



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BUT  
Title : CRYSTAL STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE  
FROM ACINETOBACTER SP. ADP1 MUTANT R457S - APO  
Authors : Vetting, M.W.; Valley, M.P.; D'Argenio, D.A.; Ornston, L.N.; Lipscomb, J.D.;  
Ohlendorf, D.H.  
Deposited on : 2005-06-17  
Resolution : 1.85 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

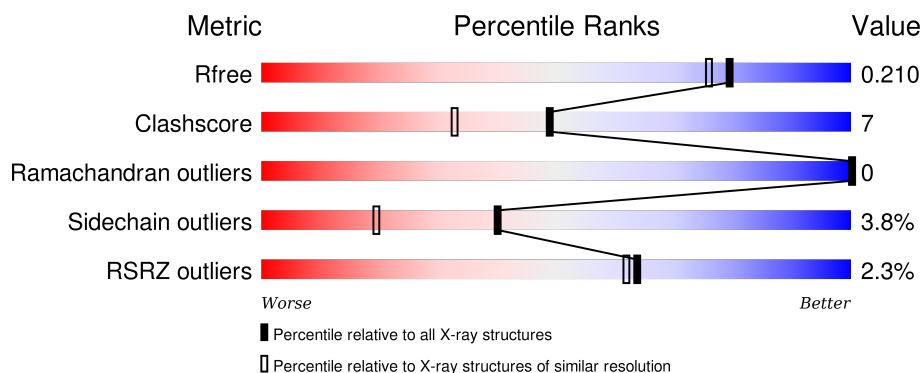
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.85 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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.

Mol	Chain	Length	Quality of chain
1	A	209	
2	B	241	

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
4	OH	B	1542	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3742 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 PROTOCATECHUATE 3,4-DIOXYGENASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	0	0	0
			1602	1010	285	307			

- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1921	1221	342	353	5			

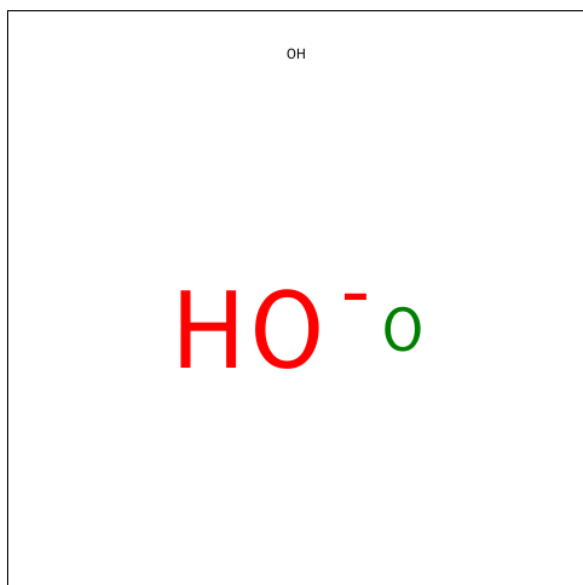
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	457	SER	ARG	ENGINEERED MUTATION	UNP P20372

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0

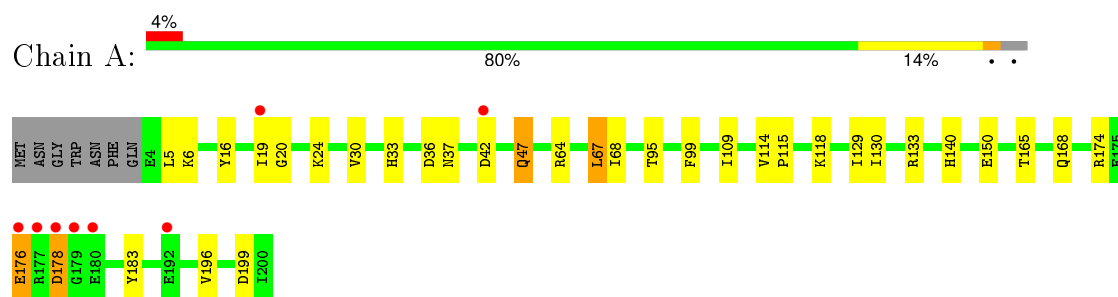
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	82	Total O 82 82	0	0
5	B	135	Total O 135 135	0	0

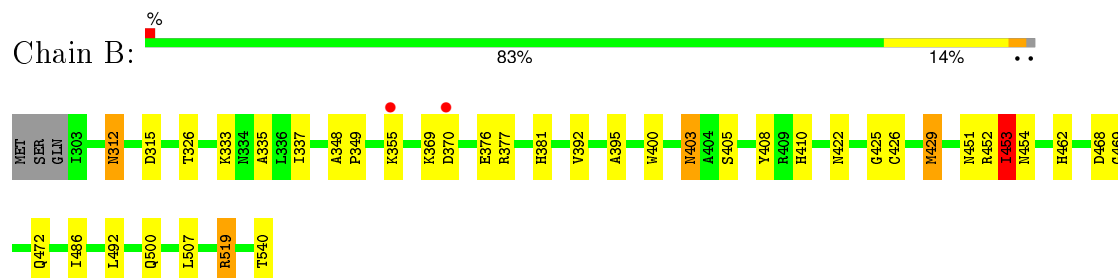
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE ALPHA CHAIN



#### • Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE BETA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.87Å 144.87Å 144.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 45.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.85) 99.5 (45.81-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 1.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.174 , 0.215 0.172 , 0.210	Depositor DCC
$R_{free}$ test set	2162 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
Estimated twinning fraction	0.048 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 42886 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FE, OH

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	1.02	4/1638 (0.2%)	0.98	2/2223 (0.1%)
2	B	0.99	2/1976 (0.1%)	1.02	7/2685 (0.3%)
All	All	1.00	6/3614 (0.2%)	1.00	9/4908 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	CG-CD	12.44	1.70	1.51
2	B	426	CYS	CB-SG	-7.67	1.69	1.82
1	A	176	GLU	CB-CG	7.46	1.66	1.52
1	A	176	GLU	CD-OE2	6.41	1.32	1.25
2	B	335	ALA	CA-CB	5.41	1.63	1.52
1	A	176	GLU	CD-OE1	5.01	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453	ILE	CB-CA-C	-7.01	97.58	111.60
2	B	429	MET	CB-CA-C	-6.45	97.50	110.40
2	B	519	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	B	451	ASN	N-CA-C	-6.16	94.36	111.00
1	A	36	ASP	CB-CG-OD1	6.02	123.72	118.30
2	B	452	ARG	N-CA-C	-5.93	94.98	111.00
1	A	199	ASP	N-CA-C	-5.20	96.97	111.00
2	B	377	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	B	453	ILE	CG1-CB-CG2	5.01	122.43	111.40

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	1602	0	1548	27	0
2	B	1921	0	1849	30	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	82	0	0	4	0
5	B	135	0	0	0	1
All	All	3742	0	3397	50	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 7.

All (50) 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:68:ILE:HD12	1:A:130:ILE:HD13	1.29	1.12
2:B:369:LYS:H	2:B:422:ASN:HD22	1.19	0.89
1:A:68:ILE:CD1	1:A:130:ILE:HD13	2.08	0.83
1:A:133:ARG:HG2	2:B:326:THR:HG21	1.68	0.76
2:B:369:LYS:H	2:B:422:ASN:ND2	1.84	0.74
1:A:20:GLY:HA3	2:B:400:TRP:HB3	1.74	0.69
2:B:469:GLY:H	2:B:472:GLN:HE21	1.40	0.68
1:A:150:GLU:HG2	5:A:2062:HOH:O	1.94	0.67
1:A:5:LEU:N	1:A:5:LEU:HD12	2.13	0.63
2:B:507:LEU:HD22	2:B:507:LEU:N	2.14	0.62
1:A:24:LYS:HG2	5:A:2012:HOH:O	2.02	0.60
1:A:196:VAL:HG13	2:B:337:ILE:HD12	1.85	0.58
2:B:403:ASN:HD22	2:B:403:ASN:C	2.07	0.57
1:A:20:GLY:CA	2:B:400:TRP:HB3	2.35	0.56
1:A:5:LEU:H	1:A:5:LEU:HD12	1.71	0.55
2:B:453:ILE:HD12	2:B:454:ASN:N	2.22	0.54
2:B:376:GLU:OE1	2:B:519:ARG:NH2	2.40	0.54
2:B:486:ILE:HG23	2:B:492:LEU:CD2	2.39	0.53
1:A:6:LYS:NZ	5:A:2003:HOH:O	2.41	0.52
2:B:468:ASP:H	2:B:472:GLN:HE22	1.58	0.51
2:B:312:ASN:C	2:B:312:ASN:HD22	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:ASP:H	2:B:422:ASN:HD21	1.59	0.49
1:A:129:ILE:HD12	1:A:140:HIS:CE1	2.47	0.49
2:B:469:GLY:H	2:B:472:GLN:NE2	2.09	0.49
1:A:118:LYS:HE3	5:A:2050:HOH:O	2.13	0.49
1:A:178:ASP:OD1	1:A:178:ASP:N	2.43	0.48
1:A:68:ILE:CD1	1:A:130:ILE:CD1	2.89	0.47
2:B:403:ASN:ND2	2:B:405:SER:H	2.13	0.47
1:A:67:LEU:O	1:A:68:ILE:HD13	2.16	0.45
1:A:174:ARG:HB2	1:A:183:TYR:CE1	2.52	0.44
1:A:33:HIS:CD2	2:B:355:LYS:HD3	2.52	0.44
2:B:400:TRP:HA	2:B:425:GLY:O	2.16	0.44
1:A:19:ILE:HD11	2:B:408:TYR:HB3	1.99	0.44
2:B:403:ASN:HD21	2:B:405:SER:HB2	1.83	0.44
1:A:37:ASN:HB3	1:A:95:THR:HB	1.99	0.44
2:B:315:ASP:HB3	2:B:500:GLN:NE2	2.33	0.43
1:A:16:TYR:HD1	2:B:410:HIS:CG	2.36	0.43
1:A:165:THR:O	1:A:168:GLN:HG2	2.18	0.43
2:B:453:ILE:HD12	2:B:454:ASN:H	1.84	0.43
2:B:403:ASN:ND2	2:B:403:ASN:C	2.71	0.42
2:B:392:VAL:HG12	2:B:395:ALA:HB2	2.00	0.42
1:A:64:ARG:HD2	1:A:99:PHE:O	2.19	0.42
2:B:507:LEU:CD2	2:B:507:LEU:N	2.82	0.42
1:A:67:LEU:C	1:A:68:ILE:HD13	2.41	0.41
1:A:68:ILE:HD12	1:A:130:ILE:CD1	2.21	0.41
2:B:468:ASP:H	2:B:472:GLN:NE2	2.18	0.41
1:A:114:VAL:HG13	1:A:115:PRO:HD2	2.02	0.41
2:B:400:TRP:CE2	2:B:462:HIS:CB	3.04	0.40
2:B:348:ALA:HB1	2:B:349:PRO:HD2	2.04	0.40
1:A:47:GLN:HB2	1:A:47:GLN:HE21	1.67	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)
5:B:2057:HOH:O	5:B:2057:HOH:O[2_555]	0.70	1.50

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	200/209 (96%)	195 (98%)	5 (2%)	0	100	100
2	B	236/241 (98%)	226 (96%)	10 (4%)	0	100	100
All	All	436/450 (97%)	421 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	169/175 (97%)	162 (96%)	7 (4%)	37	17
2	B	201/204 (98%)	194 (96%)	7 (4%)	43	23
All	All	370/379 (98%)	356 (96%)	14 (4%)	40	19

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	42	ASP
1	A	47	GLN
1	A	67	LEU
1	A	109	ILE
1	A	176	GLU
1	A	178	ASP
2	B	312	ASN

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Mol	Chain	Res	Type
2	B	333	LYS
2	B	381	HIS
2	B	403	ASN
2	B	429	MET
2	B	453	ILE
2	B	540	THR

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	38	ASN
1	A	47	GLN
1	A	72	GLN
2	B	312	ASN
2	B	403	ASN
2	B	412	ASN
2	B	422	ASN
2	B	472	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic and 1 is modelled with single atom - leaving 0 for Mogul analysis.

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.

## 5.7 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	202/209 (96%)	-0.11	8 (3%) 42 39	16, 26, 44, 64	0
2	B	238/241 (98%)	-0.34	2 (0%) 87 87	15, 20, 38, 47	0
All	All	440/450 (97%)	-0.23	10 (2%) 64 62	15, 22, 43, 64	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ASP	4.3
2	B	370	ASP	4.1
1	A	179	GLY	3.6
1	A	42	ASP	3.3
1	A	19	ILE	2.9
1	A	177	ARG	2.7
1	A	192	GLU	2.6
1	A	180	GLU	2.2
2	B	355	LYS	2.1
1	A	176	GLU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OH	B	1542	1/1	1.00	0.11	2.09	25,25,25,25	0
3	FE	B	1541	1/1	1.00	0.06	-	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.