



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 11:58 am BST

PDB ID : 1GXB
Title : ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE IN COMPLEX
WITH PYROPHOSPHATE AND MAGNESIUM
Authors : Mayans, O.; Ivens, A.; Nissen, L.J.; Kirschner, K.; Wilmanns, M.
Deposited on : 2002-04-02
Resolution : 2.65 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

<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 : 2.11
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) : 2.11

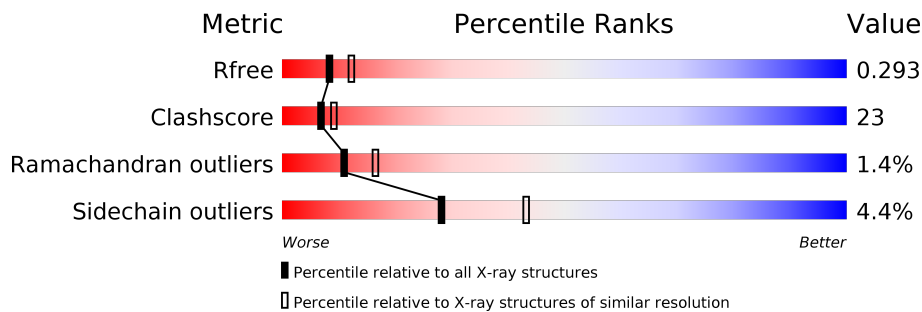
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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 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	345	63% (green), 32% (yellow), 5% (orange), 0% (red), 0% (grey)
1	B	345	58% (green), 35% (yellow), 5% (orange), 0% (red), 0% (grey)
1	C	345	55% (green), 39% (yellow), 5% (orange), 0% (red), 0% (grey)
1	D	345	60% (green), 37% (yellow), 3% (orange), 0% (red), 0% (grey)

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
3	POP	D	1349	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10753 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.

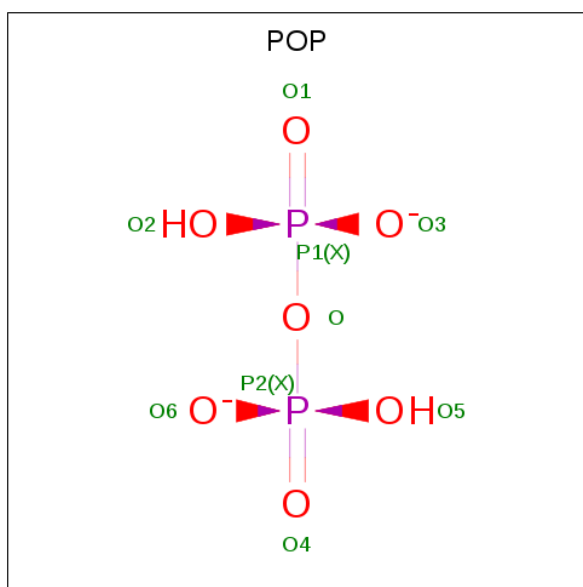
- Molecule 1 is a protein called ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	Total 2609	C 1674	N 440	O 488	S 7	0	0	1
1	B	340	Total 2611	C 1675	N 440	O 489	S 7	0	0	1
1	C	341	Total 2619	C 1679	N 441	O 492	S 7	0	0	0
1	D	345	Total 2642	C 1691	N 445	O 499	S 7	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0
3	D	1	Total O P 9 7 2	0	0

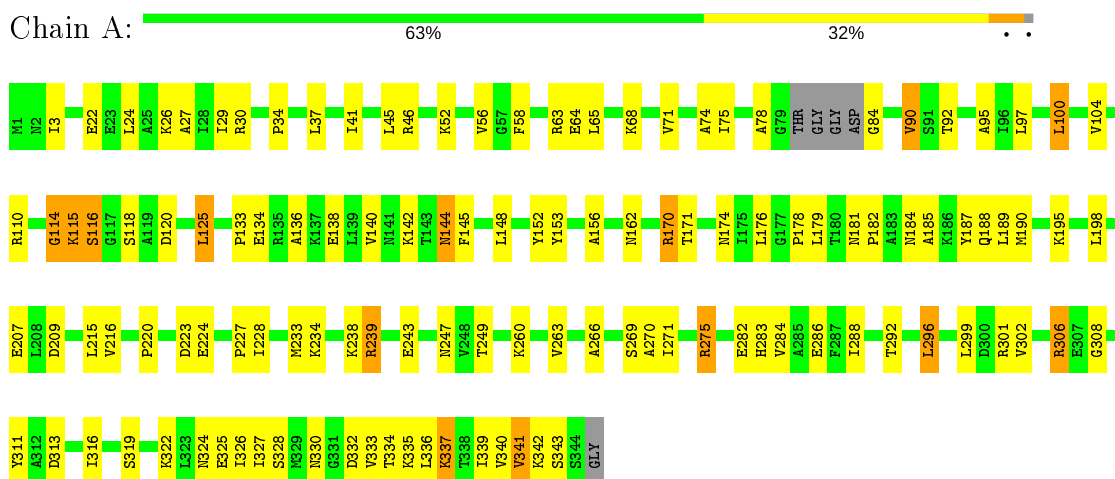
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	B	56	Total O 56 56	0	0
4	C	66	Total O 66 66	0	0
4	D	50	Total O 50 50	0	0

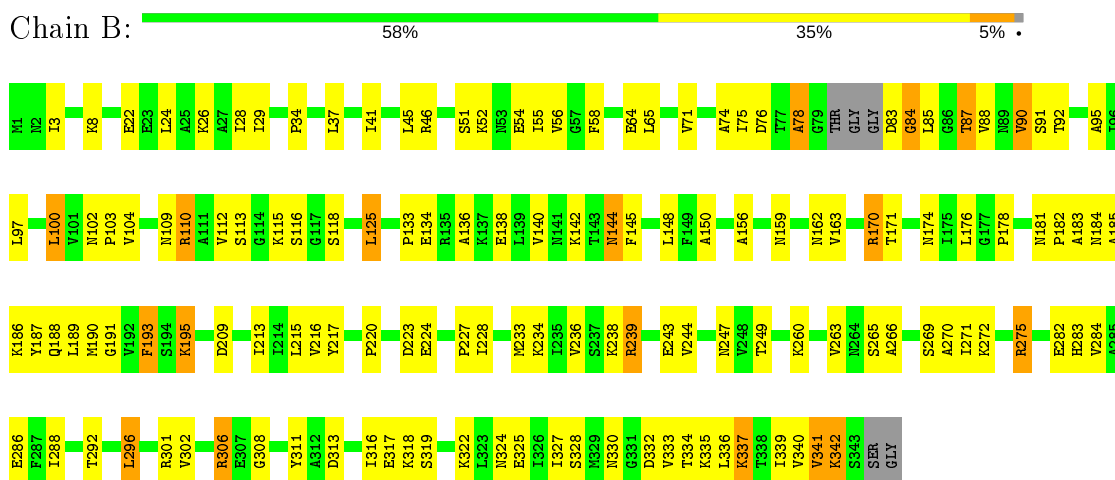
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

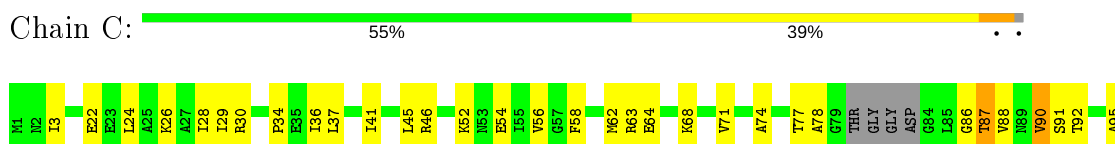
- Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

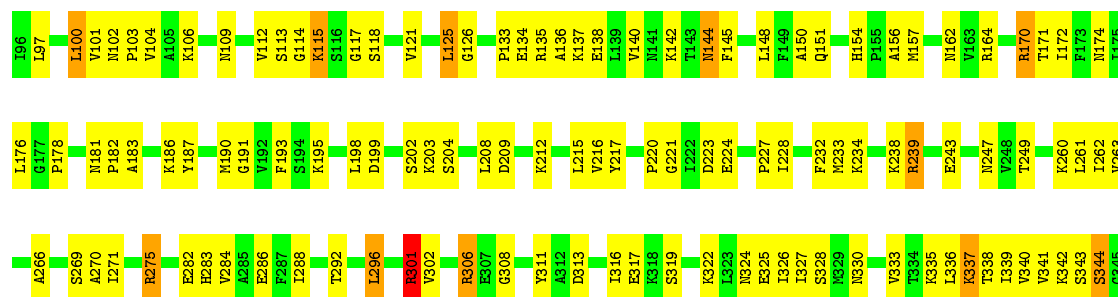


- Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE



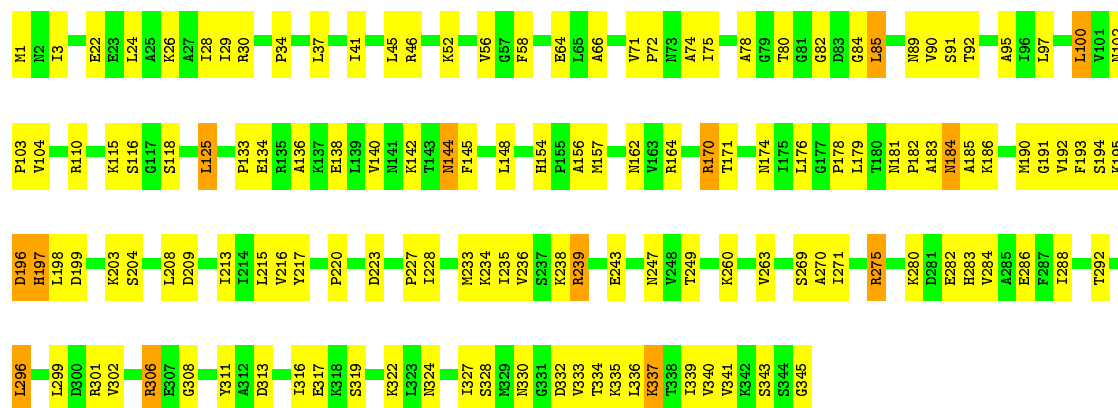
- Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE





● Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

Chain D: 60% 37%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.84Å 65.47Å 115.37Å 90.00° 107.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.69 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.0 (19.69-2.63)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.63Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.297 0.282 , 0.293	Depositor DCC
R_{free} test set	1158 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtrriage
Anisotropy	0.280	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2807e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP

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	0.40	0/2645	0.97	11/3573 (0.3%)
1	B	0.38	0/2647	0.83	10/3576 (0.3%)
1	C	0.40	0/2655	0.99	11/3584 (0.3%)
1	D	0.36	0/2679	0.82	10/3618 (0.3%)
All	All	0.39	0/10626	0.91	42/14351 (0.3%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	ARG	NE-CZ-NH1	-23.00	108.80	120.30
1	C	301	ARG	NE-CZ-NH2	20.39	130.49	120.30
1	A	306	ARG	NE-CZ-NH2	19.56	130.08	120.30
1	A	306	ARG	NE-CZ-NH1	-19.42	110.59	120.30
1	A	275	ARG	NE-CZ-NH1	-15.11	112.75	120.30

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	2609	0	2725	109	0
1	B	2611	0	2725	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2619	0	2734	127	0
1	D	2642	0	2752	130	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	2	0
3	C	9	0	0	1	0
3	D	9	0	0	4	0
4	A	61	0	0	11	0
4	B	56	0	0	14	0
4	C	66	0	0	19	0
4	D	50	0	0	23	0
All	All	10753	0	10936	496	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 23.

The worst 5 of 496 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:C:109:ASN:HD22	1:C:150:ALA:HB3	1.10	1.12
1:A:78:ALA:HB2	1:A:188:GLN:OE1	1.62	0.98
1:D:280:LYS:HE3	1:D:345:GLY:H	1.32	0.93
1:A:178:PRO:HB2	1:A:190:MET:HE2	1.48	0.93
1:C:171:THR:H	1:C:174:ASN:ND2	1.67	0.92

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	336/345 (97%)	311 (93%)	20 (6%)	5 (2%)	10	15
1	B	336/345 (97%)	311 (93%)	21 (6%)	4 (1%)	13	19
1	C	337/345 (98%)	309 (92%)	23 (7%)	5 (2%)	10	15
1	D	343/345 (99%)	313 (91%)	25 (7%)	5 (2%)	10	15
All	All	1352/1380 (98%)	1244 (92%)	89 (7%)	19 (1%)	11	16

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	341	VAL
1	B	78	ALA
1	B	341	VAL
1	C	344	SER

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	285/289 (99%)	274 (96%)	11 (4%)	32	48
1	B	285/289 (99%)	270 (95%)	15 (5%)	22	35
1	C	286/289 (99%)	274 (96%)	12 (4%)	30	45
1	D	288/289 (100%)	276 (96%)	12 (4%)	30	45
All	All	1144/1156 (99%)	1094 (96%)	50 (4%)	28	43

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

Mol	Chain	Res	Type
1	B	306	ARG
1	C	90	VAL
1	D	296	LEU
1	B	311	TYR
1	B	342	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	283	HIS
1	C	162	ASN
1	D	247	ASN
1	C	109	ASN
1	C	174	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
3	POP	D	1349	2	6,8,8	1.56	2 (33%)	13,13,13	1.04	1 (7%)
3	POP	C	1348	2	6,8,8	0.97	0	13,13,13	1.07	0
3	POP	B	1347	-	6,8,8	1.25	1 (16%)	13,13,13	1.01	1 (7%)
3	POP	A	1346	2	6,8,8	1.37	1 (16%)	13,13,13	1.20	1 (7%)

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	POP	D	1349	2	-	0/6/6/6	-
3	POP	C	1348	2	-	0/6/6/6	-
3	POP	B	1347	-	-	0/6/6/6	-
3	POP	A	1346	2	-	2/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1346	POP	P1-O1	3.06	1.60	1.50
3	D	1349	POP	P1-O1	2.78	1.59	1.50
3	B	1347	POP	P1-O3	2.13	1.63	1.54
3	D	1349	POP	P1-O3	2.01	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1349	POP	P2-O-P1	-2.27	125.03	132.83
3	B	1347	POP	P2-O-P1	-2.21	125.25	132.83
3	A	1346	POP	O2-P1-O	2.04	111.46	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1346	POP	P1-O-P2-O5
3	A	1346	POP	P1-O-P2-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1349	POP	4	0
3	C	1348	POP	1	0
3	B	1347	POP	2	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

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.