



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:33 PM GMT

PDB ID : 1XRT  
Title : The Crystal Structure of a Novel, Latent Dihydroorotase from Aquifex Aeolicus at 1.7 Å Resolution  
Authors : Martin, P.D.; Purcarea, C.; Zhang, P.; Vaishnav, A.; Sadecki, S.; Guy-Evans, H.I.; Evans, D.R.; Edwards, B.F.  
Deposited on : 2004-10-15  
Resolution : 1.61 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  
<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

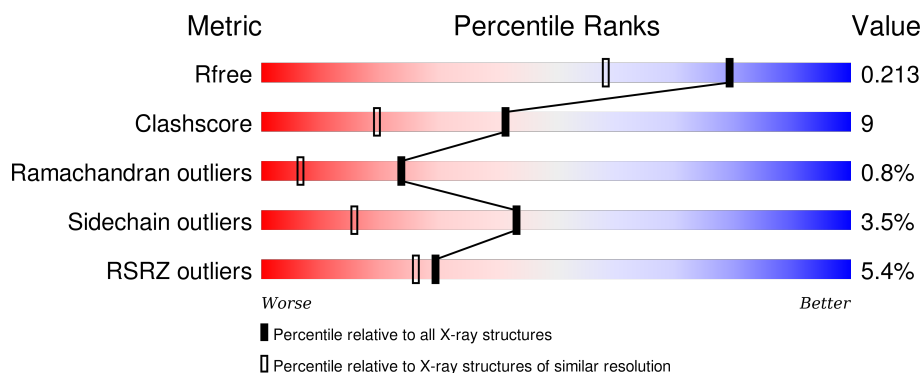
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.61 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	467	<div> <div>5%</div> <div>67%</div> <div>10%</div> <div>21%</div> </div>
1	B	467	<div> <div>4%</div> <div>66%</div> <div>12%</div> <div>21%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6940 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 Dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2849	1815	482	537	15			
1	B	369	Total	C	N	O	S	0	0	0
			2850	1818	483	534	15			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	CLONING ARTIFACT	UNP O66990
A	-43	ARG	-	CLONING ARTIFACT	UNP O66990
A	-42	PHE	-	CLONING ARTIFACT	UNP O66990
A	-41	TRP	-	CLONING ARTIFACT	UNP O66990
A	-40	GLN	-	CLONING ARTIFACT	UNP O66990
A	-39	TYR	-	CLONING ARTIFACT	UNP O66990
A	-38	ILE	-	CLONING ARTIFACT	UNP O66990
A	-37	ASN	-	CLONING ARTIFACT	UNP O66990
A	-36	GLY	-	CLONING ARTIFACT	UNP O66990
A	-35	VAL	-	CLONING ARTIFACT	UNP O66990
A	-34	ASP	-	CLONING ARTIFACT	UNP O66990
A	-33	MET	-	CLONING ARTIFACT	UNP O66990
A	-32	ARG	-	CLONING ARTIFACT	UNP O66990
A	-31	GLY	-	CLONING ARTIFACT	UNP O66990
A	-30	SER	-	CLONING ARTIFACT	UNP O66990
A	-29	HIS	-	CLONING ARTIFACT	UNP O66990
A	-28	HIS	-	CLONING ARTIFACT	UNP O66990
A	-27	HIS	-	CLONING ARTIFACT	UNP O66990
A	-26	HIS	-	CLONING ARTIFACT	UNP O66990
A	-25	HIS	-	CLONING ARTIFACT	UNP O66990
A	-24	HIS	-	CLONING ARTIFACT	UNP O66990
A	-23	GLY	-	CLONING ARTIFACT	UNP O66990
A	-22	MET	-	CLONING ARTIFACT	UNP O66990
A	-21	ALA	-	CLONING ARTIFACT	UNP O66990
A	-20	SER	-	CLONING ARTIFACT	UNP O66990

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP O66990
A	-18	THR	-	CLONING ARTIFACT	UNP O66990
A	-17	GLY	-	CLONING ARTIFACT	UNP O66990
A	-16	GLY	-	CLONING ARTIFACT	UNP O66990
A	-15	GLN	-	CLONING ARTIFACT	UNP O66990
A	-14	GLN	-	CLONING ARTIFACT	UNP O66990
A	-13	MET	-	CLONING ARTIFACT	UNP O66990
A	-12	GLY	-	CLONING ARTIFACT	UNP O66990
A	-11	ARG	-	CLONING ARTIFACT	UNP O66990
A	-10	ASP	-	CLONING ARTIFACT	UNP O66990
A	-9	LEU	-	CLONING ARTIFACT	UNP O66990
A	-8	TYR	-	CLONING ARTIFACT	UNP O66990
A	-7	ASP	-	CLONING ARTIFACT	UNP O66990
A	-6	ASP	-	CLONING ARTIFACT	UNP O66990
A	-5	ASP	-	CLONING ARTIFACT	UNP O66990
A	-4	ASP	-	CLONING ARTIFACT	UNP O66990
A	-3	LYS	-	CLONING ARTIFACT	UNP O66990
A	-2	ASP	-	CLONING ARTIFACT	UNP O66990
A	-1	ARG	-	CLONING ARTIFACT	UNP O66990
A	0	TRP	-	CLONING ARTIFACT	UNP O66990
B	-44	MET	-	CLONING ARTIFACT	UNP O66990
B	-43	ARG	-	CLONING ARTIFACT	UNP O66990
B	-42	PHE	-	CLONING ARTIFACT	UNP O66990
B	-41	TRP	-	CLONING ARTIFACT	UNP O66990
B	-40	GLN	-	CLONING ARTIFACT	UNP O66990
B	-39	TYR	-	CLONING ARTIFACT	UNP O66990
B	-38	ILE	-	CLONING ARTIFACT	UNP O66990
B	-37	ASN	-	CLONING ARTIFACT	UNP O66990
B	-36	GLY	-	CLONING ARTIFACT	UNP O66990
B	-35	VAL	-	CLONING ARTIFACT	UNP O66990
B	-34	ASP	-	CLONING ARTIFACT	UNP O66990
B	-33	MET	-	CLONING ARTIFACT	UNP O66990
B	-32	ARG	-	CLONING ARTIFACT	UNP O66990
B	-31	GLY	-	CLONING ARTIFACT	UNP O66990
B	-30	SER	-	CLONING ARTIFACT	UNP O66990
B	-29	HIS	-	CLONING ARTIFACT	UNP O66990
B	-28	HIS	-	CLONING ARTIFACT	UNP O66990
B	-27	HIS	-	CLONING ARTIFACT	UNP O66990
B	-26	HIS	-	CLONING ARTIFACT	UNP O66990
B	-25	HIS	-	CLONING ARTIFACT	UNP O66990
B	-24	HIS	-	CLONING ARTIFACT	UNP O66990
B	-23	GLY	-	CLONING ARTIFACT	UNP O66990

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	CLONING ARTIFACT	UNP O66990
B	-21	ALA	-	CLONING ARTIFACT	UNP O66990
B	-20	SER	-	CLONING ARTIFACT	UNP O66990
B	-19	MET	-	CLONING ARTIFACT	UNP O66990
B	-18	THR	-	CLONING ARTIFACT	UNP O66990
B	-17	GLY	-	CLONING ARTIFACT	UNP O66990
B	-16	GLY	-	CLONING ARTIFACT	UNP O66990
B	-15	GLN	-	CLONING ARTIFACT	UNP O66990
B	-14	GLN	-	CLONING ARTIFACT	UNP O66990
B	-13	MET	-	CLONING ARTIFACT	UNP O66990
B	-12	GLY	-	CLONING ARTIFACT	UNP O66990
B	-11	ARG	-	CLONING ARTIFACT	UNP O66990
B	-10	ASP	-	CLONING ARTIFACT	UNP O66990
B	-9	LEU	-	CLONING ARTIFACT	UNP O66990
B	-8	TYR	-	CLONING ARTIFACT	UNP O66990
B	-7	ASP	-	CLONING ARTIFACT	UNP O66990
B	-6	ASP	-	CLONING ARTIFACT	UNP O66990
B	-5	ASP	-	CLONING ARTIFACT	UNP O66990
B	-4	ASP	-	CLONING ARTIFACT	UNP O66990
B	-3	LYS	-	CLONING ARTIFACT	UNP O66990
B	-2	ASP	-	CLONING ARTIFACT	UNP O66990
B	-1	ARG	-	CLONING ARTIFACT	UNP O66990
B	0	TRP	-	CLONING ARTIFACT	UNP O66990

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

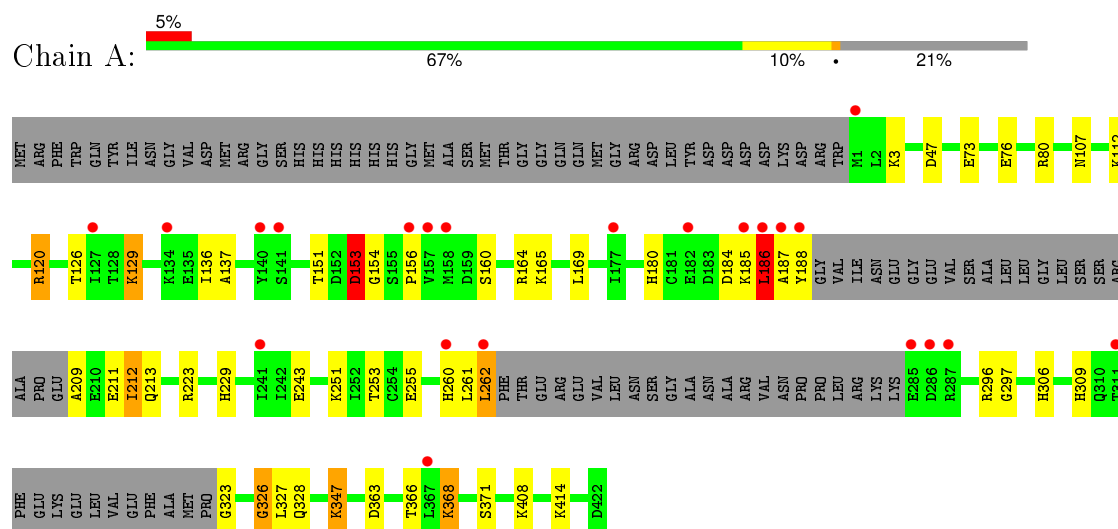
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	625	Total O 625 625	0	0
3	B	614	Total O 614 614	0	0

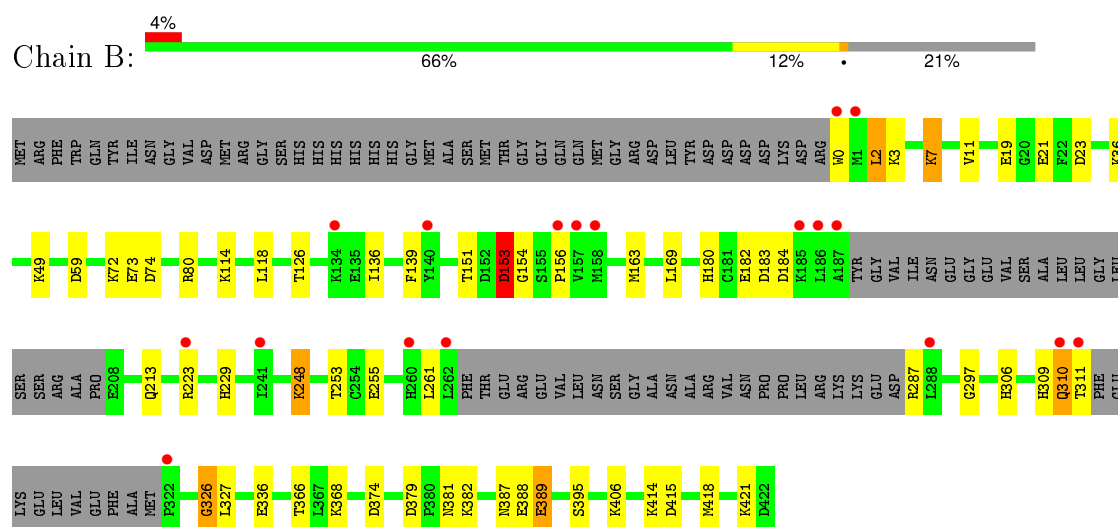
### 3 Residue-property plots [i](#)

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: Dihydroorotase



#### • Molecule 1: Dihydroorotase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.20 Å   91.23 Å   61.18 Å 90.00°   93.15°   90.00°	Depositor
Resolution (Å)	20.00 – 1.61 19.95 – 1.61	Depositor EDS
% Data completeness (in resolution range)	77.6 (20.00-1.61) 77.6 (19.95-1.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.61 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.165   ,   0.208 0.172   ,   0.213	Depositor DCC
$R_{free}$ test set	4873 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 95834 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6940	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 6.01% 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: ZN

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	0.87	0/2893	0.91	3/3904 (0.1%)
1	B	0.90	1/2896 (0.0%)	0.95	7/3909 (0.2%)
All	All	0.88	1/5789 (0.0%)	0.93	10/7813 (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	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	MET	SD-CE	-5.69	1.46	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ASP	CB-CG-OD2	6.87	124.49	118.30
1	B	74	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	153	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	2	LEU	CB-CG-CD2	6.09	121.36	111.00
1	B	59	ASP	CB-CG-OD2	5.91	123.61	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	153	ASP	Peptide
1	A	185	LYS	Peptide
1	A	186	LEU	Peptide
1	B	153	ASP	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	2849	0	2945	57	0
1	B	2850	0	2950	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	625	0	0	28	1
3	B	614	0	0	12	1
All	All	6940	0	5895	99	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 9.

The worst 5 of 99 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:371:SER:HB2	3:A:1872:HOH:O	1.09	1.27
1:A:366:THR:HG22	3:A:1846:HOH:O	1.42	1.20
1:A:186:LEU:O	1:A:309:HIS:HE1	1.26	1.15
1:A:186:LEU:O	1:A:309:HIS:CE1	2.01	1.12
1:B:156:PRO:HB3	1:B:213:GLN:HE22	1.18	1.08

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)
3:A:1493:HOH:O	3:B:1889:HOH:O[4_545]	2.14	0.06

## 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	361/467 (77%)	342 (95%)	16 (4%)	3 (1%)	24	6
1	B	361/467 (77%)	343 (95%)	15 (4%)	3 (1%)	24	6
All	All	722/934 (77%)	685 (95%)	31 (4%)	6 (1%)	24	6

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	ASP
1	A	153	ASP
1	A	180	HIS
1	B	326	GLY
1	A	326	GLY

### 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	318/400 (80%)	309 (97%)	9 (3%)	51	22
1	B	318/400 (80%)	305 (96%)	13 (4%)	37	11
All	All	636/800 (80%)	614 (96%)	22 (4%)	43	16

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LEU

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Mol	Chain	Res	Type
1	B	223	ARG
1	B	389	GLU
1	B	7	LYS
1	B	182	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	180	HIS
1	B	306	HIS
1	A	381	ASN
1	B	231	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, 2 are monoatomic - 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 [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 [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	369/467 (79%)	0.32	22 (5%) 25 22	12, 18, 35, 57	0
1	B	369/467 (79%)	0.37	18 (4%) 33 30	12, 18, 34, 51	0
All	All	738/934 (79%)	0.35	40 (5%) 29 26	12, 18, 35, 57	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	11.2
1	A	186	LEU	11.0
1	B	311	THR	8.2
1	A	285	GLU	6.1
1	A	187	ALA	5.2

### 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
2	ZN	B	1424	1/1	1.00	0.08	-0.95	33,33,33,33	0
2	ZN	A	1423	1/1	1.00	0.08	-1.08	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.