C	16	LEU
1	C	20	LYS
1	C	41	ASP
1	C	97	ASP
1	C	113[A]	ASP
1	C	113[B]	ASP
1	C	186	SER
1	C	187	ASN
2	D	520	HIS
1	E	16	LEU

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Mol	Chain	Res	Type
1	E	20	LYS
1	E	97	ASP
1	E	113[A]	ASP
1	E	113[B]	ASP
1	E	184	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 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	255/261 (97%)	0.35	9 (3%) 44 55	29, 43, 73, 117	0
1	C	255/261 (97%)	0.38	11 (4%) 36 47	24, 34, 74, 97	0
1	E	255/261 (97%)	0.61	18 (7%) 17 26	27, 41, 101, 126	0
2	B	10/15 (66%)	0.70	2 (20%) 1 1	51, 57, 80, 92	0
2	D	11/15 (73%)	1.53	5 (45%) 0 0	42, 56, 81, 89	0
2	F	11/15 (73%)	0.86	1 (9%) 10 16	39, 52, 69, 73	0
All	All	797/828 (96%)	0.47	46 (5%) 24 33	24, 40, 77, 126	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	96	ALA	9.2
1	C	189	ASP	6.5
1	C	107	ASN	5.8
2	F	526	PHE	5.6
1	E	95	ASN	5.2
2	D	527	VAL	5.0
1	E	94	ASP	4.6
1	C	106	PRO	4.5
1	E	122	ASP	4.5
1	E	126	LEU	4.3
1	C	95	ASN	4.2
1	E	189	ASP	4.2
1	C	128	ILE	4.0
1	E	127	GLY	3.7
2	D	517	GLU	3.7
1	E	187	ASN	3.6
1	E	107	ASN	3.5
1	E	124	GLU	3.5
1	C	125	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	3.5
1	C	187	ASN	3.4
1	E	188	VAL	3.4
1	A	122	ASP	3.3
1	E	125	GLN	3.3
1	E	128	ILE	3.3
1	E	8	GLN	3.3
2	B	527	VAL	3.2
1	A	124	GLU	3.2
1	A	243	ASP	3.1
2	B	526	PHE	2.9
1	A	96	ALA	2.9
2	D	526	PHE	2.9
1	C	188	VAL	2.8
1	E	106	PRO	2.7
1	C	123	VAL	2.6
1	C	122	ASP	2.5
2	D	518	LYS	2.5
2	D	520	HIS	2.3
1	E	56	GLY	2.3
1	E	255	ILE	2.3
1	E	243	ASP	2.2
1	A	94	ASP	2.2
1	A	123	VAL	2.2
1	C	255	ILE	2.1
1	A	125	GLN	2.1
1	A	203	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, 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(\AA^2)	Q<0.9
3	NA	A	301	1/1	0.76	0.18	1.61	48,48,48,48	0
3	NA	A	302	1/1	0.97	0.14	0.90	32,32,32,32	0
3	NA	E	301	1/1	0.73	0.11	-0.73	63,63,63,63	0
3	NA	C	301	1/1	0.91	0.15	-	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.