



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P77  
Title : CRYSTAL STRUCTURE OF SHIKIMATE DEHYDROGENASE (AROE)  
FROM HAEMOPHILUS INFLUENZAE  
Authors : Ye, S.; von Delft, F.; Brooun, A.; Knuth, M.W.; Swanson, R.V.; McRee, D.E.  
Deposited on : 2003-04-30  
Resolution : 1.95 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

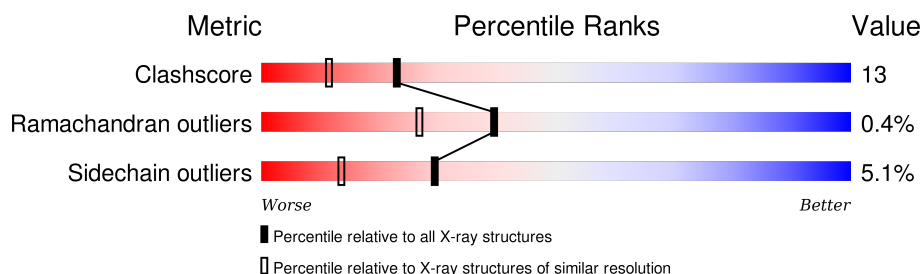
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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	272	

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	ATR	A	300	X	-	X	-

## 2 Entry composition [i](#)

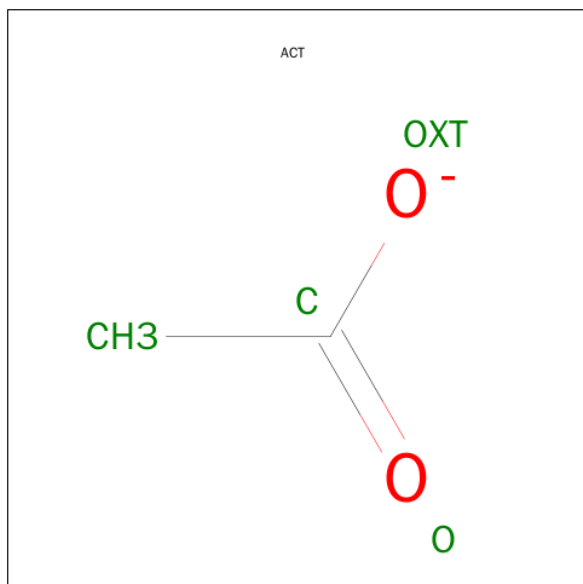
There are 4 unique types of molecules in this entry. The entry contains 2347 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Shikimate 5-dehydrogenase.

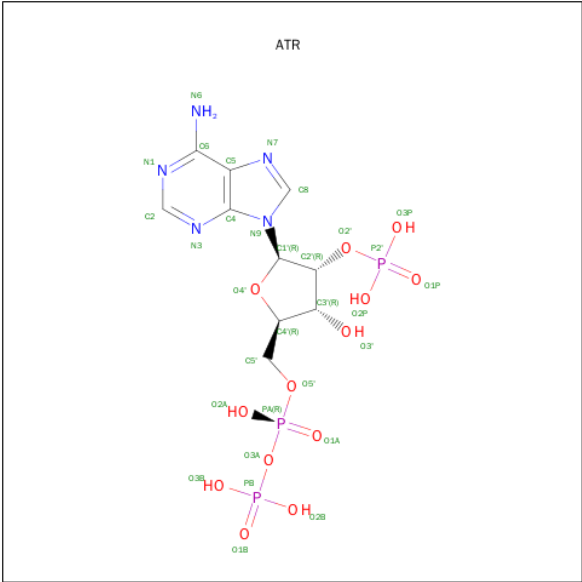
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2055	1312	345	388	10	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 3 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (three-letter code: ATR) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is water.

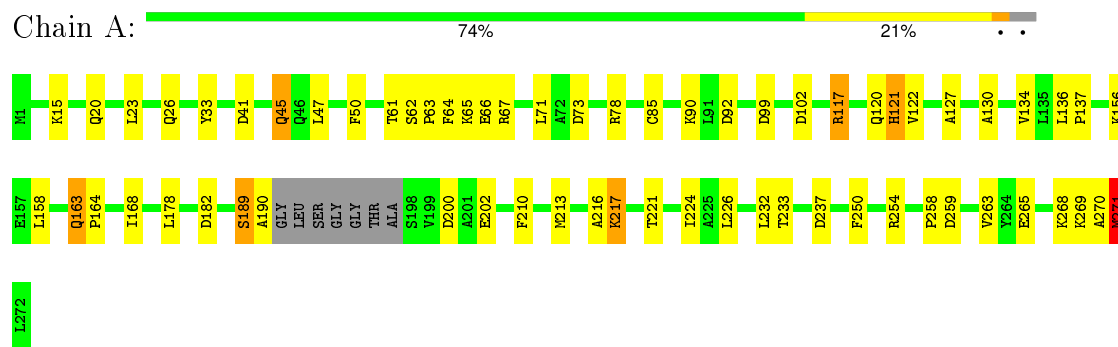
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	257	Total	O	0	0
			257	257		

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

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 ( $\text{RSRZ} > 2$ ). 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: Shikimate 5-dehydrogenase



## 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, $\alpha$ , $\beta$ , $\gamma$	84.05Å 82.73Å 82.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	100.0 (20.00-1.95)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.203 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	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: ATR, ACT

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	0.70	2/2093 (0.1%)	1.01	17/2833 (0.6%)

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	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	C-O	-6.58	1.10	1.23
1	A	122	VAL	C-O	-5.56	1.12	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	A	237	ASP	CB-CG-OD2	8.02	125.51	118.30
1	A	189	SER	C-N-CA	7.20	139.71	121.70
1	A	99	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	254	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	270	ALA	C-N-CA	6.29	137.43	121.70
1	A	73	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	271	MET	N-CA-CB	5.87	121.16	110.60
1	A	182	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	102	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	271	MET	CA-CB-CG	5.68	122.95	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	254	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	41	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	121	HIS	ND1-CE1-NE2	-5.33	98.17	109.90
1	A	121	HIS	CG-ND1-CE1	-5.25	98.87	105.70
1	A	200	ASP	CB-CG-OD2	5.23	123.01	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	271	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	HIS	Sidechain
1	A	189	SER	Mainchain

## 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	2055	0	2059	56	0
2	A	4	0	3	0	0
3	A	31	0	11	9	0
4	A	257	0	0	10	1
All	All	2347	0	2073	56	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 13.

All (56) 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:163:GLN:HE22	1:A:168:ILE:HG23	1.27	0.99
1:A:190:ALA:HA	3:A:300:ATR:C5	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB2	3:A:300:ATR:C4	1.96	0.96
1:A:92:ASP:O	4:A:369:HOH:O	1.91	0.87
1:A:163:GLN:NE2	1:A:168:ILE:HG23	1.92	0.83
1:A:66:GLU:HG3	4:A:558:HOH:O	1.82	0.79
1:A:163:GLN:HE21	1:A:163:GLN:HA	1.49	0.76
1:A:226:LEU:HD23	1:A:226:LEU:C	2.06	0.76
1:A:163:GLN:NE2	1:A:168:ILE:CG2	2.51	0.74
1:A:190:ALA:CA	3:A:300:ATR:C5	2.66	0.73
1:A:130:ALA:HB1	1:A:213:MET:HE1	1.70	0.73
1:A:265:GLU:OE2	4:A:325:HOH:O	2.08	0.72
1:A:190:ALA:HA	3:A:300:ATR:N7	2.05	0.71
1:A:130:ALA:HB1	1:A:213:MET:CE	2.21	0.70
1:A:190:ALA:CB	3:A:300:ATR:C5	2.69	0.70
1:A:163:GLN:HE22	1:A:168:ILE:CG2	2.02	0.70
1:A:156:LYS:HD3	1:A:156:LYS:O	1.92	0.70
1:A:23:LEU:HD23	1:A:263:VAL:HG21	1.77	0.66
1:A:117:ARG:H	1:A:117:ARG:HD3	1.60	0.65
1:A:210:PHE:CZ	1:A:232:LEU:HD13	2.32	0.64
1:A:117:ARG:O	1:A:120:GLN:HG3	1.98	0.63
1:A:26:GLN:NE2	1:A:263:VAL:HG23	2.12	0.63
1:A:190:ALA:C	4:A:456:HOH:O	2.38	0.61
1:A:163:GLN:NE2	4:A:309:HOH:O	2.35	0.59
1:A:190:ALA:HB2	3:A:300:ATR:C5	2.32	0.58
1:A:90:LYS:NZ	4:A:556:HOH:O	2.38	0.56
1:A:190:ALA:HB2	3:A:300:ATR:N3	2.21	0.56
1:A:226:LEU:C	1:A:226:LEU:CD2	2.74	0.55
1:A:20:GLN:HG3	1:A:33:TYR:CE1	2.42	0.55
1:A:190:ALA:CB	3:A:300:ATR:C4	2.76	0.54
1:A:226:LEU:O	1:A:226:LEU:HD23	2.08	0.54
1:A:190:ALA:O	4:A:456:HOH:O	2.19	0.53
1:A:163:GLN:N	1:A:164:PRO:CD	2.73	0.52
1:A:45:GLN:HE21	1:A:45:GLN:H	1.57	0.52
1:A:47:LEU:O	1:A:50:PHE:HB3	2.11	0.51
1:A:45:GLN:H	1:A:45:GLN:NE2	2.09	0.51
1:A:127:ALA:HB1	1:A:158:LEU:HD12	1.92	0.51
1:A:163:GLN:NE2	1:A:163:GLN:HA	2.24	0.49
1:A:47:LEU:HD23	1:A:71:LEU:HD12	1.95	0.49
1:A:26:GLN:NE2	1:A:263:VAL:CG2	2.76	0.49
1:A:26:GLN:HE22	1:A:263:VAL:HG23	1.77	0.48
1:A:217:LYS:HD2	1:A:217:LYS:C	2.34	0.48
1:A:221:THR:OG1	1:A:224:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HD3	4:A:464:HOH:O	2.14	0.46
1:A:117:ARG:N	1:A:117:ARG:HD3	2.30	0.46
1:A:202:GLU:OE2	4:A:357:HOH:O	2.21	0.45
1:A:61:THR:HA	1:A:65:LYS:HE3	1.98	0.44
1:A:216:ALA:HA	4:A:548:HOH:O	2.19	0.43
1:A:190:ALA:HA	3:A:300:ATR:C6	2.48	0.43
1:A:15:LYS:HA	1:A:15:LYS:HE2	2.01	0.42
1:A:63:PRO:HD2	1:A:64:PHE:CE1	2.55	0.42
1:A:163:GLN:NE2	1:A:168:ILE:HG22	2.31	0.41
1:A:134:VAL:O	1:A:137:PRO:HD2	2.19	0.41
1:A:210:PHE:N	1:A:210:PHE:CD2	2.88	0.41
1:A:136:LEU:HB3	1:A:137:PRO:HD3	2.03	0.41
1:A:250:PHE:CD1	1:A:258:PRO:HG3	2.57	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:A:411:HOH:O	4:A:416:HOH:O[4_555]	2.12	0.08

## 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	261/272 (96%)	253 (97%)	7 (3%)	1 (0%)	39 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	MET

### 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	217/220 (99%)	206 (95%)	11 (5%)	29	13

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	62	SER
1	A	85	CYS
1	A	117	ARG
1	A	163	GLN
1	A	178	LEU
1	A	217	LYS
1	A	233	THR
1	A	268	LYS
1	A	269	LYS
1	A	271	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	70	GLN
1	A	114	ASN
1	A	140	GLN
1	A	163	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
3	ATR	A	300	-	26,33,33	1.92	5 (19%)	34,52,52	2.60	9 (26%)
2	ACT	A	301	-	1,3,3	0.21	0	0,3,3	0.00	-

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	ATR	A	300	-	1/1/7/7	1/17/37/37	0/3/3/3
2	ACT	A	301	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	ATR	C5-C4	2.09	1.45	1.40
3	A	300	ATR	P2'-O2P	3.72	1.68	1.54
3	A	300	ATR	PA-O2A	3.88	1.71	1.54
3	A	300	ATR	P2'-O3P	4.13	1.69	1.54
3	A	300	ATR	PB-O1B	5.56	1.69	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	ATR	C1'-N9-C4	-7.30	115.93	126.94
3	A	300	ATR	N3-C2-N1	-7.17	123.40	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	ATR	O3'-C3'-C2'	-5.64	94.87	111.16
3	A	300	ATR	PA-O3A-PB	-2.94	122.81	132.67
3	A	300	ATR	O2B-PB-O1B	-2.37	102.94	110.58
3	A	300	ATR	C3'-C2'-C1'	2.11	106.80	102.73
3	A	300	ATR	P2'-O2'-C2'	3.46	129.87	121.56
3	A	300	ATR	O4'-C1'-N9	4.15	116.80	108.10
3	A	300	ATR	O2'-C2'-C3'	4.16	127.70	111.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	300	ATR	C2'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	ATR	P2'-O2'-C2'-C3'

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	ATR	9	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 ⓘ

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.