



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 10:53 PM EDT

PDB ID : 2NVO  
Title : Crystal structure of Deinococcus radiodurans RO (RSR) protein  
Authors : Ramesh, A.; Sacchettini, J.C.  
Deposited on : unknown  
Resolution : 1.89 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-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

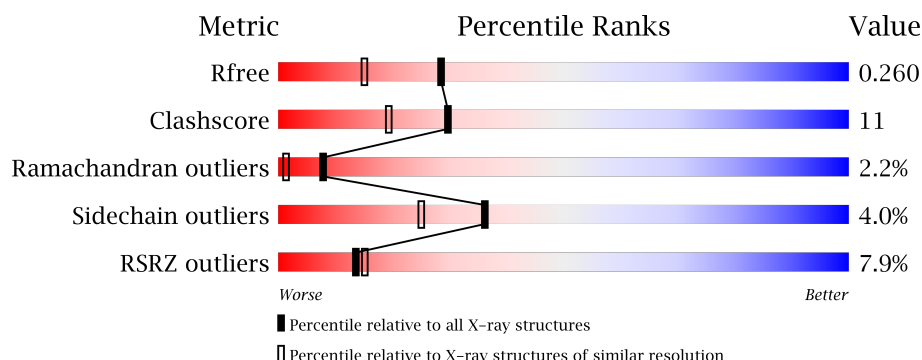
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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  $\geq 3$ , 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	535	<div> <div>7%</div> <div>73%</div> <div>17%</div> <div>•</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4141 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 Ro sixty-related protein, RSR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3739	2358	674	693	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9RUW8
A	-1	SER	-	CLONING ARTIFACT	UNP Q9RUW8
A	0	HIS	-	CLONING ARTIFACT	UNP Q9RUW8
A	433	VAL	MET	SEE REMARK 999	UNP Q9RUW8
A	532	LEU	-	CLONING ARTIFACT	UNP Q9RUW8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

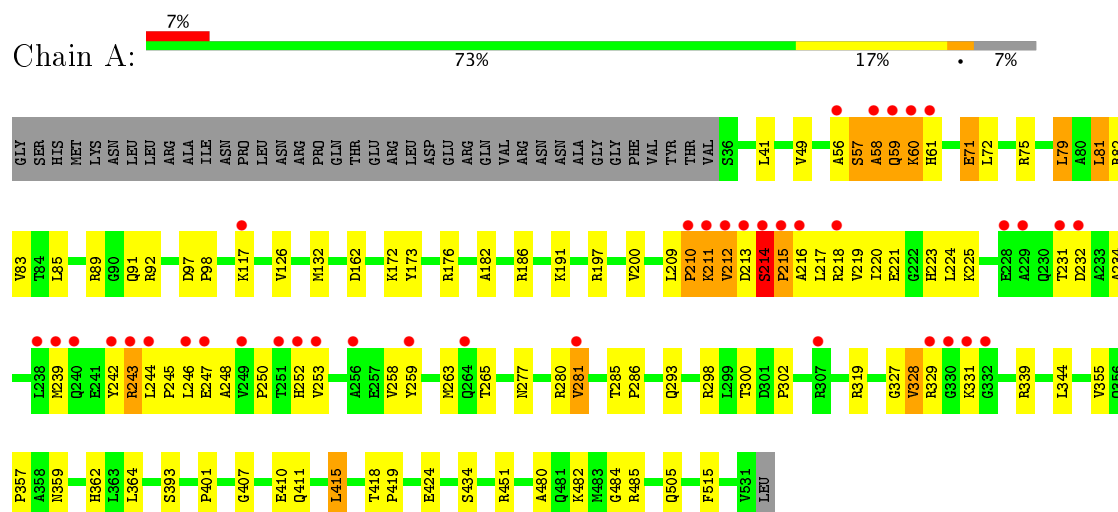
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		

### 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: Ro sixty-related protein, RSR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.56 Å   87.61 Å   70.62 Å 90.00°   96.57°   90.00°	Depositor
Resolution (Å)	46.60 – 1.89 46.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-1.89) 98.1 (46.64-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.90 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.223   ,   0.262 0.218   ,   0.260	Depositor DCC
$R_{free}$ test set	2457 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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

### 5.1 Standard geometry

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	0.39	0/3810	0.56	0/5193

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	ALA	Peptide
1	A	57	SER	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	A	3739	0	3764	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	401	0	0	6	0
All	All	4141	0	3764	80	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 11.

All (80) 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:A:242:TYR:O	1:A:243:ARG:HG3	1.81	0.80
1:A:172:LYS:HD3	1:A:173:TYR:CZ	2.17	0.78
1:A:223:HIS:CE1	1:A:248:ALA:HB2	2.19	0.78
1:A:293:GLN:HE22	1:A:339:ARG:HH22	1.32	0.77
1:A:126:VAL:O	1:A:132:MET:HE2	1.89	0.73
1:A:97:ASP:HB2	1:A:98:PRO:HD3	1.71	0.73
1:A:231:THR:HG23	1:A:234:ALA:H	1.53	0.73
1:A:252:HIS:ND1	1:A:253:VAL:HG13	2.08	0.68
1:A:362:HIS:HE1	3:A:589:HOH:O	1.78	0.65
1:A:239:MET:HE1	1:A:258:VAL:HG13	1.78	0.65
1:A:79:LEU:HB2	1:A:82:ARG:NH2	2.12	0.65
1:A:117:LYS:HB3	3:A:850:HOH:O	2.00	0.62
1:A:223:HIS:CD2	1:A:244:LEU:HD22	2.35	0.60
1:A:328:VAL:HG22	1:A:329:ARG:H	1.67	0.59
1:A:216:ALA:O	1:A:219:VAL:HG22	2.04	0.57
1:A:484:GLY:O	1:A:485:ARG:HD2	2.04	0.57
1:A:214:SER:C	1:A:216:ALA:H	2.10	0.55
1:A:451:ARG:HG2	1:A:482:LYS:HE2	1.89	0.55
1:A:72:LEU:HD11	1:A:79:LEU:HD21	1.88	0.54
1:A:71:GLU:HG2	1:A:75:ARG:HH11	1.72	0.53
1:A:219:VAL:HG11	1:A:243:ARG:NH1	2.24	0.53
1:A:209:LEU:HD22	1:A:224:LEU:HD12	1.91	0.52
1:A:259:TYR:CD2	1:A:281:VAL:HG11	2.45	0.52
1:A:250:PRO:HB3	1:A:252:HIS:CD2	2.44	0.51
1:A:328:VAL:H	1:A:331:LYS:HD2	1.73	0.51
1:A:71:GLU:CG	1:A:75:ARG:HH11	2.24	0.51
1:A:250:PRO:CB	1:A:252:HIS:CD2	2.94	0.51
1:A:328:VAL:HG13	1:A:329:ARG:N	2.25	0.50
1:A:239:MET:CE	1:A:258:VAL:HA	2.41	0.50
1:A:79:LEU:O	1:A:83:VAL:HG23	2.12	0.50
1:A:239:MET:HE2	1:A:258:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HE2	3:A:810:HOH:O	2.12	0.49
1:A:220:ILE:O	1:A:224:LEU:HG	2.11	0.49
1:A:214:SER:O	1:A:216:ALA:N	2.45	0.49
1:A:424:GLU:H	1:A:424:GLU:CD	2.15	0.49
1:A:59:GLN:CD	1:A:60:LYS:H	2.16	0.49
1:A:182:ALA:O	1:A:186:ARG:HG3	2.12	0.49
1:A:263:MET:CE	1:A:298:ARG:NH1	2.76	0.48
1:A:328:VAL:N	1:A:331:LYS:HD2	2.28	0.48
1:A:210:PRO:HG3	3:A:909:HOH:O	2.12	0.48
1:A:277:ASN:OD1	1:A:280:ARG:NH1	2.39	0.47
1:A:418:THR:HB	1:A:419:PRO:CD	2.44	0.47
1:A:197:ARG:O	1:A:200:VAL:HG12	2.14	0.47
1:A:215:PRO:HA	1:A:218:ARG:HB2	1.97	0.47
1:A:480:ALA:HA	1:A:485:ARG:O	2.15	0.47
1:A:328:VAL:HG12	1:A:331:LYS:HE3	1.97	0.46
1:A:232:ASP:OD1	1:A:258:VAL:HG23	2.14	0.46
1:A:81:LEU:HD22	1:A:85:LEU:HD13	1.97	0.46
1:A:71:GLU:CD	1:A:75:ARG:HH11	2.19	0.46
1:A:410:GLU:HG3	1:A:434:SER:OG	2.16	0.45
1:A:239:MET:HB3	1:A:244:LEU:HB2	1.99	0.45
1:A:57:SER:HB3	1:A:58:ALA:H	1.57	0.45
1:A:221:GLU:O	1:A:225:LYS:HG3	2.17	0.44
1:A:212:VAL:H	1:A:217:LEU:CD1	2.31	0.44
1:A:250:PRO:HB2	1:A:252:HIS:CD2	2.53	0.44
1:A:41:LEU:HD23	1:A:83:VAL:HB	1.99	0.44
1:A:259:TYR:HD2	1:A:281:VAL:HG11	1.82	0.44
1:A:89:ARG:O	1:A:91:GLN:HG3	2.18	0.44
1:A:407:GLY:HA3	1:A:415:LEU:HD11	2.00	0.43
1:A:327:GLY:HA3	1:A:331:LYS:HD2	1.98	0.43
1:A:505:GLN:HG3	3:A:866:HOH:O	2.17	0.43
1:A:252:HIS:CE1	1:A:253:VAL:HG13	2.54	0.43
1:A:285:THR:HB	1:A:286:PRO:HD2	2.01	0.43
1:A:243:ARG:HD2	1:A:243:ARG:O	2.19	0.42
1:A:263:MET:HE3	1:A:298:ARG:NH1	2.34	0.42
1:A:355:VAL:O	1:A:357:PRO:HD3	2.19	0.42
1:A:246:LEU:HD23	3:A:709:HOH:O	2.20	0.42
1:A:259:TYR:HB2	1:A:281:VAL:HG21	2.02	0.42
1:A:57:SER:HB3	1:A:59:GLN:H	1.85	0.42
1:A:300:THR:O	1:A:302:PRO:HD3	2.20	0.41
1:A:172:LYS:HD3	1:A:173:TYR:CE2	2.51	0.41
1:A:250:PRO:CB	1:A:252:HIS:NE2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:H	1:A:217:LEU:HD11	1.85	0.41
1:A:359:ASN:OD1	1:A:401:PRO:HG3	2.20	0.41
1:A:364:LEU:CD2	1:A:393:SER:HA	2.50	0.41
1:A:247:GLU:H	1:A:247:GLU:HG3	1.65	0.41
1:A:214:SER:C	1:A:216:ALA:N	2.74	0.41
1:A:244:LEU:HA	1:A:245:PRO:HD2	1.84	0.41
1:A:319:ARG:HA	1:A:344:LEU:HD13	2.02	0.41
1:A:418:THR:HB	1:A:419:PRO:HD2	2.03	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	494/535 (92%)	465 (94%)	18 (4%)	11 (2%)	<b>8</b> <b>1</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ALA
1	A	213	ASP
1	A	215	PRO
1	A	61	HIS
1	A	212	VAL
1	A	60	LYS
1	A	210	PRO
1	A	211	LYS
1	A	281	VAL
1	A	214	SER
1	A	328	VAL

### 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	377/414 (91%)	362 (96%)	15 (4%)	36	25

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	59	GLN
1	A	71	GLU
1	A	79	LEU
1	A	81	LEU
1	A	92	ARG
1	A	162	ASP
1	A	176	ARG
1	A	211	LYS
1	A	214	SER
1	A	243	ARG
1	A	265	THR
1	A	411	GLN
1	A	415	LEU
1	A	515	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	181	GLN
1	A	223	HIS
1	A	293	GLN
1	A	362	HIS
1	A	386	ASN
1	A	428	GLN
1	A	431	GLN
1	A	521	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](#)

Of 1 ligands modelled in this entry, 1 is 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	496/535 (92%)	0.45	39 (7%) <b>13</b> <b>15</b>	5, 22, 54, 71	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	5.3
1	A	243	ARG	5.2
1	A	329	ARG	5.1
1	A	60	LYS	5.0
1	A	212	VAL	4.8
1	A	251	THR	4.8
1	A	253	VAL	4.6
1	A	252	HIS	4.5
1	A	238	LEU	4.2
1	A	259	TYR	3.9
1	A	58	ALA	3.8
1	A	229	ALA	3.7
1	A	256	ALA	3.5
1	A	59	GLN	3.5
1	A	228	GLU	3.4
1	A	246	LEU	3.3
1	A	215	PRO	3.2
1	A	61	HIS	3.2
1	A	56	ALA	3.1
1	A	332	GLY	3.0
1	A	211	LYS	2.9
1	A	214	SER	2.9
1	A	330	GLY	2.7
1	A	213	ASP	2.7
1	A	281	VAL	2.7
1	A	240	GLN	2.6
1	A	231	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	247	GLU	2.6
1	A	210	PRO	2.6
1	A	232	ASP	2.5
1	A	331	LYS	2.4
1	A	242	TYR	2.3
1	A	307	ARG	2.3
1	A	264	GLN	2.2
1	A	239	MET	2.2
1	A	216	ALA	2.2
1	A	244	LEU	2.1
1	A	117	LYS	2.1
1	A	218	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(Å <sup>2</sup> )	Q<0.9
2	CA	A	533	1/1	0.99	0.11	-	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.