



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

PDB ID : 1P43  
Title : REVERSE PROTONATION IS THE KEY TO GENERAL ACID-BASE CATALYSIS IN ENOLASE  
Authors : Sims, P.A.; Larsen, T.M.; Poyner, R.R.; Cleland, W.W.; Reed, G.H.  
Deposited on : 2003-04-21  
Resolution : 1.80 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](mailto: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.

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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 : 1.7 (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

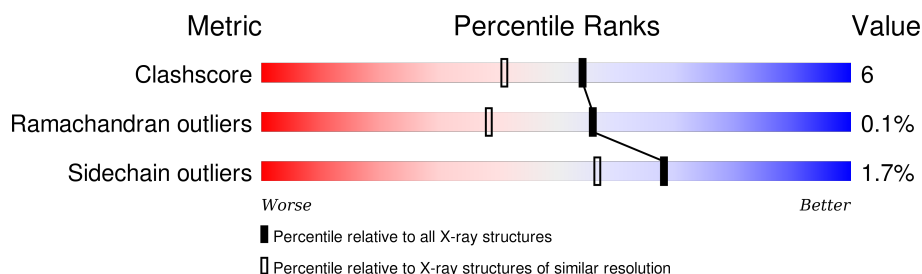
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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. 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	436	 85% 15%
1	B	436	 85% 14% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7475 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 Enolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3291	2079	571	635	6			
1	B	436	Total	C	N	O	S	0	0	0
			3291	2079	571	635	6			

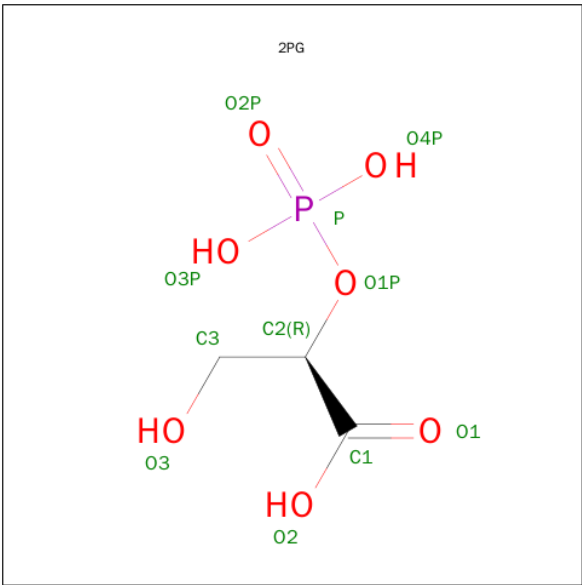
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLN	GLU	ENGINEERED	UNP P00924
B	668	GLN	GLU	ENGINEERED	UNP P00924

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



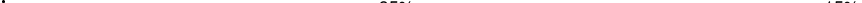
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	3	7	1		
3	B	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	402	Total	O	0	0
			402	402		
4	B	465	Total	O	0	0
			465	465		

**i**

Note EDS was not executed.

- Chain A:  85% 15%
- | Residue | Chain A | Chain B | Chain C | Chain D |
|---------|---------|---------|---------|---------|
| A1      | ✓       |         |         |         |
| V2      | ✓       |         |         |         |
| A7      | ✓       |         |         |         |
| R14     | ✓       |         |         |         |
| L23     | ✓       |         |         |         |
| G37     | ✓       |         |         |         |
| L46     | ✓       |         |         |         |
| V68     | ✓       |         |         |         |
| D97     | ✓       |         |         |         |
| N101    | ✓       |         |         |         |
| K102    | ✓       |         |         |         |
| S103    | ✓       |         |         |         |
| K104    | ✓       |         |         |         |
| I110    | ✓       |         |         |         |
| V127    | ✓       |         |         |         |
| P128    | ✓       |         |         |         |
| K131    | ✓       |         |         |         |
| K140    | ✓       |         |         |         |
| T141    | ✓       |         |         |         |
| S142    | ✓       |         |         |         |
| P143    | ✓       |         |         |         |
| L146    | ✓       |         |         |         |
| P147    | ✓       |         |         |         |
| N152    | ✓       |         |         |         |
| L164    | ✓       |         |         |         |
| Q168    | ✓       |         |         |         |
| F169    | ✓       |         |         |         |
| H191    | ✓       |         |         |         |
| L196    | ✓       |         |         |         |
| S204    | ✓       |         |         |         |
| A205    | ✓       |         |         |         |
| G206    | ✓       |         |         |         |
| N207    | ✓       |         |         |         |
| P216    | ✓       |         |         |         |
| I228    | ✓       |         |         |         |
| D246    | ✓       |         |         |         |
| S270    | ✓       |         |         |         |
| F252    | ✓       |         |         |         |
| F253    | ✓       |         |         |         |
| G256    | ✓       |         |         |         |
| K263    | ✓       |         |         |         |
| R288    | ✓       |         |         |         |
| E295    | ✓       |         |         |         |
| D296    | ✓       |         |         |         |
| P297    | ✓       |         |         |         |
| W306    | ✓       |         |         |         |
| T325    | ✓       |         |         |         |
| I330    | ✓       |         |         |         |
| I334    | ✓       |         |         |         |
| K337    | ✓       |         |         |         |
| L344    | ✓       |         |         |         |
| N347    | ✓       |         |         |         |
| Q348    | ✓       |         |         |         |
| I349    | ✓       |         |         |         |
| G350    | ✓       |         |         |         |
| E354    | ✓       |         |         |         |
| K357    | ✓       |         |         |         |
| D361    | ✓       |         |         |         |
| S362    | ✓       |         |         |         |
| W367    | ✓       |         |         |         |
| H373    | ✓       |         |         |         |
| K374    | ✓       |         |         |         |
| S375    | ✓       |         |         |         |
| T392    | ✓       |         |         |         |
| A401    | ✓       |         |         |         |
| R402    | ✓       |         |         |         |
| S403    | ✓       |         |         |         |
| E405    | ✓       |         |         |         |
| R405    | ✓       |         |         |         |
| A423    | ✓       |         |         |         |
| L436    | ✓       |         |         |         |

- Chain B:
- 
- 85% 14%
- A501 S784 L785 M786 K787 Y788 Y789 E795 D796 F797 F798 A799 E800 D801 D802 I803 I806 I815 D820 V824 R829 K836 K837 L843 N847 M870 H873 T892 K896 T897 G898 A899 P900 A901 R902 S903 E904 R905 L936 A507 B514 B543 V568 A573 P574 I580 L593 I601 A602 S603 I610 I626 K640 T641 S642 L651 I652 R659 A660 Q668 P669 M670 L693 A705 T706 I707 P716 I717 I718 L725 D726 I727 I728 V729 K733 D746 V752

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.30 Å   115.10 Å   72.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.185 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: MG, 2PG

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	0.30	0/3351	0.57	0/4534
1	B	0.31	0/3351	0.59	0/4534
All	All	0.30	0/6702	0.58	0/9068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3291	0	3303	45	0
1	B	3291	0	3300	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	4	0	0
3	B	11	0	4	0	0
4	A	402	0	0	6	0
4	B	465	0	0	2	1
All	All	7475	0	6611	85	1

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 6.

All (85) 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:B:705:ALA:HB1	1:B:716:PRO:HB3	1.69	0.75
1:B:799:ALA:HB3	1:B:802:ASP:HB2	1.73	0.69
1:B:543:HIS:HE1	1:B:801:ASP:OD2	1.80	0.64
1:B:640:LYS:HE2	1:B:642:SER:O	2.01	0.61
1:A:128:PRO:HD2	1:A:131:LYS:HE2	1.83	0.60
1:B:669:PHE:HB3	1:B:728:ILE:HD11	1.84	0.60
1:A:204:SER:HB3	4:A:1354:HOH:O	2.04	0.56
1:B:784:SER:HA	1:B:787:LYS:HE2	1.87	0.56
1:A:191:HIS:HD2	4:A:1318:HOH:O	1.88	0.55
1:A:7:ALA:HB2	1:A:68:VAL:HG11	1.88	0.55
1:B:668:GLN:HB2	1:B:746:ASP:HB3	1.89	0.54
1:B:796:ASP:OD2	1:B:820:ASP:HB3	2.08	0.54
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.89	0.53
1:A:169:PHE:HB3	1:A:228:ILE:HD11	1.90	0.53
1:A:101:ASN:ND2	1:A:103:SER:HB3	2.23	0.53
1:B:803:TRP:HB3	1:B:836:LYS:HD3	1.90	0.53
1:B:901:ALA:O	1:B:902:ARG:HB2	2.09	0.52
1:B:507:ALA:HB2	1:B:568:VAL:HG11	1.90	0.52
1:A:101:ASN:HD21	1:A:103:SER:HB3	1.74	0.52
1:A:191:HIS:HE1	1:B:514:ARG:O	1.93	0.52
1:A:401:ALA:O	1:A:402:ARG:HB2	2.10	0.52
1:A:127:VAL:HB	1:A:131:LYS:HE3	1.93	0.51
1:B:786:MET:HE1	1:B:815:ILE:HG12	1.93	0.51
1:A:168:GLN:HB2	1:A:246:ASP:HB3	1.93	0.50
1:A:164:LEU:HD21	1:A:169:PHE:CE2	2.46	0.50
1:B:746:ASP:HA	1:B:795:GLU:HB3	1.93	0.50
1:B:593:LEU:HB3	1:B:610:ILE:HG23	1.93	0.50
1:B:659:HIS:O	1:B:660:ALA:HB2	2.11	0.50
1:A:349:ILE:HG12	1:A:354:GLU:HB3	1.94	0.50
1:A:14:ARG:HH12	1:A:375:SER:HB2	1.78	0.49
1:A:404:GLU:HB3	1:B:903:SER:HB2	1.94	0.49
1:A:249:SER:HA	1:A:252:PHE:CE2	2.48	0.48
1:B:670:MET:SD	1:B:896:LYS:HD2	2.53	0.48
1:B:763:LYS:HB2	4:B:1762:HOH:O	2.12	0.48
1:A:337:LYS:HE2	4:A:1731:HOH:O	2.14	0.48
1:A:263:LYS:HB2	4:A:1313:HOH:O	2.13	0.48
1:B:693:LEU:CD1	1:B:727:LEU:HD22	2.44	0.48
1:A:97:ASP:OD2	1:A:102:LYS:HA	2.14	0.47
1:B:729:VAL:CG1	1:B:733:LYS:HE3	2.44	0.47
1:A:362:SER:O	1:A:367:TRP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG22	1:A:23:LEU:HD21	1.97	0.47
1:B:837:LYS:HD3	4:B:1828:HOH:O	2.14	0.47
1:B:784:SER:O	1:B:787:LYS:HG2	2.15	0.47
1:B:652:ASN:O	1:B:899:ALA:HB2	2.15	0.47
1:B:693:LEU:HD12	1:B:727:LEU:HD22	1.96	0.46
1:B:797:PRO:HD2	1:B:806:TRP:CH2	2.50	0.46
1:A:288:ARG:HD2	4:A:1536:HOH:O	2.15	0.46
1:A:253:PHE:CZ	1:A:256:GLY:HA2	2.51	0.46
1:B:669:PHE:HB3	1:B:728:ILE:CD1	2.45	0.46
1:A:14:ARG:HH12	1:A:375:SER:CB	2.28	0.45
1:B:904:GLU:HG2	1:B:905:ARG:NE	2.32	0.45
1:B:601:ASN:ND2	1:B:603:SER:HB3	2.32	0.44
1:A:102:LYS:HE2	1:A:350:GLY:HA3	1.99	0.44
1:A:357:LYS:HE2	1:A:361:ASP:OD1	2.17	0.44
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.53	0.44
1:B:651:LEU:O	1:B:670:MET:HA	2.18	0.43
1:A:146:LEU:CD2	1:A:423:ALA:HB1	2.48	0.43
1:A:37:GLY:HA3	1:A:374:ARG:NH2	2.34	0.43
1:A:373:HIS:CD2	1:A:373:HIS:H	2.36	0.43
1:B:725:LEU:HD13	1:B:789:TYR:CD2	2.52	0.43
1:A:97:ASP:OD1	1:A:104:LYS:HB3	2.18	0.43
1:A:196:LEU:HD21	4:A:1615:HOH:O	2.19	0.42
1:B:899:ALA:HB1	1:B:900:PRO:HD2	2.01	0.42
1:B:716:PRO:HG2	1:B:718:ILE:HG13	2.00	0.42
1:B:870:MET:SD	1:B:896:LYS:HB2	2.59	0.42
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.53	0.42
1:A:373:HIS:ND1	1:A:405:ARG:NH1	2.67	0.42
1:B:873:HIS:H	1:B:873:HIS:CD2	2.38	0.42
1:B:824:VAL:HG22	1:B:829:ARG:HD3	2.00	0.42
1:A:97:ASP:HB2	1:A:110:ILE:HD11	2.00	0.42
1:B:601:ASN:HD21	1:B:603:SER:HB3	1.84	0.42
1:A:404:GLU:HB3	1:B:903:SER:CB	2.50	0.41
1:A:344:LEU:HD23	1:A:344:LEU:C	2.40	0.41
1:A:46:LEU:HD23	1:A:103:SER:HA	2.01	0.41
1:A:207:ASN:HB3	1:B:707:ASN:HB3	2.02	0.41
1:B:901:ALA:O	1:B:902:ARG:CB	2.69	0.41
1:B:795:GLU:OE2	1:B:843:LEU:HD22	2.21	0.41
1:A:205:ALA:HB1	1:A:216:PRO:HB3	2.03	0.41
1:A:325:THR:O	1:A:325:THR:HG22	2.21	0.41
1:A:140:LYS:HE2	1:A:142:SER:O	2.21	0.41
1:B:573:ALA:N	1:B:574:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:HIS:CG	1:B:897:THR:HA	2.56	0.40
1:B:652:ASN:HA	1:B:670:MET:HG2	2.04	0.40
1:A:330:ILE:O	1:A:334:ILE:HG13	2.21	0.40
1:A:207:ASN:HB3	1:B:707:ASN:CB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1847:HOH:O	4:B:1847:HOH:O[2_565]	1.21	0.99

## 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	434/436 (100%)	424 (98%)	10 (2%)	0	100	100
1	B	434/436 (100%)	421 (97%)	12 (3%)	1 (0%)	52	35
All	All	868/872 (100%)	845 (97%)	22 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	902	ARG

### 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	344/344 (100%)	338 (98%)	6 (2%)	68	57
1	B	344/344 (100%)	338 (98%)	6 (2%)	68	57
All	All	688/688 (100%)	676 (98%)	12 (2%)	68	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	147	PRO
1	A	152	ASN
1	A	347	ASN
1	A	373	HIS
1	A	392	THR
1	B	580	ASN
1	B	626	ASN
1	B	727	LEU
1	B	847	ASN
1	B	873	HIS
1	B	892	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	152	ASN
1	A	191	HIS
1	B	516	ASN
1	B	543	HIS
1	B	580	ASN
1	B	626	ASN
1	B	652	ASN
1	B	659	HIS
1	B	717	ASN
1	B	922	ASN

### 5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	2PG	A	441	2	6,10,10	1.88	2 (33%)	5,14,14	0.97	0
3	2PG	B	941	2	6,10,10	2.02	2 (33%)	5,14,14	1.07	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
3	2PG	A	441	2	-	0/7/11/11	0/0/0/0
3	2PG	B	941	2	-	0/7/11/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	441	2PG	P-O1P	2.29	1.66	1.60
3	B	941	2PG	P-O1P	2.54	1.67	1.60
3	A	441	2PG	C3-C2	3.61	1.59	1.52
3	B	941	2PG	C3-C2	3.97	1.60	1.52

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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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