



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2022 – 04:18 PM JST

PDB ID : 7YNW  
Title : Crystal structure of O-(2-nitrobenzyl)-L-tyrosine-tRNA synthetase in complex with O-(2-nitrobenzyl)-L-tyrosine  
Authors : Hosaka, T.; Shirouzu, M.  
Deposited on : 2022-08-01  
Resolution : 2.79 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

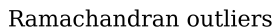
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Ramachandran outliers

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.

			13%
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ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	J2F	B	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5039 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 Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2449	1561	417	458	13			
1	B	308	Total	C	N	O	S	0	0	0
			2463	1568	419	463	13			

There are 30 discrepancies between the modelled and reference sequences:

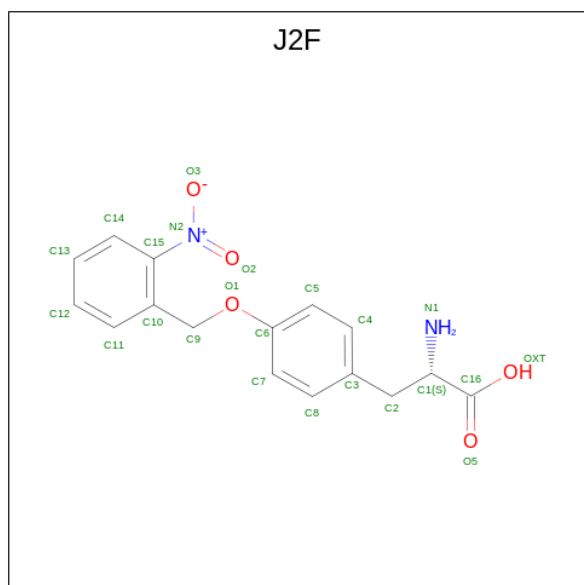
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	TYR	conflict	UNP Q57834
A	65	GLY	LEU	conflict	UNP Q57834
A	108	GLU	PHE	conflict	UNP Q57834
A	158	SER	ASP	conflict	UNP Q57834
A	162	GLU	LEU	conflict	UNP Q57834
A	286	ARG	ASP	conflict	UNP Q57834
A	307	SER	-	expression tag	UNP Q57834
A	308	ASP	-	expression tag	UNP Q57834
A	309	PRO	-	expression tag	UNP Q57834
A	310	GLU	-	expression tag	UNP Q57834
A	311	ASN	-	expression tag	UNP Q57834
A	312	LEU	-	expression tag	UNP Q57834
A	313	TYR	-	expression tag	UNP Q57834
A	314	PHE	-	expression tag	UNP Q57834
A	315	GLN	-	expression tag	UNP Q57834
B	32	GLY	TYR	conflict	UNP Q57834
B	65	GLY	LEU	conflict	UNP Q57834
B	108	GLU	PHE	conflict	UNP Q57834
B	158	SER	ASP	conflict	UNP Q57834
B	162	GLU	LEU	conflict	UNP Q57834
B	286	ARG	ASP	conflict	UNP Q57834
B	307	SER	-	expression tag	UNP Q57834
B	308	ASP	-	expression tag	UNP Q57834
B	309	PRO	-	expression tag	UNP Q57834
B	310	GLU	-	expression tag	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
B	311	ASN	-	expression tag	UNP Q57834
B	312	LEU	-	expression tag	UNP Q57834
B	313	TYR	-	expression tag	UNP Q57834
B	314	PHE	-	expression tag	UNP Q57834
B	315	GLN	-	expression tag	UNP Q57834

- Molecule 2 is (2 {S})-2-azanyl-3-[4-[(2-nitrophenyl)methoxy]phenyl]propanoic acid (three-letter code: J2F) (formula: C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	2	5		
2	B	1	Total	C	N	O	0	0
			23	16	2	5		

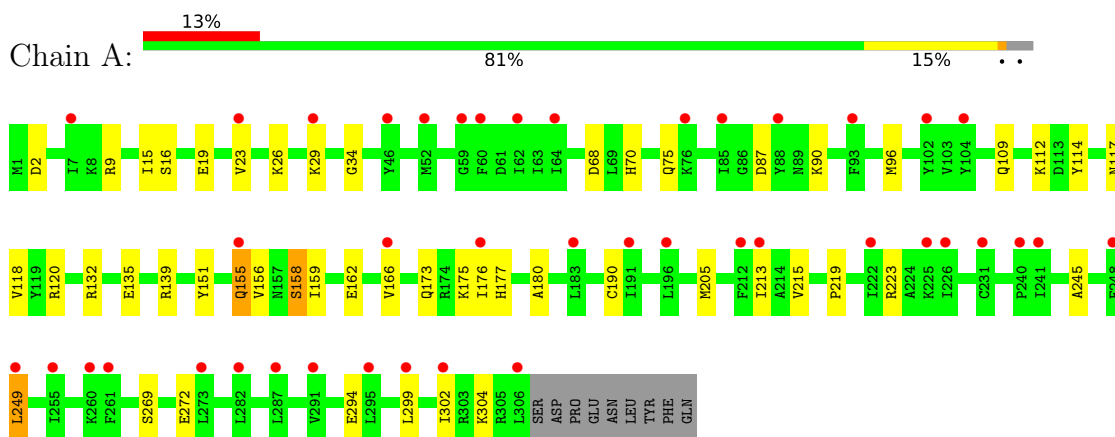
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	31	Total	O	0	0
			31	31		

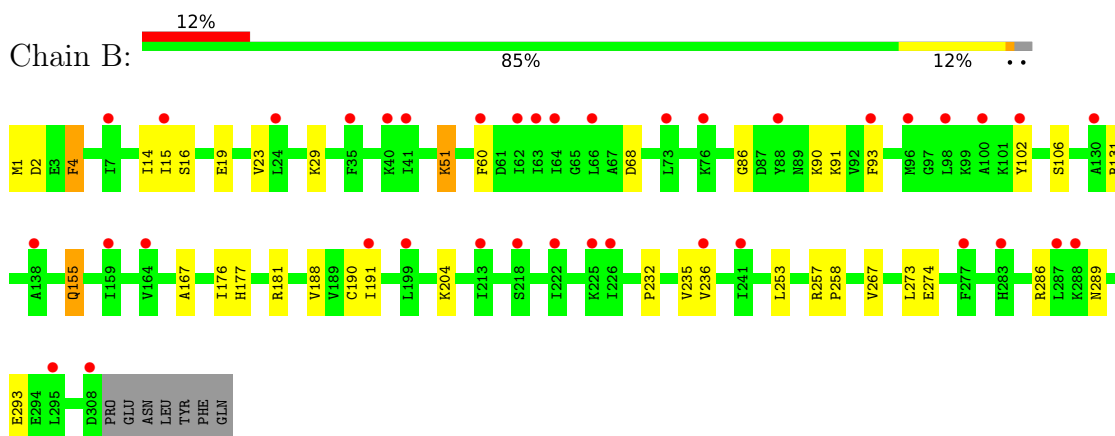
### 3 Residue-property plots [i](#)

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: Tyrosine-tRNA ligase



#### • Molecule 1: Tyrosine-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.48Å 83.48Å 488.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.59 – 2.79 46.66 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.59-2.79) 99.9 (46.66-2.64)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.260 , 0.297 0.273 , 0.311	Depositor DCC
$R_{free}$ test set	2000 reflections (6.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 94.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8123e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: J2F

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	0.28	0/2488	0.48	0/3337
1	B	0.26	0/2502	0.48	0/3356
All	All	0.27	0/4990	0.48	0/6693

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	2449	0	2525	33	0
1	B	2463	0	2534	21	0
2	A	23	0	0	2	0
2	B	23	0	0	0	0
3	A	50	0	0	3	0
3	B	31	0	0	0	0
All	All	5039	0	5059	54	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 5.

The worst 5 of 54 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:245:ALA:HA	1:A:249:LEU:HG	1.68	0.74
1:A:23:VAL:HG13	1:A:26:LYS:HD3	1.70	0.73
1:A:19:GLU:O	1:A:23:VAL:HG23	1.99	0.62
1:A:96:MET:HA	1:A:302:ILE:HD12	1.81	0.62
1:A:304:LYS:NZ	3:A:602:HOH:O	2.30	0.61

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	304/315 (96%)	297 (98%)	7 (2%)	0	100	100
1	B	306/315 (97%)	299 (98%)	7 (2%)	0	100	100
All	All	610/630 (97%)	596 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	266/275 (97%)	262 (98%)	4 (2%)	65	89
1	B	268/275 (98%)	261 (97%)	7 (3%)	46	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	534/550 (97%)	523 (98%)	11 (2%)	53 84

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	ARG
1	B	155	GLN
1	B	253	LEU
1	B	204	LYS
1	B	4	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	155	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 monosaccharides 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
2	J2F	B	501	-	22,24,24	2.39	1 (4%)	28,32,32	1.56	2 (7%)
2	J2F	A	501	-	22,24,24	2.36	1 (4%)	28,32,32	1.09	2 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	J2F	B	501	-	-	6/15/17/17	0/2/2/2
2	J2F	A	501	-	-	6/15/17/17	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	J2F	O2-N2	10.80	1.41	1.22
2	A	501	J2F	O2-N2	10.68	1.40	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	J2F	C9-C10-C15	-6.29	120.45	123.94
2	A	501	J2F	C9-C10-C15	-3.97	121.74	123.94
2	B	501	J2F	C14-C15-N2	3.21	119.90	116.47
2	A	501	J2F	OXT-C16-C1	2.02	120.25	113.38

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

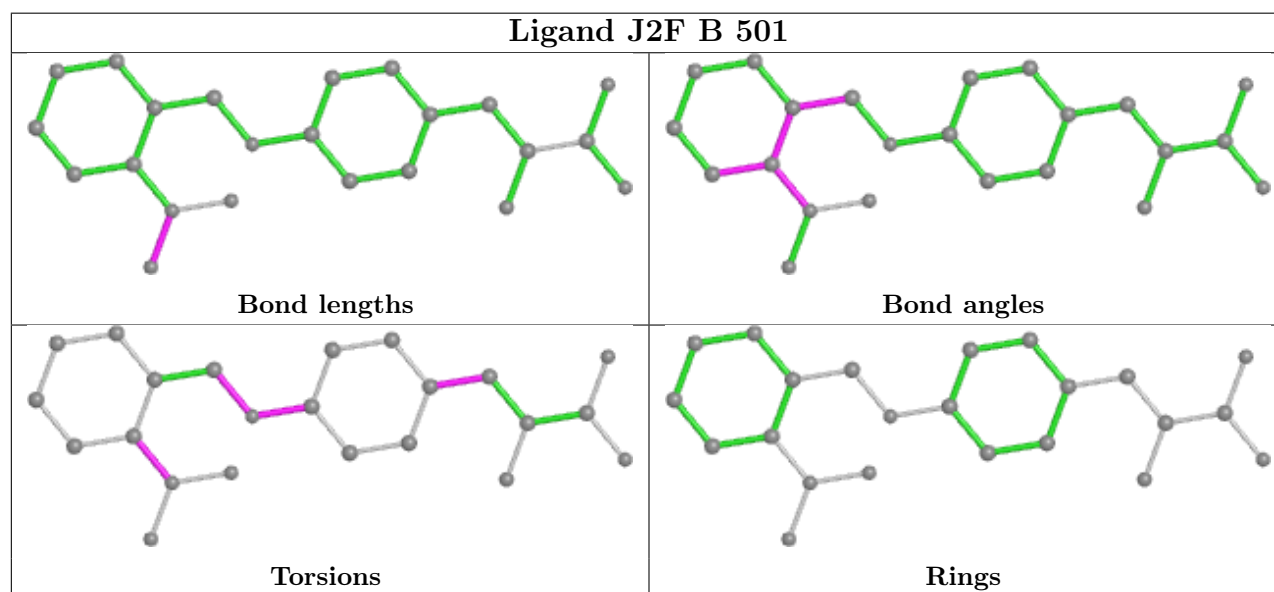
Mol	Chain	Res	Type	Atoms
2	B	501	J2F	C5-C6-O1-C9
2	B	501	J2F	C7-C6-O1-C9
2	A	501	J2F	C5-C6-O1-C9
2	A	501	J2F	C7-C6-O1-C9
2	B	501	J2F	C10-C9-O1-C6

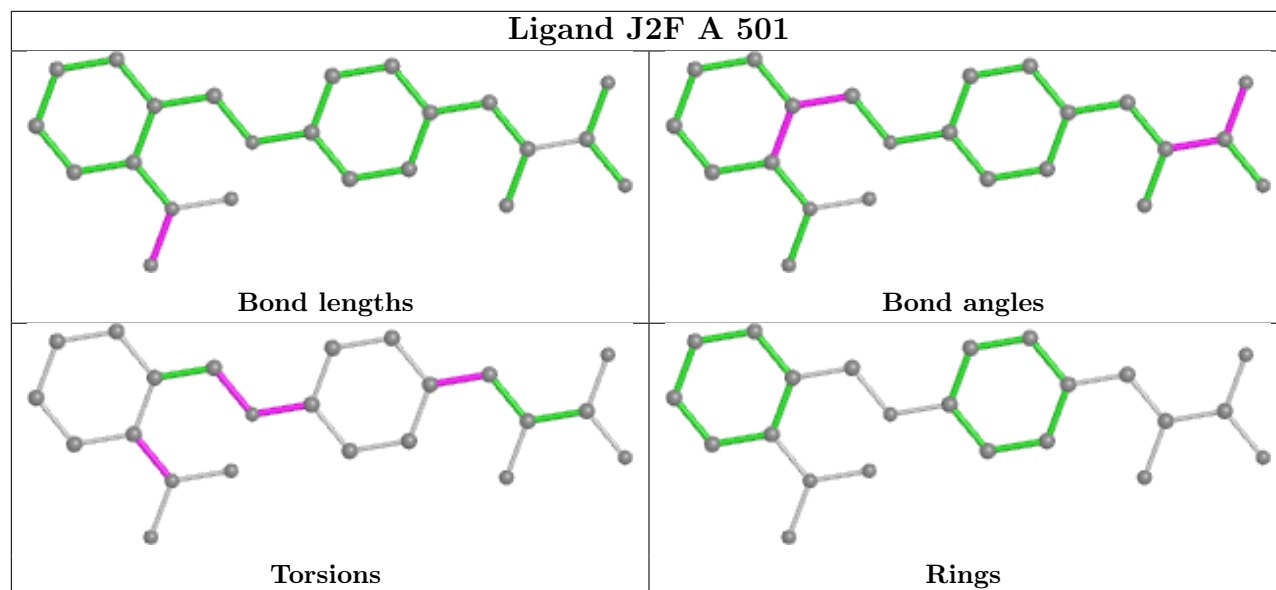
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	J2F	2	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 [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	306/315 (97%)	0.83	42 (13%)	3 1	76, 136, 195, 228	0
1	B	308/315 (97%)	0.74	38 (12%)	4 2	81, 131, 196, 242	0
All	All	614/630 (97%)	0.79	80 (13%)	3 2	76, 134, 196, 242	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	LYS	6.5
1	A	29	LYS	5.8
1	A	248	PHE	5.4
1	B	213	ILE	5.4
1	A	225	LYS	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

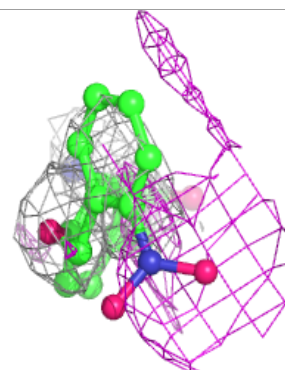
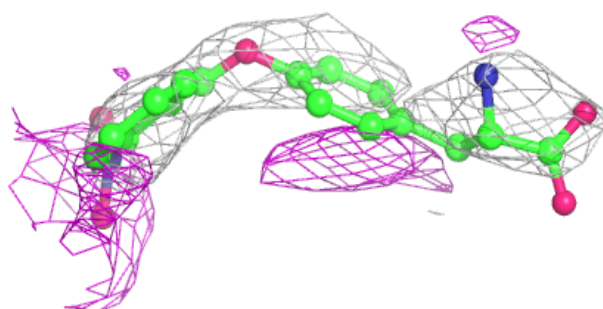
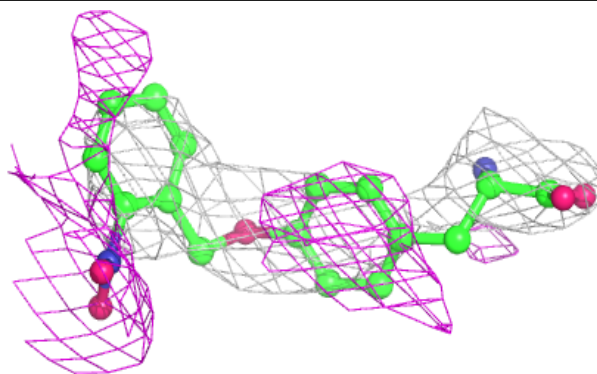
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	J2F	B	501	23/23	0.74	0.74	97,121,132,139	0
2	J2F	A	501	23/23	0.87	0.48	103,119,128,131	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.

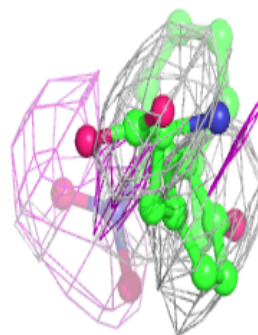
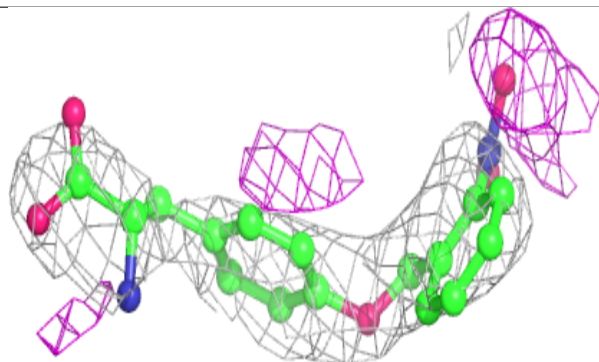
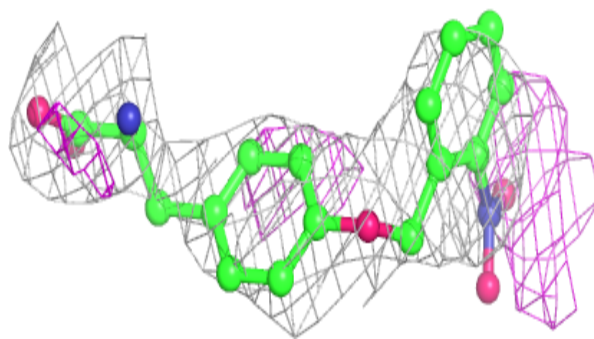
**Electron density around J2F B 501:**

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



**Electron density around J2F A 501:**

$2mF_o - DF_c$  (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.