



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2024 – 02:30 PM EST

PDB ID : 7UI3  
Title : Apo-form of Human Tryptophan 2,3-Dioxygenase Induced by NADH Binding  
Authors : Yeh, S.-R.; Geeraerts, Z.  
Deposited on : 2022-03-28  
Resolution : 3.18 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

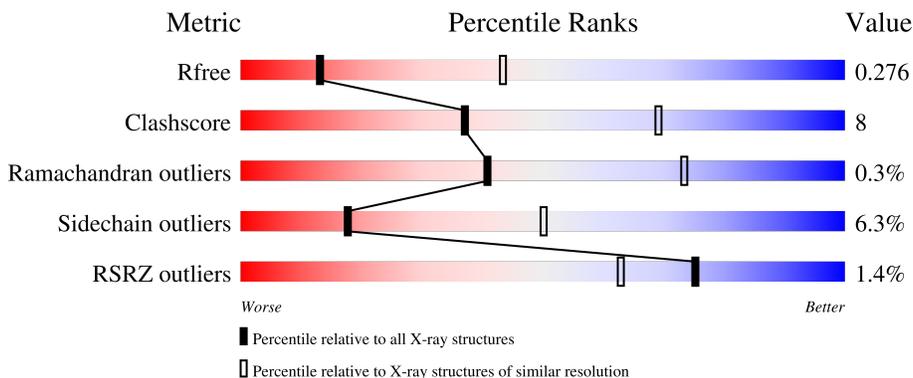
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	380	
1	B	380	
1	C	380	
1	D	380	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17673 atoms, of which 8569 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	309	4443	1452	2159	403	421	8	133	0	0
1	B	302	4693	1524	2316	414	429	10	102	0	0
1	C	293	4082	1357	1955	368	393	9	140	0	0
1	D	303	4335	1436	2083	388	418	10	131	0	0

There are 32 discrepancies between the modelled and reference sequences:

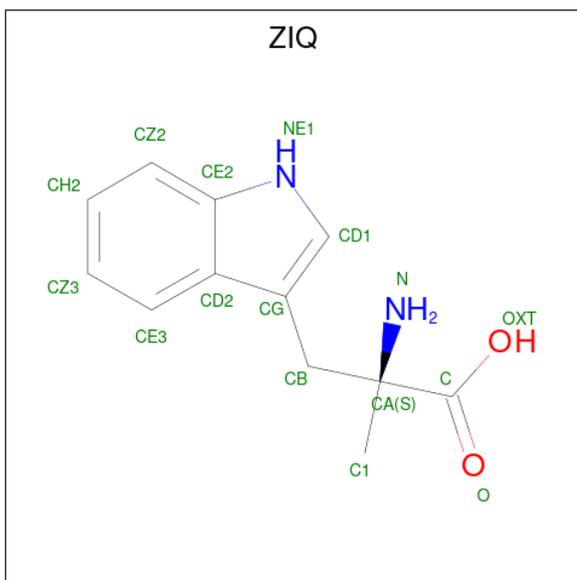
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

- Molecule 2 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>).

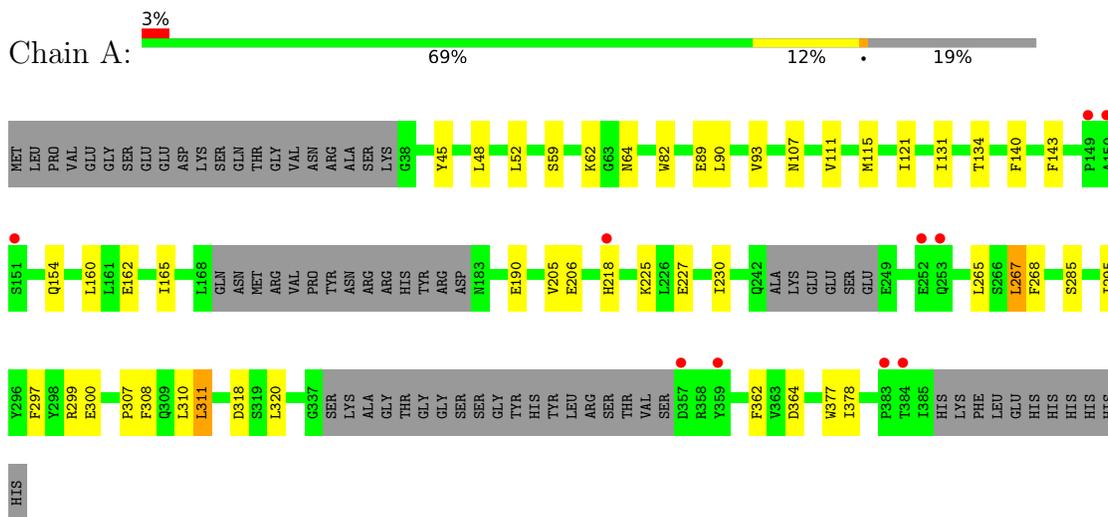


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
2	A	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	B	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	C	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	D	1	Total	C	H	N	O	0	0
			30	12	14	2	2		

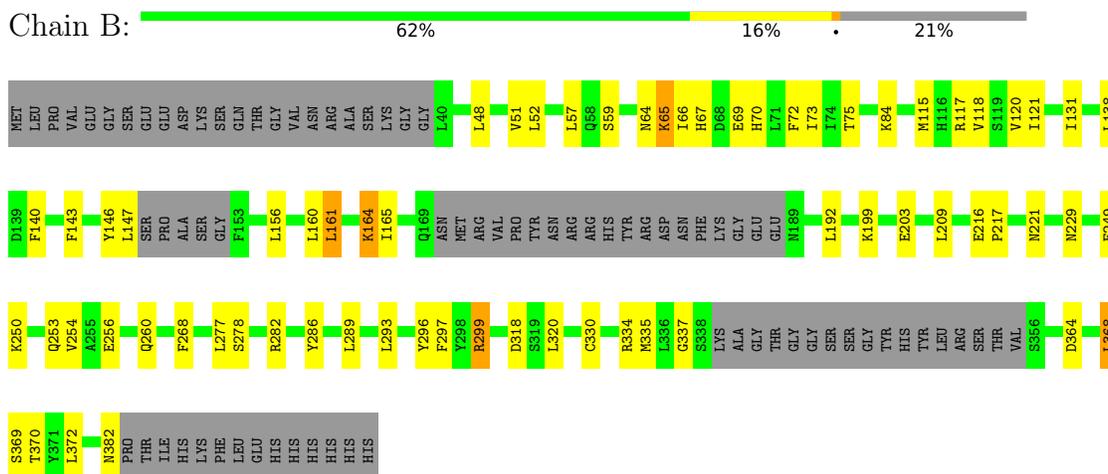
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: Tryptophan 2,3-dioxygenase

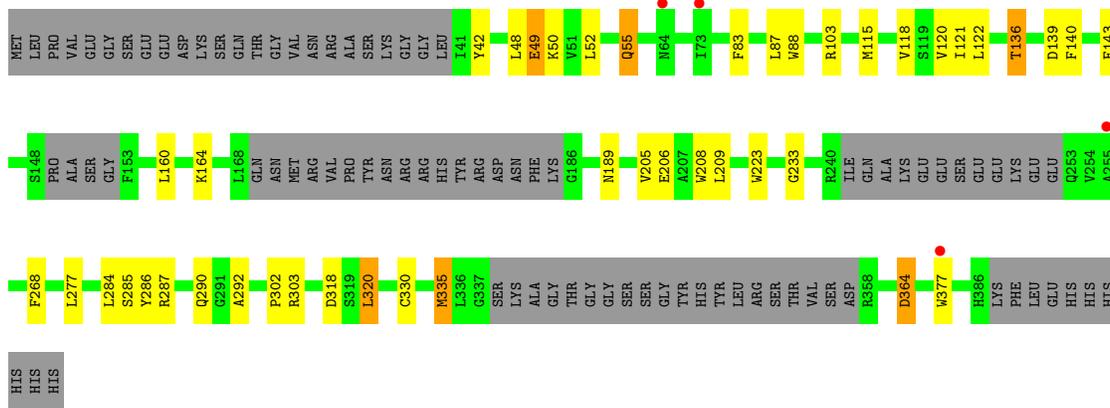


- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





● Molecule 1: Tryptophan 2,3-dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.85Å 156.26Å 88.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.18 19.97 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.97-3.18) 99.6 (19.97-3.18)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.15Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.244 , 0.278 0.245 , 0.276	Depositor DCC
$R_{free}$ test set	1774 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.5	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 103.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.333 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: ZIQ

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	0.69	0/2330	0.75	0/3166
1	B	0.69	0/2425	0.75	0/3280
1	C	0.70	0/2172	0.75	0/2958
1	D	0.69	0/2300	0.75	0/3130
All	All	0.69	0/9227	0.75	0/12534

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 [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	2284	2159	1990	35	0
1	B	2377	2316	2210	43	0
1	C	2127	1955	1767	30	0
1	D	2252	2083	1913	45	0
2	A	16	14	0	0	0
2	B	16	14	0	0	0
2	C	16	14	0	1	0
2	D	16	14	0	1	0
All	All	9104	8569	7880	133	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 8.

The worst 5 of 133 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:131:ILE:O	1:A:134:THR:HG22	1.77	0.85
1:A:307:PRO:O	1:A:311:LEU:HD22	1.83	0.78
1:B:293:LEU:HD13	1:B:368:LEU:HD12	1.66	0.77
1:A:90:LEU:O	1:A:93:VAL:HG22	1.85	0.76
1:D:361:VAL:HG13	1:D:362:PHE:CD1	2.22	0.74

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	301/380 (79%)	281 (93%)	19 (6%)	1 (0%)	41	73
1	B	294/380 (77%)	275 (94%)	18 (6%)	1 (0%)	41	73
1	C	283/380 (74%)	268 (95%)	14 (5%)	1 (0%)	34	69
1	D	295/380 (78%)	277 (94%)	18 (6%)	0	100	100
All	All	1173/1520 (77%)	1101 (94%)	69 (6%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	LEU
1	C	42	TYR
1	A	154	GLN

### 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	203/348 (58%)	193 (95%)	10 (5%)	25	59
1	B	234/348 (67%)	216 (92%)	18 (8%)	13	42
1	C	179/348 (51%)	170 (95%)	9 (5%)	24	58
1	D	198/348 (57%)	184 (93%)	14 (7%)	14	45
All	All	814/1392 (58%)	763 (94%)	51 (6%)	18	50

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	GLU
1	C	335	MET
1	D	363	VAL
1	C	55	GLN
1	C	318	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	ASN
1	D	367	ASN
1	C	70	HIS
1	C	141	ASN
1	C	163	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
2	ZIQ	A	401	-	13,17,17	0.79	0	14,25,25	0.96	0
2	ZIQ	C	401	-	13,17,17	0.82	0	14,25,25	1.21	2 (14%)
2	ZIQ	B	401	-	13,17,17	0.82	0	14,25,25	1.26	3 (21%)
2	ZIQ	D	401	-	13,17,17	0.77	0	14,25,25	1.15	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZIQ	A	401	-	-	0/9/11/11	0/2/2/2
2	ZIQ	C	401	-	-	1/9/11/11	0/2/2/2
2	ZIQ	B	401	-	-	4/9/11/11	0/2/2/2
2	ZIQ	D	401	-	-	2/9/11/11	0/2/2/2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ZIQ	C1-CA-CB	-2.78	107.18	110.94
2	D	401	ZIQ	C1-CA-CB	-2.67	107.32	110.94
2	B	401	ZIQ	C1-CA-CB	-2.67	107.33	110.94
2	B	401	ZIQ	CB-CA-C	2.30	112.26	109.02
2	B	401	ZIQ	CH2-CZ2-CE2	-2.18	116.94	120.08

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ZIQ	O-C-CA-N
2	D	401	ZIQ	O-C-CA-CB
2	D	401	ZIQ	OXT-C-CA-CB
2	B	401	ZIQ	OXT-C-CA-C1
2	B	401	ZIQ	O-C-CA-C1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ZIQ	1	0
2	D	401	ZIQ	1	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 [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	309/380 (81%)	-0.05	10 (3%) 47 31	82, 127, 186, 212	0
1	B	302/380 (79%)	-0.18	0 100 100	78, 106, 155, 194	0
1	C	293/380 (77%)	-0.14	4 (1%) 75 63	84, 135, 184, 215	0
1	D	303/380 (79%)	-0.18	3 (0%) 82 72	89, 129, 172, 206	0
All	All	1207/1520 (79%)	-0.14	17 (1%) 75 63	78, 126, 179, 215	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	TRP	4.8
1	A	218	HIS	3.1
1	C	64	ASN	3.0
1	D	338	SER	2.9
1	A	359	TYR	2.8

### 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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZIQ	C	401	16/16	0.88	0.19	115,120,133,136	0
2	ZIQ	B	401	16/16	0.94	0.17	82,86,95,97	0
2	ZIQ	D	401	16/16	0.94	0.15	125,131,135,135	0
2	ZIQ	A	401	16/16	0.96	0.16	82,89,94,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.