



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TL1
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW451211
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

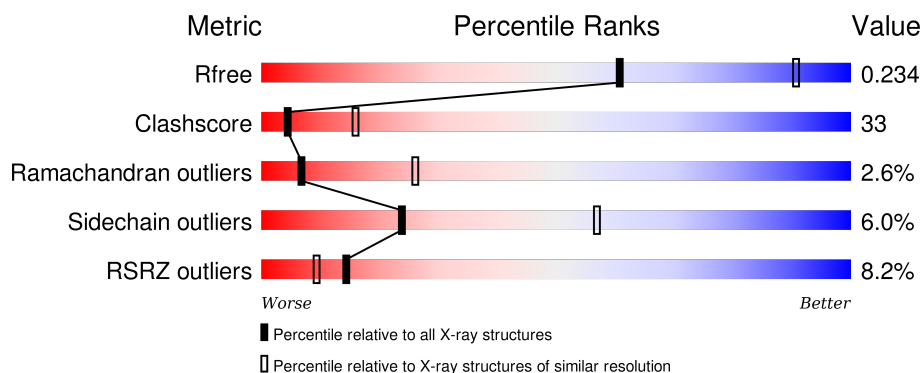
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 ≥ 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	560	<div> <div>7%</div> <div>41%</div> <div>46%</div> <div>5%</div> <div>8%</div> </div>
2	B	440	<div> <div>8%</div> <div>45%</div> <div>43%</div> <div>•</div> <div>9%</div> </div>

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	H18	A	999	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7604 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4247	2754	701	784	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

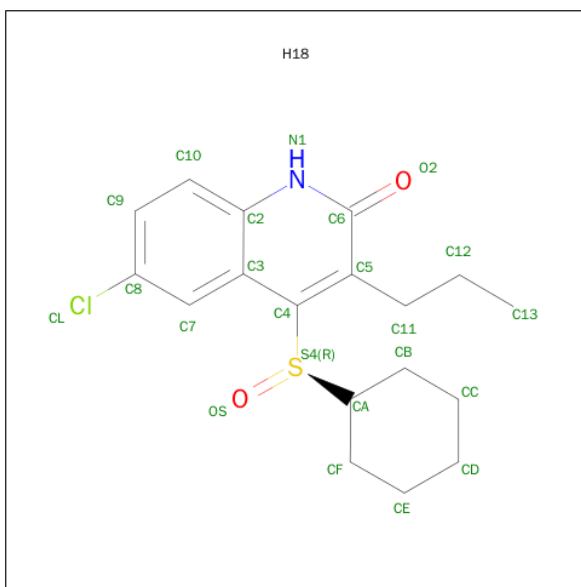
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3319	2168	546	598	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLSULFINYL)-3-PROPYLQUINOLIN-2(1H)-ONE (three-letter code: H18) (formula: C₁₈H₂₂ClNO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0
			23	18	1	1	2	1	0

V372	L228	L303	V372	V88	T165	L228	L303	V372	V88
T375	W229	A304	T375	GLU	K166	W229	A304	GLU	GLU
T376	M230	E305	T376	VAL	I167	M230	E305	VAL	VAL
T377	G231	N306	T377	GLN	L168	G231	N306	GLN	GLN
E378	E232	L310	E378	LEU	E169	E232	L310	LEU	LEU
S379	E233	V311	S379	GLY	P170	E233	V311	GLY	GLY
I380	L234	K311	I380	ILE	F171	L234	K311	ILE	ILE
	H235	E312		P95	A172	H235	E312	P95	P95
	P236	P313		H96	K173	P236	P313	H96	H96
W383	G237	G316	W383	P97	Q174	G237	G316	P97	P97
G384	K238	V317	G384	A98	N175	K238	V317	A98	A98
K385	W239	Y318	K385	G99	P176	W239	Y318	G99	G99
T386	T240	Y319	T386	L100	D177	T240	Y319	L100	L100
	V241	S322		K101	I178	V241	S322	K101	K101
F389	Q242	L325	F389	K102	Q182	Q242	L325	K102	K102
K390	P243	E328	K390	K104	Y183	P243	E328	K104	K104
	I244	I329		T107	M184	I244	I329	T107	T107
	D250	E328		V108	D185	D250	E328	V108	V108
G396	S251	I329	G396	L109	D186	S251	I329	L109	L109
W398	W252	K330	W398	G112	L187	W252	K330	G112	G112
E399	T253	K331	E399		Y188	T253	K331		
	V254	Q332		Y115	V189	V254	Q332	Y115	Y115
T400	G333	G333	T400	F116	G190	G333	G333	F116	F116
W401	Q334	Q334	W401	S117	S191	Q334	Q334	S117	S117
	G335	Q335		V118	D192	G335	Q335	V118	V118
Y405	Q336	Q336	Y405	P119	T195	Q336	Q336	P119	P119
	W337	W337		E122	G196	W337	W337	E122	E122
P413	T338	T338	P413	R125	Q197	T338	T338	R125	R125
W414	Y339	Y339	W414	T131	H198	Y339	Y339	T131	T131
E415	Q340	Q340	E415	I135	R199	Q340	Q340	I135	I135
F416	I341	I341	F416	N136	T200	I341	I341	N136	N136
V417	Y342	Y342	V417	E138	K201	Y342	Y342	E138	E138
N418	F346	F346	N418	T139	I202	F346	F346	T139	T139
T419	K347	K347	T419	P140	E203	K347	K347	P140	P140
P420	N348	N348	P420	B143	E204	N348	N348	B143	B143
L422	T351	T351	L422	Y144	L205	T351	T351	Y144	Y144
K424	G352	G352	K424	Q145	R206	G352	G352	Q145	Q145
L425	K353	K353	L425	Y146	Q207	K353	K353	Y146	Y146
W426	Y354	Y354	W426	P150	H208	Y354	Y354	P150	P150
Q428	A355	A355	Q428	Q151	L210	A355	A355	Q151	Q151
L429	K356	K356	L429	G152	R211	K356	K356	G152	G152
E430	MET	MET	E430	K154	W212	MET	MET	K154	K154
	ARG	ARG		P157	G213	ARG	ARG	P157	P157
LYS	GLY	GLY	LYS	F160	L214	GLY	GLY	F160	F160
GLU	ALA	ALA	GLU	S163	THR	ALA	ALA	S163	S163
PRO	HIS	HIS	PRO	M164	PRO	HIS	HIS	M164	M164
ILE	T362	T362	ILE		ASP	T362	T362		
VAL	N363	N363	VAL		ASP	N363	N363		
GLY	D364	D364	GLY		LYS	D364	D364		
ALA	V365	V365	ALA		LYS	V365	V365		
GLU	K366	K366	GLU		HIS	K366	K366		
THR	Q367	Q367	THR		GLN	Q367	Q367		
PHE	L368	L368	PHE		LYS	L368	L368		
	T369	T369			GLU	T369	T369		
	E370	E370			P226	E370	E370		
	A371	A371			F227	A371	A371		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.50 Å 115.30 Å 65.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.90 24.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.91-2.90) 99.3 (24.91-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.89 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.281 0.217 , 0.234	Depositor DCC
R_{free} test set	1135 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 88.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23552 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: H18, CSD, PO4

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	0/4352	0.72	0/5918
2	B	0.50	1/3415 (0.0%)	0.72	0/4639
All	All	0.51	1/7767 (0.0%)	0.72	0/10557

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TRP	CB-CG	5.12	1.59	1.50

There are no bond angle outliers.

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	4247	0	4274	309	0
2	B	3319	0	3341	210	0
3	A	15	0	0	1	0
4	A	23	0	22	5	0
All	All	7604	0	7637	497	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 33.

The worst 5 of 497 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:178:ILE:HD11	1:A:201:LYS:HG2	1.31	1.13
1:A:91:GLN:NE2	2:B:137:ASN:HB3	1.72	1.05
1:A:253:THR:HG22	1:A:255:ASN:H	1.17	1.02
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.43	1.00
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.44	0.99

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	510/560 (91%)	449 (88%)	45 (9%)	16 (3%)	5	21
2	B	390/440 (89%)	349 (90%)	34 (9%)	7 (2%)	11	37
All	All	900/1000 (90%)	798 (89%)	79 (9%)	23 (3%)	7	26

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	195	ILE
1	A	222	GLN
1	A	412	PRO
2	B	116	PHE

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	466/499 (93%)	433 (93%)	33 (7%)	18	47
2	B	365/400 (91%)	348 (95%)	17 (5%)	32	68
All	All	831/899 (92%)	781 (94%)	50 (6%)	24	57

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	443	ASP
2	B	303	LEU
1	A	340	GLN
1	A	356	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	487	GLN
2	B	278	GLN
1	A	475	GLN
1	A	480	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
1	CSD	A	280	1	3,7,8	0.69	0	3,8,10	5.06	1 (33%)

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
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	8.55	119.66	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
3	PO4	A	1300	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	A	1301	-	4,4,4	1.20	0	6,6,6	0.27	0
3	PO4	A	1302	-	4,4,4	1.06	0	6,6,6	0.27	0
4	H18	A	999	-	21,25,25	2.86	12 (57%)	25,35,35	2.98	8 (32%)

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
3	PO4	A	1300	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	H18	A	999	-	-	0/11/19/19	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H18	C8-CL	-2.56	1.68	1.74
4	A	999	H18	CB-CA	2.10	1.55	1.52
4	A	999	H18	CE-CF	2.21	1.59	1.53
4	A	999	H18	O2-C6	2.23	1.30	1.24
4	A	999	H18	C5-C4	2.55	1.44	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H18	C3-C2-N1	-3.71	120.06	123.45
4	A	999	H18	C12-C11-C5	-2.82	107.85	112.84
4	A	999	H18	CF-CA-CB	2.28	113.76	111.59
4	A	999	H18	CD-CE-CF	2.61	116.90	111.44
4	A	999	H18	OS-S4-C4	2.69	110.34	106.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	PO4	1	0
4	A	999	H18	5	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	A	516/560 (92%)	0.26	39 (7%)	17 11	28, 65, 110, 139	0
2	B	400/440 (90%)	0.17	36 (9%)	12 7	28, 60, 117, 148	0
All	All	916/1000 (91%)	0.22	75 (8%)	14 9	28, 64, 113, 148	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	334	GLN	8.1
2	B	214	LEU	6.3
1	A	138	GLU	5.2
2	B	421	PRO	5.2
1	A	116	PHE	5.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.94	0.17	-	51,55,65,74	0

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	H18	A	999	23/23	0.86	0.26	2.50	45,66,78,88	0
3	PO4	A	1301	5/5	0.87	0.23	0.78	123,124,129,131	0
3	PO4	A	1302	5/5	0.88	0.26	-0.28	150,150,150,150	0
3	PO4	A	1300	5/5	0.61	0.20	-0.39	137,140,144,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.