



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:26 PM GMT

PDB ID : 3RC7  
Title : Crystal Structure of the Y186F mutant of KijD10, a 3-ketoreductase from Actinomadura kijaniata in complex with TDP-benzene and NADP  
Authors : Holden, H.M.; Kubiak, R.L.  
Deposited on : 2011-03-30  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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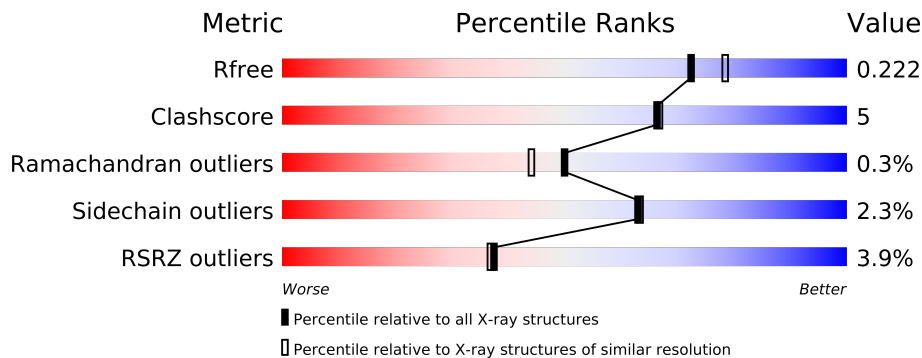
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	350	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	334	-	X
5	PO4	A	336	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2920 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

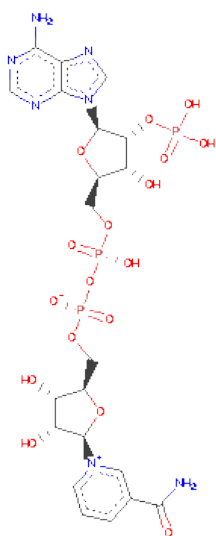
- Molecule 1 is a protein called Sugar 3-ketoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	2	0
			2581	1636	475	464	6			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP B3TMR8
A	-16	GLY	-	EXPRESSION TAG	UNP B3TMR8
A	-15	SER	-	EXPRESSION TAG	UNP B3TMR8
A	-14	SER	-	EXPRESSION TAG	UNP B3TMR8
A	-13	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-12	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-11	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-10	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-9	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-8	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	-7	GLU	-	EXPRESSION TAG	UNP B3TMR8
A	-6	ASN	-	EXPRESSION TAG	UNP B3TMR8
A	-5	LEU	-	EXPRESSION TAG	UNP B3TMR8
A	-4	TYR	-	EXPRESSION TAG	UNP B3TMR8
A	-3	PHE	-	EXPRESSION TAG	UNP B3TMR8
A	-2	GLN	-	EXPRESSION TAG	UNP B3TMR8
A	-1	GLY	-	EXPRESSION TAG	UNP B3TMR8
A	0	HIS	-	EXPRESSION TAG	UNP B3TMR8
A	186	PHE	TYR	ENGINEERED MUTATION	UNP B3TMR8

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

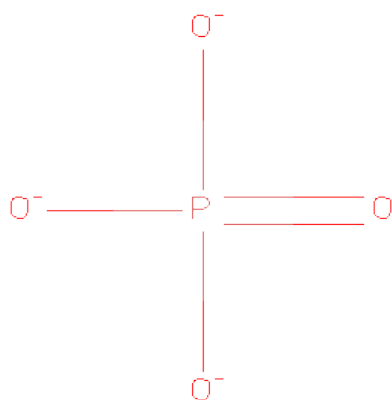
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

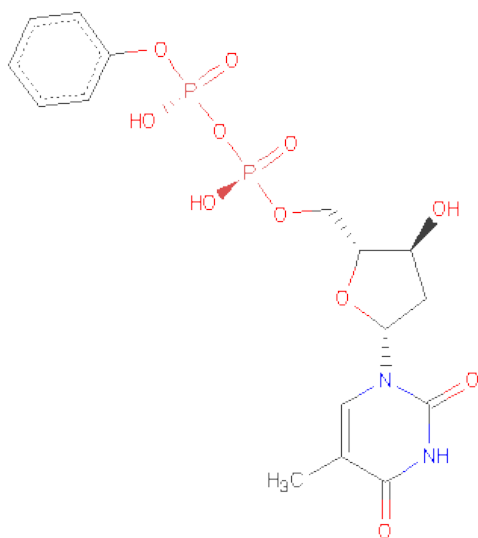
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	P		0	0
			5	4	1			

- Molecule 6 is 5'-O-[(S)-HYDROXY{[(S)-HYDROXY(PHENOXY)PHOSPHORYL]OXY}P HOSPHORYL]THYMIDINE (three-letter code: TLO) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	
			31	16	2	11	2	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	252	Total 252	O 252	0	0

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- Molecule 1: Sugar 3-ketoreductase

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.82Å 104.22Å 145.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.00 65.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.00-2.00) 96.9 (65.12-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.191 , 0.232 0.185 , 0.222	Depositor DCC
$R_{free}$ test set	1835 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 36598 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, TLO, NAP, CL

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	0.51	0/2651	1.24	15/3601 (0.4%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	A	138	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	A	119	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	182	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	142	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	121	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	170	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	24	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	138	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	182	ASP	OD1-CG-OD2	6.54	135.72	123.30
1	A	257	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	182	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	61	GLU	OE1-CD-OE2	-5.84	116.30	123.30
1	A	306	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	245	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2581	0	2542	21	0
2	A	48	0	25	8	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
6	A	31	0	18	2	0
7	A	252	0	0	2	0
All	All	2920	0	2585	27	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:ARG:NH2	2:A:333:NAP:O7N	2.04	0.91
2:A:333:NAP:O2N	2:A:333:NAP:C7N	2.25	0.84
1:A:169:ILE:O	1:A:176:GLY:HA3	1.88	0.71
2:A:333:NAP:H2N	2:A:333:NAP:O5D	1.92	0.69
1:A:20:ILE:HD11	1:A:24:ARG:HG3	1.87	0.57
2:A:333:NAP:O7N	2:A:333:NAP:O2N	2.23	0.55
1:A:172:GLN:NE2	1:A:175:VAL:HG21	2.27	0.50
2:A:333:NAP:H4N	6:A:337:TLO:O3B	2.13	0.49
1:A:166:GLN:NE2	1:A:212:ARG:NH1	2.60	0.49
1:A:138:ARG:O	1:A:138:ARG:HD3	2.13	0.49
1:A:170:ARG:O	1:A:214:VAL:HG21	2.14	0.48
1:A:164:LYS:HE3	7:A:530:HOH:O	2.14	0.47
1:A:11:ARG:HB3	1:A:38:THR:HG21	1.96	0.47
1:A:63:TYR:OH	2:A:333:NAP:H8A	2.16	0.46
1:A:166:GLN:HA	1:A:166:GLN:HE21	1.80	0.46
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.63	0.46
2:A:333:NAP:H4N	6:A:337:TLO:CG	2.47	0.45
1:A:293:ARG:O	1:A:297:GLN:HG3	2.17	0.45
1:A:161:ILE:O	1:A:236:MET:HA	2.16	0.44
1:A:110:GLN:NE2	1:A:113:ARG:HH11	2.16	0.43
2:A:333:NAP:H2N	2:A:333:NAP:PN	2.59	0.42
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.84	0.42
1:A:314:ARG:HD2	7:A:375:HOH:O	2.19	0.41
1:A:20:ILE:HA	1:A:20:ILE:HD12	1.93	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:GLN:NE2	1:A:113:ARG:NH1	2.69	0.41
1:A:331:PHE:HB2	1:A:332:PRO:HA	2.02	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	325/350 (93%)	317 (98%)	7 (2%)	1 (0%)	50 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	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	262/281 (93%)	256 (98%)	6 (2%)	63 63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	159	PHE
1	A	166	GLN
1	A	174	ASP
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	244	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	166	GLN
1	A	172	GLN
1	A	297	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 6 ligands modelled in this entry, 3 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$
2	NAP	A	333	-	52,52,52	0.82	1 (1%)	80,80,80	2.10	16 (20%)
5	PO4	A	336	-	4,4,4	0.23	0	6,6,6	0.38	0
6	TLO	A	337	-	33,33,33	1.00	1 (3%)	44,49,49	1.82	9 (20%)

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
2	NAP	A	333	-	-	0/35/67/67	0/3/5/5
5	PO4	A	336	-	-	0/0/0/0	0/0/0/0
6	TLO	A	337	-	-	0/18/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	337	TLO	C2-N1	-3.72	1.34	1.38
2	A	333	NAP	C4A-N9A	-2.66	1.33	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	333	NAP	N3A-C2A-N1A	-9.71	120.59	128.71
2	A	333	NAP	C3N-C7N-N7N	7.16	125.92	117.77
6	A	337	TLO	N3-C2-N1	5.29	120.39	115.97
6	A	337	TLO	C6-N1-C2	-5.06	120.97	122.41
2	A	333	NAP	O4B-C1B-N9A	4.98	113.08	108.44
2	A	333	NAP	O7N-C7N-C3N	-4.73	114.24	119.58
2	A	333	NAP	C4B-O4B-C1B	4.28	114.40	109.75
6	A	337	TLO	C2'-C3'-C4'	3.83	111.31	102.73
2	A	333	NAP	C8A-N9A-C4A	3.66	109.69	106.90
2	A	333	NAP	N3A-C4A-N9A	3.57	131.87	125.43
2	A	333	NAP	O2B-C2B-C1B	-3.25	98.30	110.36
2	A	333	NAP	O4B-C1B-C2B	-3.07	104.08	106.95
2	A	333	NAP	O3X-P2B-O1X	2.95	120.09	110.44
6	A	337	TLO	O1B-PB-O3B	2.94	114.36	104.44
6	A	337	TLO	CZ-CE2-CD2	-2.87	115.39	120.17
2	A	333	NAP	O3-PN-O1N	2.55	114.91	108.83
2	A	333	NAP	C2A-N1A-C6A	2.48	123.25	118.77
6	A	337	TLO	O1B-PB-O2B	2.47	126.00	112.21
6	A	337	TLO	C4-N3-C2	-2.43	120.41	125.39
6	A	337	TLO	CE1-CD1-CG	-2.28	114.87	118.91
2	A	333	NAP	O5D-PN-O1N	2.15	117.74	108.61
2	A	333	NAP	O2A-PA-O1A	2.14	124.14	112.21
2	A	333	NAP	C3B-C2B-C1B	2.08	106.78	102.73
6	A	337	TLO	O1A-PA-O3A	2.03	114.75	105.14
2	A	333	NAP	N6A-C6A-N1A	2.00	123.30	119.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	325/350 (92%)	-0.24	13 (4%) 36 36	5, 13, 38, 58	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	5.6
1	A	171	TYR	5.5
1	A	169	ILE	4.5
1	A	167	GLY	4.4
1	A	166	GLN	4.1
1	A	174	ASP	3.6
1	A	175	VAL	3.4
1	A	172	GLN	3.3
1	A	332	PRO	2.8
1	A	177	GLY	2.5
1	A	173	ALA	2.3
1	A	165	PRO	2.2
1	A	8	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	334	1/1	0.27	25.93	42,42,42,42	0
5	PO4	A	336	5/5	0.12	3.17	27,41,42,46	0
4	NA	A	335	1/1	0.14	1.70	12,12,12,12	0
2	NAP	A	333	48/48	0.13	-0.03	15,25,51,58	0
6	TLO	A	337	31/31	0.10	-0.40	7,12,24,25	0
3	CL	A	338	1/1	0.06	-2.59	15,15,15,15	0

## 6.5 Other polymers

There are no such residues in this entry.