



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:07 pm BST

PDB ID : 3JZF  
Title : Crystal structure of biotin carboxylase from E. Coli in complex with benzimidazoles series  
Authors : Orth, P.  
Deposited on : 2009-09-23  
Resolution : 2.13 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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)	:	2.11

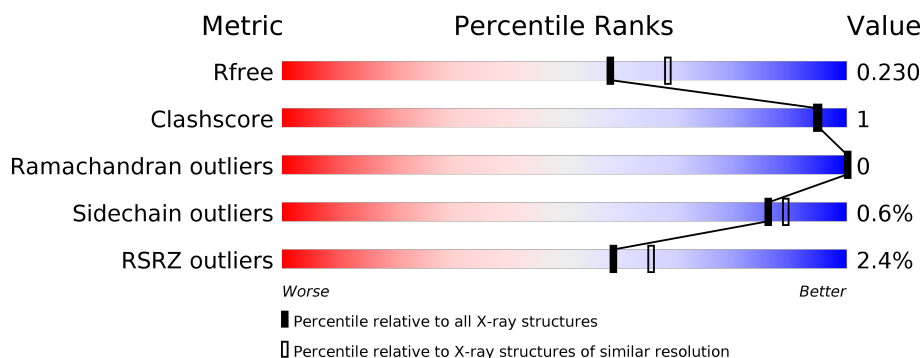
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 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	486	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	486	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6942 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 Biotin carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2933	1857	518	541	17			
1	B	447	Total	C	N	O	S	0	0	0
			3434	2163	613	636	22			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P24182
A	-19	GLY	-	EXPRESSION TAG	UNP P24182
A	-18	HIS	-	EXPRESSION TAG	UNP P24182
A	-17	HIS	-	EXPRESSION TAG	UNP P24182
A	-16	HIS	-	EXPRESSION TAG	UNP P24182
A	-15	HIS	-	EXPRESSION TAG	UNP P24182
A	-14	HIS	-	EXPRESSION TAG	UNP P24182
A	-13	HIS	-	EXPRESSION TAG	UNP P24182
A	-12	HIS	-	EXPRESSION TAG	UNP P24182
A	-11	HIS	-	EXPRESSION TAG	UNP P24182
A	-10	HIS	-	EXPRESSION TAG	UNP P24182
A	-9	HIS	-	EXPRESSION TAG	UNP P24182
A	-8	SER	-	EXPRESSION TAG	UNP P24182
A	-7	SER	-	EXPRESSION TAG	UNP P24182
A	-6	GLY	-	EXPRESSION TAG	UNP P24182
A	-5	HIS	-	EXPRESSION TAG	UNP P24182
A	-4	ILE	-	EXPRESSION TAG	UNP P24182
A	-3	GLU	-	EXPRESSION TAG	UNP P24182
A	-2	GLY	-	EXPRESSION TAG	UNP P24182
A	-1	ARG	-	EXPRESSION TAG	UNP P24182
A	0	HIS	-	EXPRESSION TAG	UNP P24182
A	450	SER	-	EXPRESSION TAG	UNP P24182
A	451	ASP	-	EXPRESSION TAG	UNP P24182
A	452	PRO	-	EXPRESSION TAG	UNP P24182
A	453	ASN	-	EXPRESSION TAG	UNP P24182

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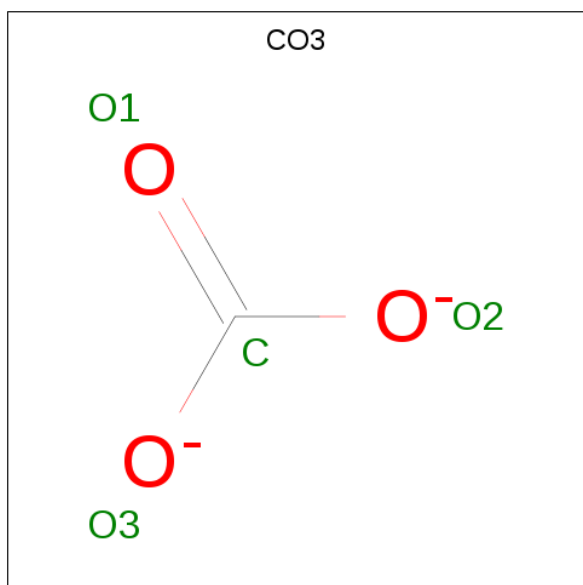
Chain	Residue	Modelled	Actual	Comment	Reference
A	454	SER	-	EXPRESSION TAG	UNP P24182
A	455	SER	-	EXPRESSION TAG	UNP P24182
A	456	SER	-	EXPRESSION TAG	UNP P24182
A	457	VAL	-	EXPRESSION TAG	UNP P24182
A	458	ASP	-	EXPRESSION TAG	UNP P24182
A	459	LYS	-	EXPRESSION TAG	UNP P24182
A	460	LEU	-	EXPRESSION TAG	UNP P24182
A	461	ALA	-	EXPRESSION TAG	UNP P24182
A	462	ALA	-	EXPRESSION TAG	UNP P24182
A	463	ALA	-	EXPRESSION TAG	UNP P24182
A	464	LEU	-	EXPRESSION TAG	UNP P24182
A	465	GLU	-	EXPRESSION TAG	UNP P24182
B	-20	MET	-	EXPRESSION TAG	UNP P24182
B	-19	GLY	-	EXPRESSION TAG	UNP P24182
B	-18	HIS	-	EXPRESSION TAG	UNP P24182
B	-17	HIS	-	EXPRESSION TAG	UNP P24182
B	-16	HIS	-	EXPRESSION TAG	UNP P24182
B	-15	HIS	-	EXPRESSION TAG	UNP P24182
B	-14	HIS	-	EXPRESSION TAG	UNP P24182
B	-13	HIS	-	EXPRESSION TAG	UNP P24182
B	-12	HIS	-	EXPRESSION TAG	UNP P24182
B	-11	HIS	-	EXPRESSION TAG	UNP P24182
B	-10	HIS	-	EXPRESSION TAG	UNP P24182
B	-9	HIS	-	EXPRESSION TAG	UNP P24182
B	-8	SER	-	EXPRESSION TAG	UNP P24182
B	-7	SER	-	EXPRESSION TAG	UNP P24182
B	-6	GLY	-	EXPRESSION TAG	UNP P24182
B	-5	HIS	-	EXPRESSION TAG	UNP P24182
B	-4	ILE	-	EXPRESSION TAG	UNP P24182
B	-3	GLU	-	EXPRESSION TAG	UNP P24182
B	-2	GLY	-	EXPRESSION TAG	UNP P24182
B	-1	ARG	-	EXPRESSION TAG	UNP P24182
B	0	HIS	-	EXPRESSION TAG	UNP P24182
B	450	SER	-	EXPRESSION TAG	UNP P24182
B	451	ASP	-	EXPRESSION TAG	UNP P24182
B	452	PRO	-	EXPRESSION TAG	UNP P24182
B	453	ASN	-	EXPRESSION TAG	UNP P24182
B	454	SER	-	EXPRESSION TAG	UNP P24182
B	455	SER	-	EXPRESSION TAG	UNP P24182
B	456	SER	-	EXPRESSION TAG	UNP P24182
B	457	VAL	-	EXPRESSION TAG	UNP P24182
B	458	ASP	-	EXPRESSION TAG	UNP P24182

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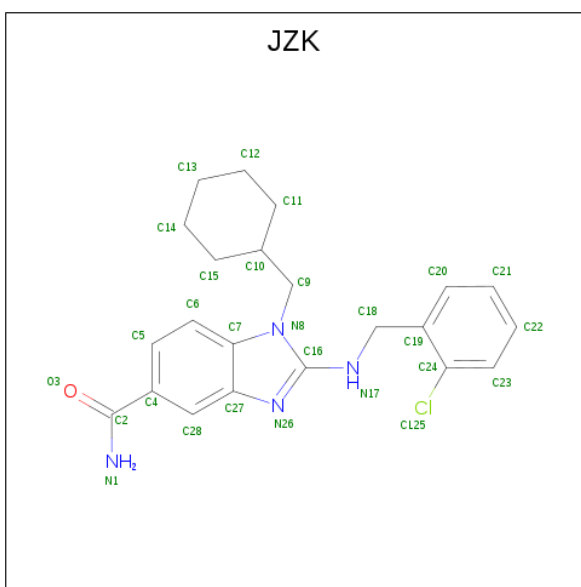
Chain	Residue	Modelled	Actual	Comment	Reference
B	459	LYS	-	EXPRESSION TAG	UNP P24182
B	460	LEU	-	EXPRESSION TAG	UNP P24182
B	461	ALA	-	EXPRESSION TAG	UNP P24182
B	462	ALA	-	EXPRESSION TAG	UNP P24182
B	463	ALA	-	EXPRESSION TAG	UNP P24182
B	464	LEU	-	EXPRESSION TAG	UNP P24182
B	465	GLU	-	EXPRESSION TAG	UNP P24182

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is 2-[(2-chlorobenzyl)amino]-1-(cyclohexylmethyl)-1H-benzimidazole-5-carboxamide (three-letter code: JZK) (formula: C<sub>22</sub>H<sub>25</sub>ClN<sub>4</sub>O).



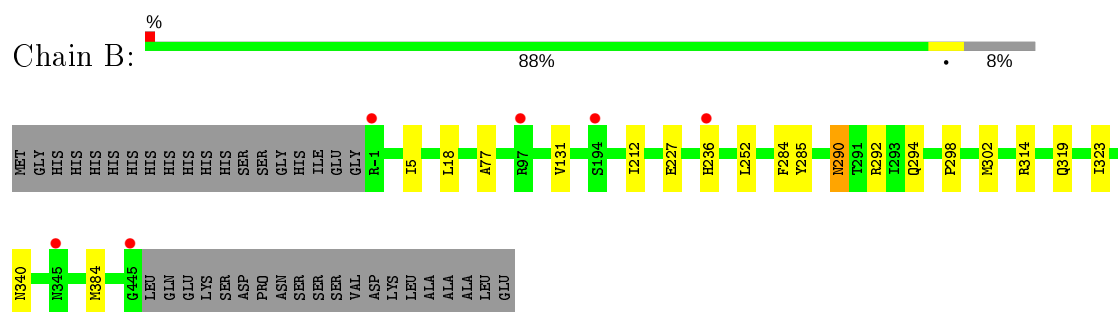
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		
4	B	310	Total	O	0	0
			310	310		



- Molecule 1: Biotin carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.37Å 107.51Å 122.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.13 19.94 – 2.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.94-2.13) 99.4 (19.94-2.13)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.13Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.203 , 0.236 0.196 , 0.230	Depositor DCC
$R_{free}$ test set	3151 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, JZK

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	0.43	0/2989	0.59	0/4042
1	B	0.44	0/3498	0.60	0/4722
All	All	0.44	0/6487	0.59	0/8764

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	2933	0	2937	5	0
1	B	3434	0	3446	10	0
2	A	4	0	0	0	0
3	B	28	0	25	1	0
4	A	233	0	0	0	0
4	B	310	0	0	0	0
All	All	6942	0	6408	15	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 1.

All (15) 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:236:HIS:HD2	3:B:466:JZK:H12	1.59	0.68
1:B:314:ARG:HH11	1:B:319:GLN:HE22	1.41	0.67
1:B:212:ILE:HD13	1:B:227:GLU:HB3	1.93	0.49
1:A:298:PRO:O	1:A:302:MET:HG2	2.14	0.47
1:B:5:ILE:HG22	1:B:77:ALA:HB3	1.97	0.46
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.98	0.45
1:B:340:ASN:HD22	1:B:384:MET:HA	1.80	0.45
1:B:290:ASN:OD1	1:B:292:ARG:CZ	2.66	0.42
1:A:441:GLU:HG2	1:A:446:LEU:HB2	2.01	0.42
1:B:252:LEU:HG	1:B:284:PHE:HE1	1.84	0.41
1:A:63:ILE:HG12	1:A:91:PHE:CD2	2.55	0.41
1:B:292:ARG:HH12	1:B:294:GLN:HG3	1.85	0.41
1:A:5:ILE:HG22	1:A:77:ALA:HB3	2.02	0.41
1:A:340:ASN:HD22	1:A:384:MET:HA	1.86	0.40
1:B:298:PRO:O	1:B:302:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

## 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	376/486 (77%)	367 (98%)	9 (2%)	0	100	100
1	B	445/486 (92%)	436 (98%)	9 (2%)	0	100	100
All	All	821/972 (84%)	803 (98%)	18 (2%)	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	307/392 (78%)	306 (100%)	1 (0%)	92	94
1	B	357/392 (91%)	354 (99%)	3 (1%)	81	85
All	All	664/784 (85%)	660 (99%)	4 (1%)	86	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	B	18	LEU
1	B	290	ASN
1	B	323	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	319	GLN
1	A	340	ASN
1	A	404	ASN
1	B	145	ASN
1	B	236	HIS
1	B	319	GLN
1	B	340	ASN
1	B	404	ASN
1	B	431	GLN

### 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](#)

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	JZK	B	466	-	28,31,31	2.06	7 (25%)	31,43,43	2.15	4 (12%)
2	CO3	A	466	-	0,3,3	0.00	-	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	JZK	B	466	-	-	0/9/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	466	JZK	C6-C5	6.38	1.50	1.36
3	B	466	JZK	C2-N1	4.08	1.40	1.33
3	B	466	JZK	C6-C7	3.88	1.48	1.41
3	B	466	JZK	C28-C4	3.19	1.43	1.37
3	B	466	JZK	C24-C19	2.39	1.43	1.39
3	B	466	JZK	C21-C20	2.24	1.43	1.38
3	B	466	JZK	C5-C4	2.17	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	466	JZK	C5-C6-C7	-8.07	107.31	119.70
3	B	466	JZK	C6-C5-C4	5.28	126.75	120.79
3	B	466	JZK	C6-C7-C27	3.68	127.31	121.30
3	B	466	JZK	C18-C19-C24	-3.55	116.43	121.13

There are no chirality outliers.

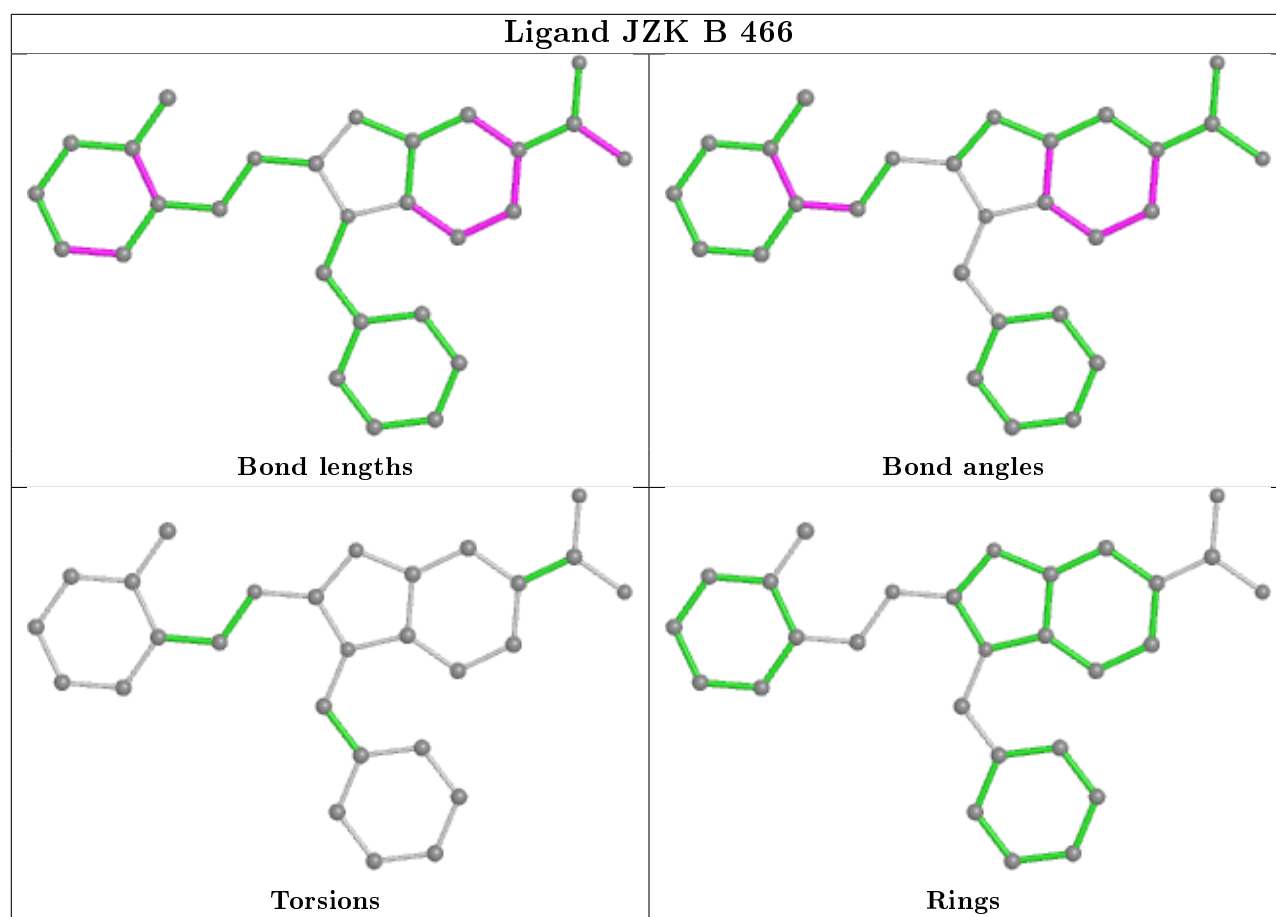
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	466	JZK	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

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	380/486 (78%)	-0.00	14 (3%) 41 49	18, 28, 53, 122	0
1	B	447/486 (91%)	-0.19	6 (1%) 77 81	19, 29, 47, 78	0
All	All	827/972 (85%)	-0.10	20 (2%) 59 65	18, 28, 50, 122	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LYS	12.0
1	A	446	LEU	11.2
1	A	448	GLU	8.9
1	A	447	GLN	7.6
1	A	445	GLY	4.9
1	B	-1	ARG	4.7
1	A	117	VAL	3.2
1	A	322	SER	3.2
1	B	345	ASN	3.0
1	A	203	TYR	2.9
1	A	344	PRO	2.9
1	A	347	PHE	2.8
1	A	281	ASN	2.7
1	A	132	PRO	2.5
1	B	97	ARG	2.4
1	B	236	HIS	2.2
1	B	445	GLY	2.1
1	B	194	SER	2.1
1	A	345	ASN	2.0
1	A	131	VAL	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. 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.

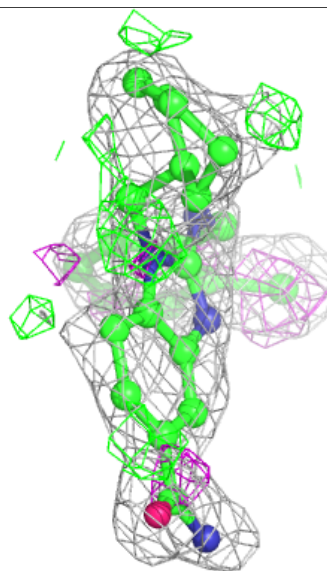
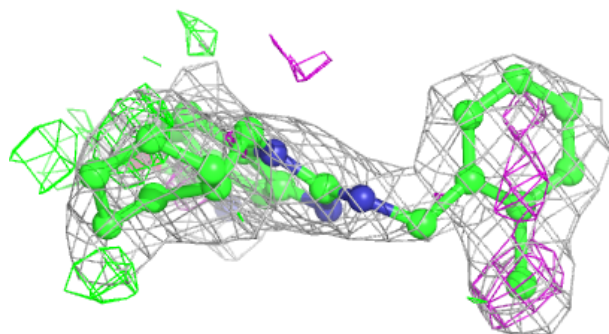
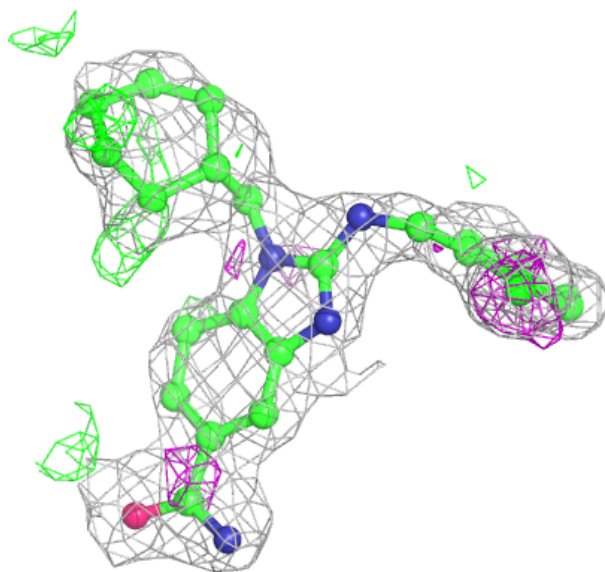
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	JZK	B	466	28/28	0.88	0.20	35,42,46,47	0
2	CO3	A	466	4/4	0.94	0.17	30,30,31,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around JZK B 466:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.