



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2020 – 01:55 PM BST

PDB ID : 2UZP  
Title : Crystal structure of the C2 domain of human protein kinase C gamma.  
Authors : Pike, A.C.W.; Amos, A.; Johansson, C.; Sobott, F.; Savitsky, P.; Berridge, G.; Fedorov, O.; Umeano, C.; Gorrec, F.; Bunkoczi, G.; Debreczeni, J.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Weigelt, J.; Sundstrom, M.; Knapp, S.  
Deposited on : 2007-04-30  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.3.dev2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.3.dev2

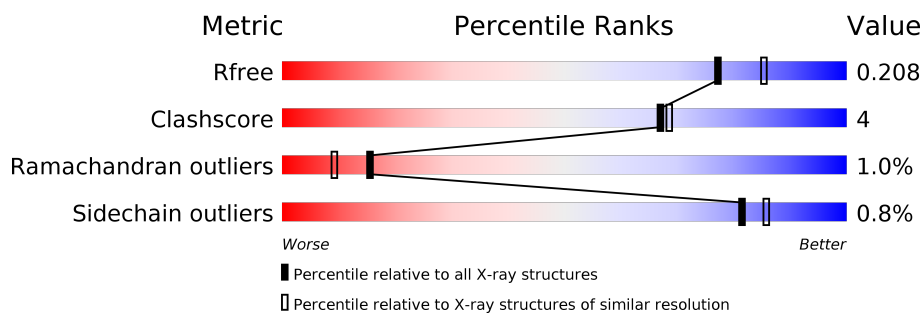
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	144	90% 6% ..
1	B	144	94% 5% .
1	C	144	95% ..

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4078 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 PROTEIN KINASE C GAMMA TYPE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	8	0
			1203	757	216	226	4			
1	B	142	Total	C	N	O	S	0	3	0
			1139	722	200	213	4			
1	C	142	Total	C	N	O	S	0	2	0
			1143	725	200	214	4			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			21	9	1	9	2		
2	B	1	Total	C	N	O	P	0	1
			21	9	1	9	2		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

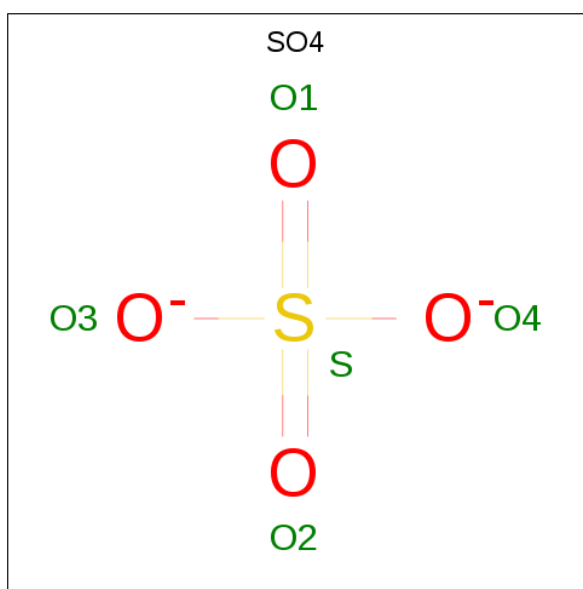
- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		
3	A	1	Total	Co	0	0
			1	1		
3	C	1	Total	Co	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Ca	0	0
			3	3		
4	A	3	Total	Ca	0	0
			3	3		
4	C	3	Total	Ca	0	0
			3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	145	Total	O	0	0
			145	145		
7	B	115	Total	O	0	0
			115	115		
7	C	132	Total	O	0	0
			132	132		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: PROTEIN KINASE C GAMMA TYPE

Chain A:  90% 6% ..



- Molecule 1: PROTEIN KINASE C GAMMA TYPE

Chain B:  94% 5% ..



- Molecule 1: PROTEIN KINASE C GAMMA TYPE

Chain C:  95% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50 Å   138.50 Å   68.36 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.00 48.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 100.0 (48.97-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.171   ,   0.205 0.173   ,   0.208	Depositor DCC
$R_{free}$ test set	2294 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CO, PLP, CA, EDO, DSN, SO4

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	0.59	2/1239 (0.2%)	0.84	6/1684 (0.4%)
1	B	0.49	0/1173	0.61	0/1597
1	C	0.48	0/1173	0.63	0/1595
All	All	0.53	2/3585 (0.1%)	0.70	6/4876 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207[A]	LEU	CB-CG	6.65	1.71	1.52
1	A	207[B]	LEU	CB-CG	6.65	1.71	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207[A]	LEU	CB-CG-CD2	-8.91	95.85	111.00
1	A	207[B]	LEU	CB-CG-CD2	-8.91	95.85	111.00
1	A	207[A]	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	A	207[B]	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	A	207[A]	LEU	CA-CB-CG	-7.36	98.38	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202[B]	PRO	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	1203	0	1189	24	0
1	B	1139	0	1114	3	0
1	C	1143	0	1123	2	0
2	A	21	0	4	0	0
2	B	21	0	4	0	0
2	C	15	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
5	A	30	0	0	0	0
5	B	35	0	0	0	0
5	C	35	0	0	0	0
6	A	8	0	12	0	0
6	B	8	0	12	0	0
6	C	16	0	24	0	0
7	A	145	0	0	0	0
7	B	115	0	0	0	0
7	C	132	0	0	0	0
All	All	4078	0	3488	28	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 4.

The worst 5 of 28 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:205[A]:ARG:HB3	1:A:207[A]:LEU:HD11	1.26	1.14
1:A:205[A]:ARG:CB	1:A:207[A]:LEU:HD11	1.80	1.10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HG22	1:A:203[B]:ASP:HB3	1.50	0.92
1:A:205[A]:ARG:HB2	1:A:207[A]:LEU:HD11	1.68	0.74
1:A:203[B]:ASP:N	1:A:204[B]:PRO:HD2	2.11	0.66

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	148/144 (103%)	139 (94%)	6 (4%)	3 (2%)	7	3
1	B	143/144 (99%)	140 (98%)	2 (1%)	1 (1%)	22	16
1	C	142/144 (99%)	138 (97%)	3 (2%)	1 (1%)	22	16
All	All	433/432 (100%)	417 (96%)	11 (2%)	5 (1%)	15	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	B	0	MET
1	C	0	MET
1	A	203[A]	ASP
1	A	203[B]	ASP

### 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	133/127 (105%)	132 (99%)	1 (1%)	81	86
1	B	123/127 (97%)	122 (99%)	1 (1%)	81	86
1	C	124/127 (98%)	123 (99%)	1 (1%)	81	86
All	All	380/381 (100%)	377 (99%)	3 (1%)	81	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	B	154	HIS
1	C	154	HIS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 12 are monoatomic - leaving 33 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$
6	EDO	B	1307	-	3,3,3	0.41	0	2,2,2	0.40	0
6	EDO	C	1309	-	3,3,3	0.52	0	2,2,2	0.24	0
2	PLP	A	1294[B]	-	15,15,16	1.14	2 (13%)	20,22,23	1.25	3 (15%)
5	SO4	C	1305	-	4,4,4	0.07	0	6,6,6	0.40	0
5	SO4	C	1301	-	4,4,4	0.17	0	6,6,6	0.28	0
6	EDO	B	1306	-	3,3,3	0.44	0	2,2,2	0.12	0
2	PLP	A	1294[A]	-	15,15,16	1.12	2 (13%)	20,22,23	1.21	3 (15%)
5	SO4	A	1299	4	4,4,4	0.25	0	6,6,6	0.40	0
5	SO4	C	1302	-	4,4,4	0.18	0	6,6,6	0.58	0
6	EDO	C	1308	-	3,3,3	0.38	0	2,2,2	0.48	0
5	SO4	B	1302	-	4,4,4	0.22	0	6,6,6	0.25	0
2	PLP	B	1294[A]	-	15,15,16	1.15	2 (13%)	20,22,23	1.04	0
5	SO4	C	1303	-	4,4,4	0.13	0	6,6,6	0.20	0
2	PLP	B	1294[B]	-	15,15,16	1.17	2 (13%)	20,22,23	1.12	0
5	SO4	C	1300	-	4,4,4	0.12	0	6,6,6	0.40	0
5	SO4	A	1303	-	4,4,4	0.11	0	6,6,6	0.55	0
5	SO4	C	1304	-	4,4,4	0.17	0	6,6,6	0.50	0
6	EDO	A	1305	-	3,3,3	0.35	0	2,2,2	0.43	0
5	SO4	B	1303	-	4,4,4	0.18	0	6,6,6	0.47	0
5	SO4	B	1300	-	4,4,4	0.11	0	6,6,6	0.36	0
5	SO4	B	1299	4	4,4,4	0.25	0	6,6,6	0.69	0
5	SO4	B	1301	-	4,4,4	0.28	0	6,6,6	0.37	0
5	SO4	B	1305	-	4,4,4	0.28	0	6,6,6	0.67	0
5	SO4	A	1300	-	4,4,4	0.16	0	6,6,6	0.19	0
2	PLP	C	1294	1,3	15,15,16	1.00	2 (13%)	20,22,23	1.10	1 (5%)
5	SO4	A	1301	-	4,4,4	0.20	0	6,6,6	0.83	0
6	EDO	A	1306	-	3,3,3	0.54	0	2,2,2	0.06	0
5	SO4	C	1299	4	4,4,4	0.29	0	6,6,6	0.59	0
5	SO4	A	1302	-	4,4,4	0.19	0	6,6,6	0.36	0
6	EDO	C	1307	-	3,3,3	0.60	0	2,2,2	0.08	0
5	SO4	B	1304	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	A	1304	-	4,4,4	0.20	0	6,6,6	0.41	0
6	EDO	C	1306	-	3,3,3	0.45	0	2,2,2	0.08	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
6	EDO	C	1308	-	-	0/1/1/1	-
6	EDO	B	1307	-	-	1/1/1/1	-
6	EDO	C	1309	-	-	1/1/1/1	-
6	EDO	C	1307	-	-	0/1/1/1	-
2	PLP	A	1294[B]	-	-	3/6/6/8	0/1/1/1
2	PLP	B	1294[B]	-	-	3/6/6/8	0/1/1/1
6	EDO	B	1306	-	-	0/1/1/1	-
2	PLP	A	1294[A]	-	-	2/6/6/8	0/1/1/1
6	EDO	A	1305	-	-	1/1/1/1	-
2	PLP	B	1294[A]	-	-	0/6/6/8	0/1/1/1
2	PLP	C	1294	1,3	-	0/6/6/8	0/1/1/1
6	EDO	C	1306	-	-	0/1/1/1	-
6	EDO	A	1306	-	-	1/1/1/1	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1294[B]	PLP	C2-N1	2.88	1.39	1.33
2	A	1294[A]	PLP	C2-N1	2.88	1.39	1.33
2	C	1294	PLP	C2-N1	2.24	1.38	1.33
2	A	1294[B]	PLP	C6-N1	2.16	1.39	1.34
2	A	1294[A]	PLP	C6-N1	2.16	1.39	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1294[B]	PLP	C2A-C2-C3	2.44	123.91	120.89
2	A	1294[A]	PLP	C2A-C2-C3	2.44	123.91	120.89
2	A	1294[B]	PLP	O3-C3-C2	2.31	122.52	117.49
2	A	1294[A]	PLP	O3-C3-C2	2.31	122.52	117.49
2	C	1294	PLP	C5-C6-N1	-2.20	120.16	123.82

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1294[B]	PLP	C5A-O4P-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1294[B]	PLP	C5A-O4P-P-O3P
2	A	1294[A]	PLP	C4-C5-C5A-O4P
2	B	1294[B]	PLP	C5A-O4P-P-O1P
2	B	1294[B]	PLP	C5A-O4P-P-O2P

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.