



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2025 – 02:19 pm BST

PDB ID : 9S8I / pdb\_00009s8i  
Title : Crystal Structure of UDP-N-acetylmuramate-L-alanine ligase (MurC) from Pseudomonas aeruginosa in complex with compound OSA\_001176 (WYH78)  
Authors : Diaz-Saez, L.; Lloyd, A.J.; Wang, Y.; Todd, M.H.; Dowson, C.G.  
Deposited on : 2025-08-05  
Resolution : 2.30 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	:	<b>FAILED</b>
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

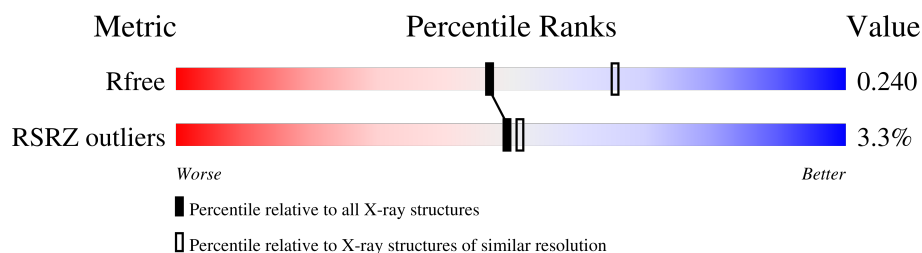
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
5	EDO	B	508	-	-	-	X
7	DMS	A	516	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7679 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.

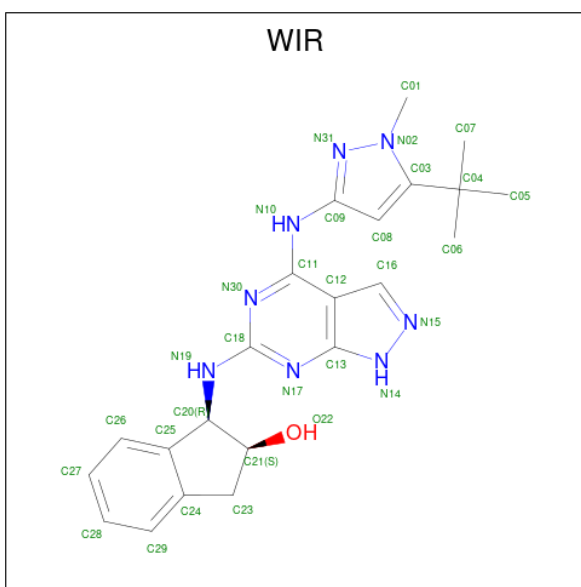
- Molecule 1 is a protein called UDP-N-acetylmuramate--L-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	23	0
			3621	2304	646	655	16			
1	B	452	Total	C	N	O	S	0	9	0
			3529	2234	636	644	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	ALA	-	expression tag	UNP Q9HW02
A	482	GLU	-	expression tag	UNP Q9HW02
A	483	ASN	-	expression tag	UNP Q9HW02
A	484	LEU	-	expression tag	UNP Q9HW02
A	485	TYR	-	expression tag	UNP Q9HW02
A	486	PHE	-	expression tag	UNP Q9HW02
A	487	GLN	-	expression tag	UNP Q9HW02
B	481	ALA	-	expression tag	UNP Q9HW02
B	482	GLU	-	expression tag	UNP Q9HW02
B	483	ASN	-	expression tag	UNP Q9HW02
B	484	LEU	-	expression tag	UNP Q9HW02
B	485	TYR	-	expression tag	UNP Q9HW02
B	486	PHE	-	expression tag	UNP Q9HW02
B	487	GLN	-	expression tag	UNP Q9HW02

- Molecule 2 is (1R,2S)-1-({4-[(5-tert-butyl-1-methyl-1H-pyrazol-3-yl)amino]-1H-pyrazolo[3,4-d]pyrimidin-6-yl}amino)-2,3-dihydro-1H-inden-2-ol (CCD ID: WIR) (formula: C<sub>22</sub>H<sub>26</sub>N<sub>8</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	8	1		
2	B	1	Total	C	N	O	0	0
			31	22	8	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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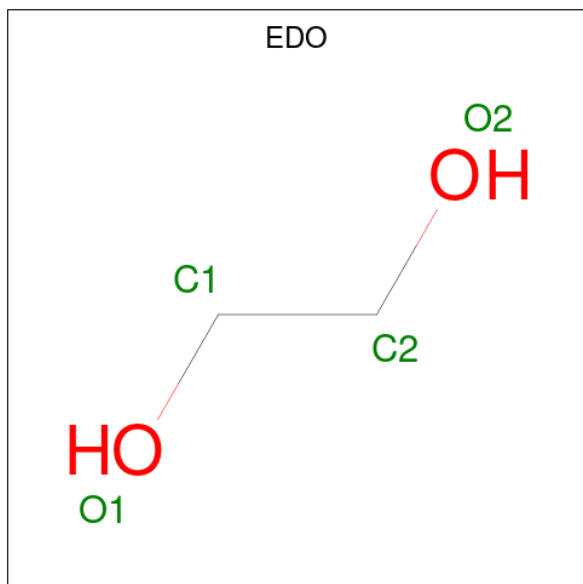
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	X	0	0
			1	1		
4	B	1	Total	X	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



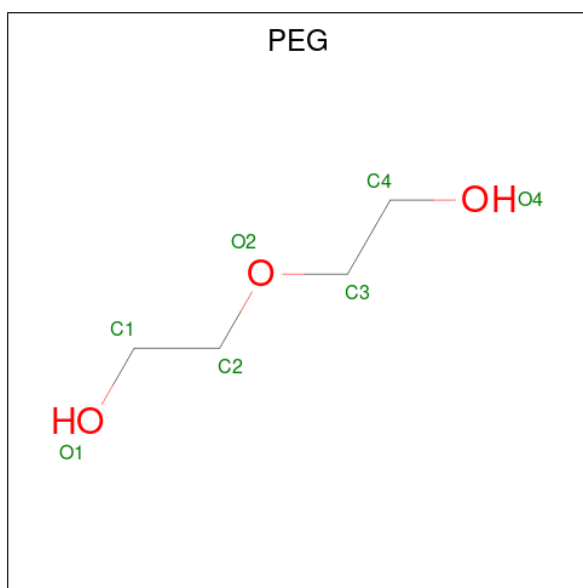
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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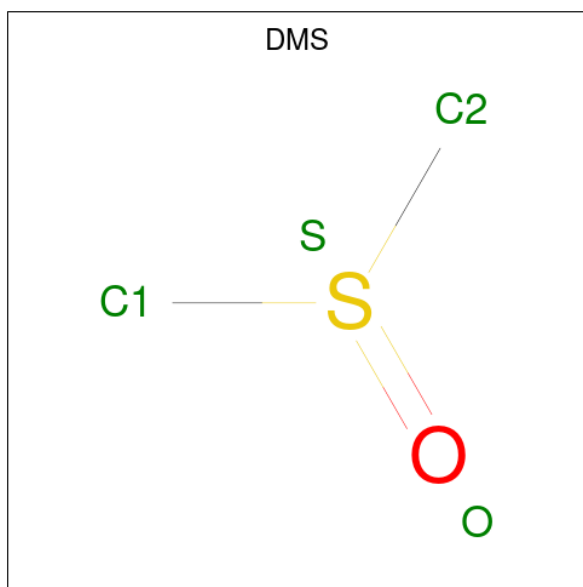
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	204	Total	O	0	0
			204	204		
8	B	149	Total	O	0	0
			149	149		

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.58Å 99.11Å 192.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.28 – 2.30 88.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.28-2.30) 100.0 (88.28-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.188 , 0.239 0.197 , 0.240	Depositor DCC
$R_{free}$ test set	2705 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.6	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	0.95	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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.



## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are unknown - leaving 27 for Mogul analysis.

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
5	EDO	A	511	-	3,3,3	0.13	0	2,2,2	0.13	0
5	EDO	B	508	-	3,3,3	0.06	0	2,2,2	0.16	0
5	EDO	B	510	-	3,3,3	0.15	0	2,2,2	0.17	0
3	PO4	A	503	-	4,4,4	0.56	0	6,6,6	0.46	0
5	EDO	A	506	-	3,3,3	0.12	0	2,2,2	0.46	0
5	EDO	A	513	-	3,3,3	0.17	0	2,2,2	0.13	0
7	DMS	A	514	-	3,3,3	0.27	0	3,3,3	0.26	0
6	PEG	A	507	-	6,6,6	0.21	0	5,5,5	0.12	0
3	PO4	B	504	-	4,4,4	0.93	0	6,6,6	0.42	0
5	EDO	A	510	-	3,3,3	0.09	0	2,2,2	0.06	0
5	EDO	B	509	-	3,3,3	0.07	0	2,2,2	0.22	0
7	DMS	A	516	-	3,3,3	0.20	0	3,3,3	0.16	0
2	WIR	A	501	-	33,35,35	4.13	12 (36%)	38,53,53	2.62	10 (26%)
5	EDO	A	512	-	3,3,3	0.13	0	2,2,2	0.11	0
3	PO4	A	502	-	4,4,4	0.80	0	6,6,6	0.48	0
5	EDO	B	506	-	3,3,3	0.17	0	2,2,2	0.04	0
5	EDO	B	507	-	3,3,3	0.07	0	2,2,2	0.21	0
3	PO4	A	504	-	4,4,4	0.80	0	6,6,6	0.40	0
2	WIR	B	501	-	33,35,35	3.83	13 (39%)	38,53,53	2.80	13 (34%)
5	EDO	B	511	-	3,3,3	0.06	0	2,2,2	0.25	0
6	PEG	A	517	-	6,6,6	0.15	0	5,5,5	0.10	0
5	EDO	B	512	-	3,3,3	0.12	0	2,2,2	0.20	0
5	EDO	A	508	-	3,3,3	0.13	0	2,2,2	0.29	0
3	PO4	B	502	-	4,4,4	0.67	0	6,6,6	0.44	0
3	PO4	B	503	-	4,4,4	0.74	0	6,6,6	0.43	0
5	EDO	A	515	-	3,3,3	0.04	0	2,2,2	0.14	0
5	EDO	A	509	-	3,3,3	0.08	0	2,2,2	0.26	0

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
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	B	508	-	-	0/1/1/1	-
5	EDO	B	510	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	513	-	-	1/1/1/1	-
6	PEG	A	507	-	-	1/4/4/4	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	B	509	-	-	0/1/1/1	-
2	WIR	A	501	-	-	0/12/32/32	0/5/5/5
5	EDO	A	512	-	-	1/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
5	EDO	B	507	-	-	1/1/1/1	-
2	WIR	B	501	-	1/1/3/7	3/12/32/32	0/5/5/5
6	PEG	A	517	-	-	0/4/4/4	-
5	EDO	B	511	-	-	1/1/1/1	-
5	EDO	B	512	-	-	0/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	A	515	-	-	1/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	WIR	C25-C20	-13.73	1.37	1.51
2	A	501	WIR	C21-C20	-13.70	1.41	1.55
2	B	501	WIR	C25-C20	-12.82	1.38	1.51
2	B	501	WIR	C21-C20	-11.39	1.43	1.55
2	A	501	WIR	C23-C24	-7.76	1.38	1.50

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	WIR	C25-C20-C21	10.56	110.09	102.58
2	B	501	WIR	C25-C20-C21	7.06	107.60	102.58
2	B	501	WIR	C25-C20-N19	6.37	126.08	114.39
2	A	501	WIR	C25-C20-N19	6.27	125.90	114.39
2	B	501	WIR	C24-C25-C20	-5.90	105.30	110.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	WIR	C20

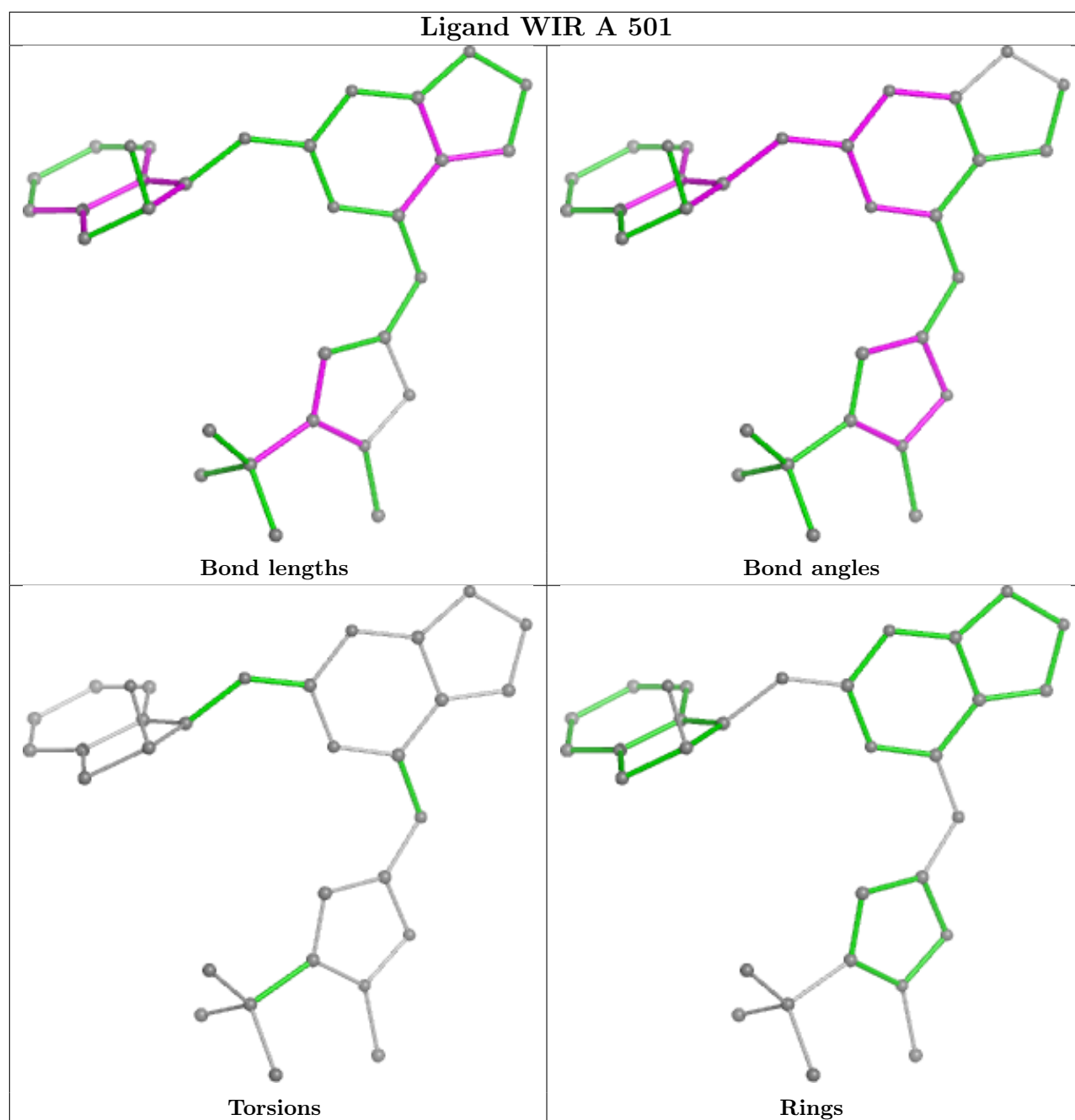
5 of 12 torsion outliers are listed below:

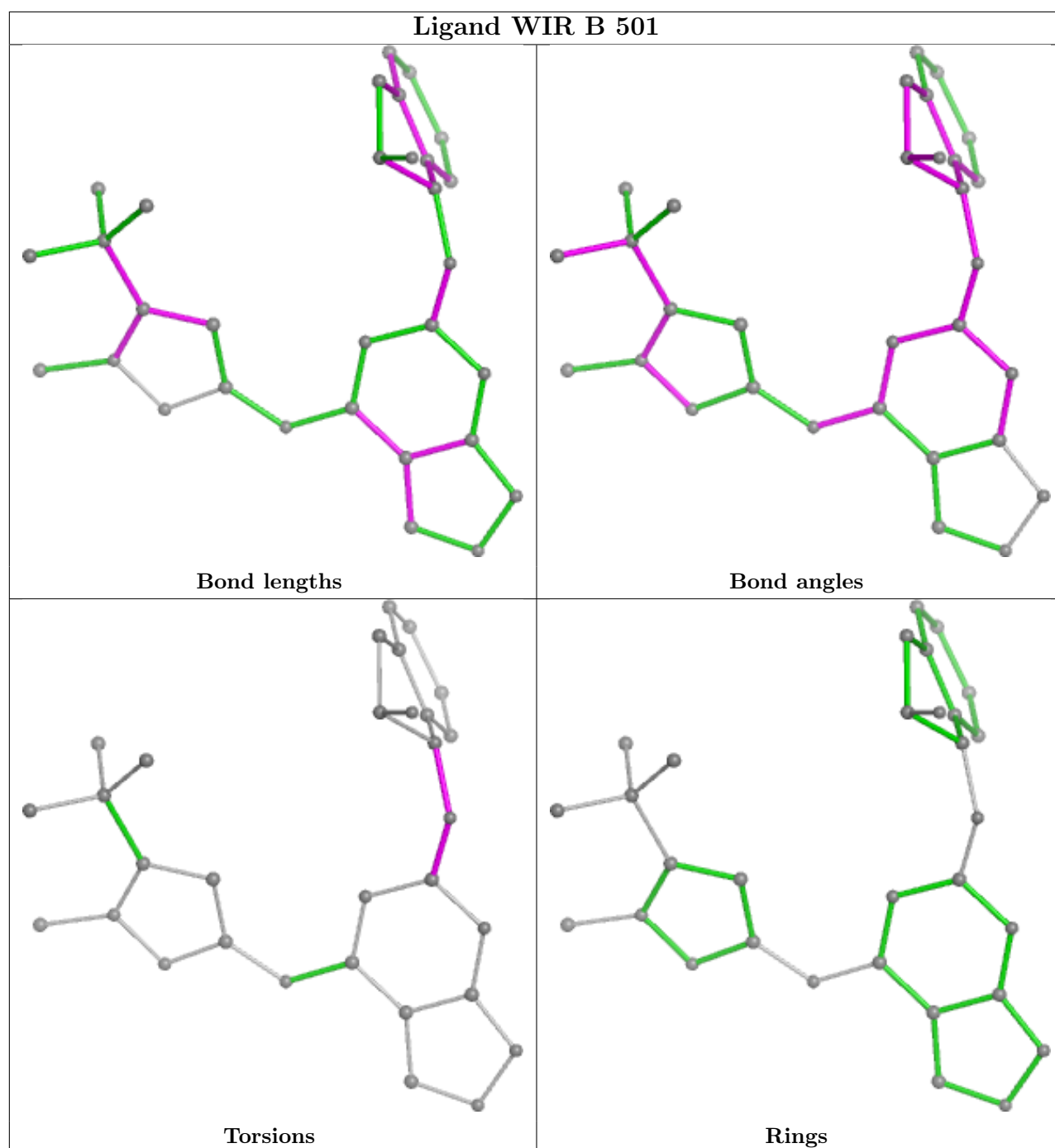
Mol	Chain	Res	Type	Atoms
2	B	501	WIR	N17-C18-N19-C20
2	B	501	WIR	N30-C18-N19-C20
6	A	507	PEG	O2-C3-C4-O4
5	A	509	EDO	O1-C1-C2-O2
5	A	510	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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	454/487 (93%)	-0.02	10 (2%) 62 63	19, 40, 69, 105	24 (5%)
1	B	452/487 (92%)	0.36	20 (4%) 39 40	21, 48, 81, 105	9 (1%)
All	All	906/974 (93%)	0.17	30 (3%) 49 51	19, 44, 76, 105	33 (3%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	5.3
1	B	159	ALA	4.3
1	A	155	ALA	3.7
1	A	196	MET	3.6
1	B	196	MET	3.4

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

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

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 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.

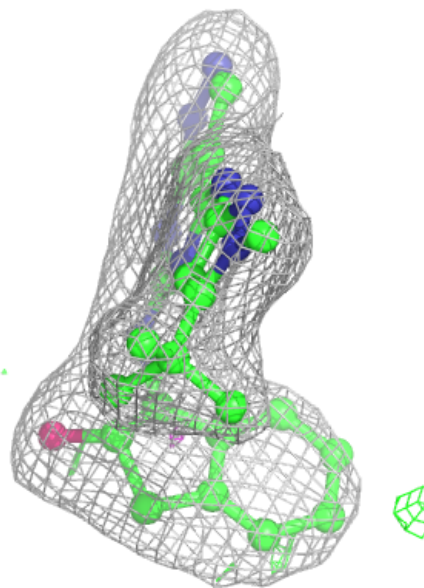
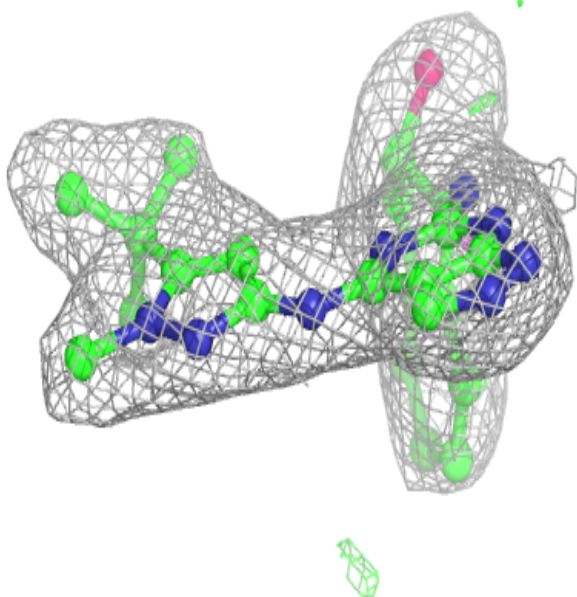
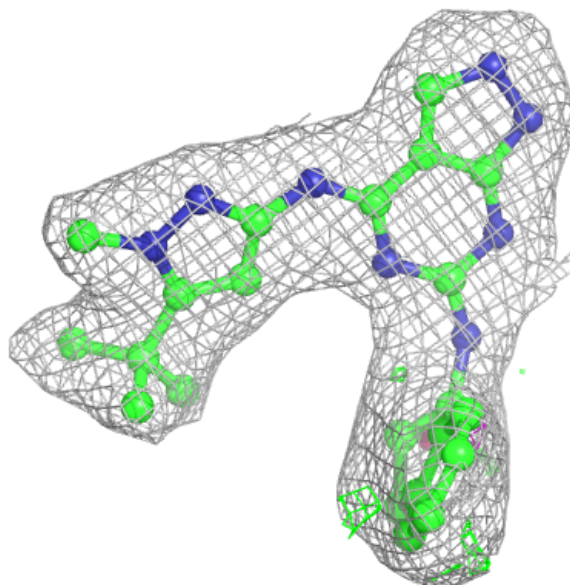
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	510	4/4	0.66	0.21	77,80,80,90	0
7	DMS	A	516	4/4	0.71	0.40	48,52,57,60	4
7	DMS	A	514	4/4	0.74	0.32	28,32,34,51	4
5	EDO	B	508	4/4	0.77	0.41	40,44,45,50	4
6	PEG	A	517	7/7	0.80	0.20	74,82,91,96	0
5	EDO	B	507	4/4	0.81	0.18	66,66,70,70	0
3	PO4	A	504	5/5	0.82	0.11	65,73,79,86	0
5	EDO	A	513	4/4	0.84	0.16	51,54,56,58	0
6	PEG	A	507	7/7	0.85	0.20	59,75,83,84	0
5	EDO	A	509	4/4	0.87	0.19	71,74,74,79	0
3	PO4	B	503	5/5	0.88	0.16	37,40,45,52	5
3	PO4	B	504	5/5	0.89	0.14	41,42,45,49	5
5	EDO	A	515	4/4	0.90	0.18	61,61,66,78	0
5	EDO	A	508	4/4	0.91	0.19	38,54,58,70	0
5	EDO	B	512	4/4	0.91	0.12	46,50,55,68	0
5	EDO	B	510	4/4	0.92	0.25	48,49,49,55	0
5	EDO	B	511	4/4	0.93	0.12	45,46,48,57	0
3	PO4	A	503	5/5	0.94	0.18	54,63,69,70	0
5	EDO	B	506	4/4	0.94	0.09	38,39,40,45	0
5	EDO	A	511	4/4	0.94	0.15	36,48,48,62	0
5	EDO	A	512	4/4	0.94	0.12	39,40,50,55	0
5	EDO	B	509	4/4	0.94	0.08	44,46,50,59	0
2	WIR	B	501	31/31	0.94	0.09	30,39,68,69	0
4	UNX	B	505	1/1	0.96	0.13	18,18,18,18	0
5	EDO	A	506	4/4	0.96	0.07	31,35,35,36	0
3	PO4	A	502	5/5	0.96	0.12	39,53,55,76	0
3	PO4	B	502	5/5	0.96	0.09	44,46,46,59	0
2	WIR	A	501	31/31	0.98	0.05	21,28,37,40	0
4	UNX	A	505	1/1	0.99	0.11	8,8,8,8	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.



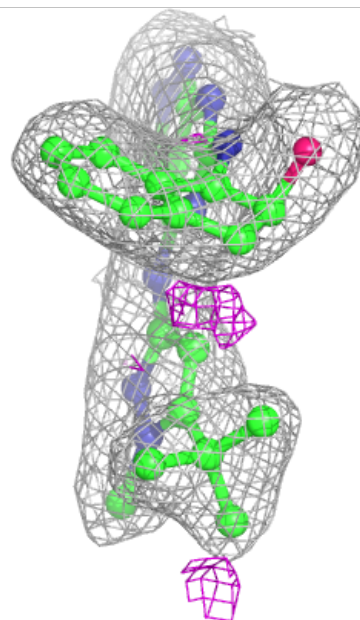
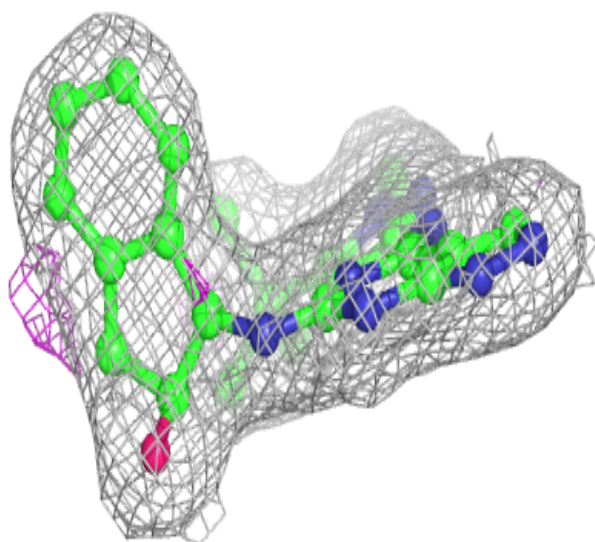
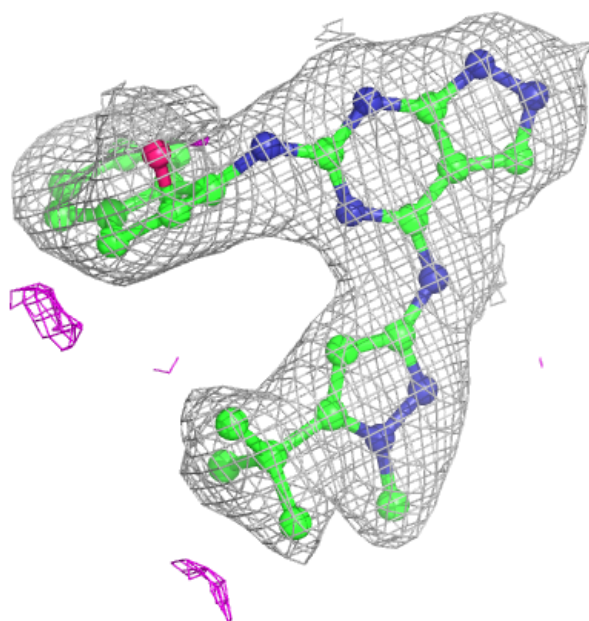
**Electron density around WIR B 501:**

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



**Electron density around WIR 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)



## 5.5 Other polymers ⓘ

There are no such residues in this entry.