



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GRC
Title : CRYSTAL STRUCTURE OF GLYCINAMIDE RIBONUCLEOTIDE
TRANSFORMYLASE FROM ESCHERICHIA COLI AT 3.0 ANGSTROMS
RESOLUTION: A TARGET ENZYME FOR CHEMOTHERAPY
Authors : Chen, P.; Wilson, I.A.
Deposited on : 1992-07-21
Resolution : 3.00 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

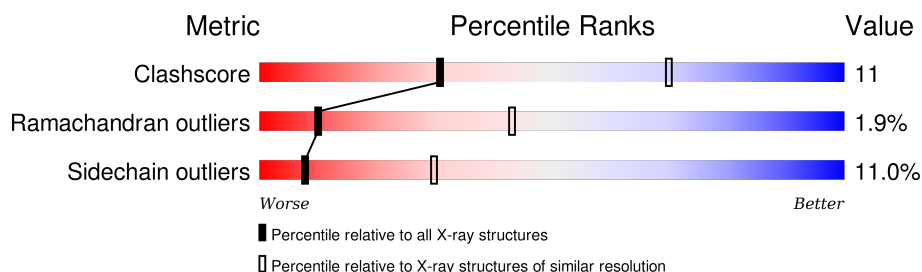
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2963 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 GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	1
			1487	943	262	277	5			
1	B	192	Total	C	N	O	S	0	0	1
			1466	932	258	271	5			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



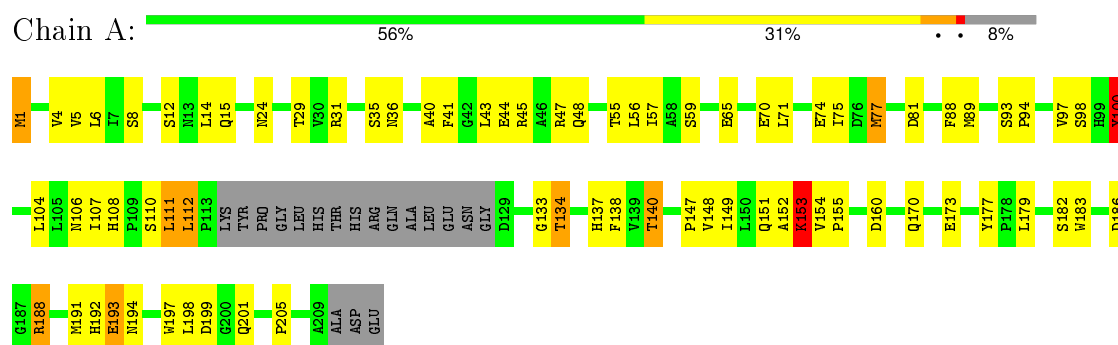
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

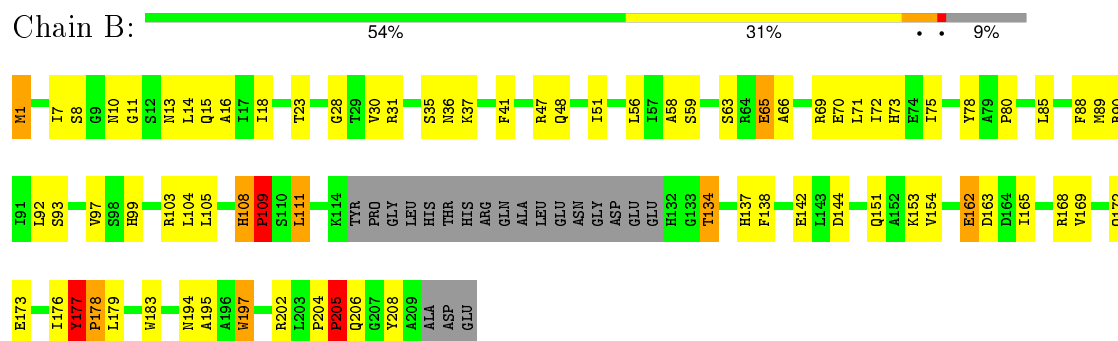
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE



• Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.50 Å 98.20 Å 103.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2963	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.96	1/1518 (0.1%)	1.67	18/2062 (0.9%)
1	B	0.98	0/1497	1.76	27/2035 (1.3%)
All	All	0.97	1/3015 (0.0%)	1.72	45/4097 (1.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	LEU	C-N	-5.88	1.23	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	47	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	177	TYR	CB-CG-CD2	-9.09	115.55	121.00
1	B	208	TYR	CB-CG-CD1	-8.75	115.75	121.00
1	B	1	MET	CG-SD-CE	8.14	113.23	100.20
1	B	47	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	A	197	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	B	197	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	197	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	197	TRP	CD1-CG-CD2	6.93	111.85	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	TRP	CD1-CG-CD2	6.91	111.83	106.30
1	A	100	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	B	103	ARG	CG-CD-NE	-6.61	97.93	111.80
1	A	89	MET	CA-CB-CG	6.56	124.46	113.30
1	A	183	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	B	183	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	B	168	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	23	THR	N-CA-CB	-6.33	98.27	110.30
1	A	31	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	153	LYS	CA-C-N	-6.12	103.73	117.20
1	A	188	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	140	THR	N-CA-CB	-6.05	98.81	110.30
1	A	183	TRP	CD1-CG-CD2	6.04	111.13	106.30
1	A	47	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	78	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	B	65	GLU	CA-C-N	-5.78	104.47	117.20
1	B	154	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	A	4	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	B	177	TYR	CB-CG-CD1	5.53	124.32	121.00
1	B	89	MET	CA-CB-CG	5.50	122.65	113.30
1	B	31	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	202	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	208	TYR	N-CA-C	-5.34	96.57	111.00
1	B	168	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	177	TYR	CA-CB-CG	5.23	123.34	113.40
1	B	108	HIS	CA-CB-CG	-5.20	104.75	113.60
1	B	109	PRO	N-CA-C	5.20	125.63	112.10
1	B	104	LEU	N-CA-C	-5.12	97.17	111.00
1	B	105	LEU	CB-CA-C	-5.11	100.50	110.20
1	A	77	MET	CA-CB-CG	5.10	121.96	113.30
1	A	153	LYS	CA-CB-CG	5.09	124.60	113.40
1	A	100	TYR	CD1-CG-CD2	5.08	123.48	117.90
1	A	24	ASN	CA-C-N	-5.05	106.10	117.20
1	B	205	PRO	N-CA-C	5.03	125.18	112.10
1	A	193	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain

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	1487	0	1466	29	0
1	B	1466	0	1454	36	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
All	All	2963	0	2920	64	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 (64) 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:134:THR:HG21	1:A:173:GLU:HG2	1.39	1.04
1:A:137:HIS:HA	1:A:149:ILE:HD12	1.74	0.69
1:B:134:THR:HG21	1:B:173:GLU:HG2	1.77	0.66
1:A:138:PHE:HB2	1:A:147:PRO:HG2	1.78	0.64
1:B:162:GLU:O	1:B:165:ILE:HB	1.98	0.64
1:A:148:VAL:HG11	1:A:151:GLN:HG3	1.80	0.63
1:A:108:HIS:O	1:A:134:THR:HG22	1.98	0.63
1:B:111:LEU:HD21	1:B:153:LYS:HG2	1.82	0.61
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.81	0.60
1:A:106:ASN:ND2	1:A:107:ILE:H	2.01	0.58
1:A:93:SER:O	1:A:97:VAL:HG23	2.02	0.58
1:A:70:GLU:O	1:A:74:GLU:HG3	2.04	0.57
1:B:195:ALA:HB3	1:B:197:TRP:HE1	1.69	0.56
1:A:71:LEU:O	1:A:75:ILE:HG13	2.06	0.56
1:A:15:GLN:OE1	1:A:45:ARG:HD3	2.06	0.55
1:B:111:LEU:HB3	1:B:151:GLN:NE2	2.23	0.54
1:B:8:SER:O	1:B:37:LYS:HD2	2.09	0.53
1:B:11:GLY:O	1:B:14:LEU:HB3	2.09	0.53
1:B:56:LEU:HD12	1:B:71:LEU:HD12	1.91	0.53
1:B:93:SER:O	1:B:97:VAL:HG23	2.10	0.52
1:B:15:GLN:O	1:B:18:ILE:HB	2.09	0.52
1:B:30:VAL:HB	1:B:51:ILE:HD13	1.92	0.52
1:B:7:ILE:O	1:B:35:SER:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:SER:O	1:A:55:THR:HA	2.11	0.51
1:B:65:GLU:O	1:B:69:ARG:HB2	2.11	0.50
1:A:36:ASN:HA	1:A:56:LEU:O	2.12	0.49
1:B:85:LEU:HG	1:B:88:PHE:HB3	1.94	0.49
1:B:70:GLU:O	1:B:73:HIS:HB3	2.13	0.49
1:B:13:ASN:O	1:B:16:ALA:HB3	2.13	0.48
1:B:176:ILE:O	1:B:179:LEU:HB3	2.13	0.48
1:B:162:GLU:HA	1:B:165:ILE:HD12	1.94	0.48
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.58	0.48
1:A:153:LYS:H	1:A:153:LYS:NZ	2.12	0.48
1:A:192:HIS:O	1:A:193:GLU:HG2	2.13	0.48
1:A:12:SER:O	1:A:15:GLN:HB3	2.13	0.48
1:B:75:ILE:HG22	1:B:80:PRO:HG2	1.96	0.48
1:A:133:GLY:HA3	1:A:152:ALA:O	2.14	0.48
1:B:165:ILE:O	1:B:169:VAL:HG23	2.16	0.46
1:A:188:ARG:O	1:A:198:LEU:HA	2.15	0.46
1:B:63:SER:O	1:B:66:ALA:HB3	2.14	0.46
1:B:197:TRP:CD1	1:B:197:TRP:N	2.83	0.46
1:A:77:MET:SD	1:B:70:GLU:OE1	2.74	0.45
1:B:108:HIS:HA	1:B:109:PRO:HD2	1.82	0.45
1:A:1:MET:SD	1:A:81:ASP:HB2	2.57	0.44
1:A:100:TYR:HB2	1:A:104:LEU:HD22	1.99	0.44
1:A:111:LEU:HB3	1:A:151:GLN:OE1	2.17	0.44
1:B:1:MET:HB3	1:B:28:GLY:HA3	1.99	0.44
1:A:5:VAL:HG12	1:A:6:LEU:N	2.32	0.43
1:B:137:HIS:CD2	1:B:138:PHE:O	2.72	0.43
1:A:6:LEU:HD12	1:A:6:LEU:N	2.34	0.42
1:A:41:PHE:O	1:A:44:GLU:HB3	2.19	0.42
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.49	0.42
1:A:154:VAL:HA	1:A:155:PRO:HD2	1.90	0.42
1:B:10:ASN:HA	1:B:41:PHE:HB3	2.01	0.42
1:B:72:ILE:HG23	1:B:99:HIS:CD2	2.55	0.42
1:B:30:VAL:HG12	1:B:51:ILE:HG21	2.01	0.42
1:A:8:SER:OG	1:A:88:PHE:HA	2.20	0.42
1:B:142:GLU:HG3	1:B:194:ASN:ND2	2.34	0.42
1:B:92:LEU:HD23	1:B:97:VAL:HG22	2.01	0.41
1:A:40:ALA:O	1:A:43:LEU:HB2	2.21	0.41
1:A:138:PHE:CD2	1:A:149:ILE:HD11	2.56	0.41
1:A:106:ASN:ND2	1:A:107:ILE:N	2.68	0.40
1:B:172:GLN:O	1:B:176:ILE:HG12	2.21	0.40
1:B:36:ASN:HD22	1:B:88:PHE:HE1	1.65	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	190/212 (90%)	176 (93%)	11 (6%)	3 (2%)	12	48
1	B	188/212 (89%)	174 (93%)	10 (5%)	4 (2%)	9	40
All	All	378/424 (89%)	350 (93%)	21 (6%)	7 (2%)	10	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	PRO
1	B	205	PRO
1	B	162	GLU
1	A	112	LEU
1	B	58	ALA
1	A	94	PRO
1	A	205	PRO

5.3.2 Protein sidechains [i](#)

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	155/171 (91%)	132 (85%)	23 (15%)	4	17
1	B	153/171 (90%)	142 (93%)	11 (7%)	18	53
All	All	308/342 (90%)	274 (89%)	34 (11%)	8	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	LEU
1	A	29	THR
1	A	48	GLN
1	A	57	ILE
1	A	59	SER
1	A	65	GLU
1	A	98	SER
1	A	110	SER
1	A	111	LEU
1	A	134	THR
1	A	140	THR
1	A	153	LYS
1	A	160	ASP
1	A	170	GLN
1	A	177	TYR
1	A	179	LEU
1	A	182	SER
1	A	186	ASP
1	A	191	MET
1	A	194	ASN
1	A	199	ASP
1	A	201	GLN
1	B	48	GLN
1	B	59	SER
1	B	111	LEU
1	B	134	THR
1	B	144	ASP
1	B	163	ASP
1	B	177	TYR
1	B	178	PRO
1	B	204	PRO
1	B	205	PRO
1	B	206	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	108	HIS
1	A	174	HIS

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Mol	Chain	Res	Type
1	A	206	GLN
1	B	106	ASN
1	B	137	HIS
1	B	194	ASN
1	B	206	GLN

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](#)

2 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	$\# Z > 2$
2	PO4	A	301	-	4,4,4	2.09	2 (50%)	6,6,6	0.45	0
2	PO4	B	301	-	4,4,4	1.79	1 (25%)	6,6,6	0.40	0

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	PO4	A	301	-	-	0/0/0/0	0/0/0/0
2	PO4	B	301	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PO4	P-O1	2.11	1.61	1.52
2	B	301	PO4	P-O4	2.76	1.63	1.53
2	A	301	PO4	P-O4	2.99	1.64	1.53

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.