

# Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2023 – 03:17 pm GMT

PDB ID : 7ZTL

Title: Crystal structure of a covalently linked Aurora-A N-Myc complex

Authors: Diebold, M.; Schindelin, H.

Deposited on : 2022-05-11

Resolution : 1.90 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.31.3 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

 $\begin{tabular}{lll} CCP4 & : & 7.0.044 & (Gargrove) \end{tabular}$ 

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

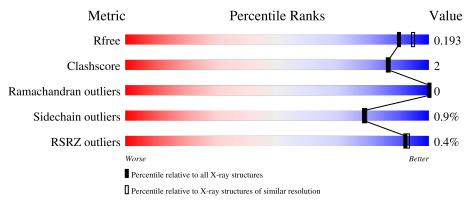
Validation Pipeline (wwPDB-VP) : 2.31.3

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.90 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 >=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 <=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	309			80%	5%	15%				
2	В	62	24%	5%	71%						



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 2589 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 Aurora kinase A.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2161	C 1395	N 368	O 389	P 1	S 8	0	6	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	MET	-	initiating methionine	UNP O14965
A	96	LYS	-	expression tag	UNP O14965
A	97	HIS	-	expression tag	UNP O14965
A	98	HIS	-	expression tag	UNP O14965
A	99	HIS	-	expression tag	UNP O14965
A	100	HIS	-	expression tag	UNP O14965
A	101	HIS	-	expression tag	UNP O14965
A	102	HIS	-	expression tag	UNP O14965
A	103	PRO	_	expression tag	UNP O14965
A	104	MET	-	expression tag	UNP O14965
A	105	SER	-	expression tag	UNP O14965
A	106	ASP	-	expression tag	UNP O14965
A	107	TYR	-	- expression tag	
A	108	ASP	-	expression tag	UNP O14965
A	109	ILE	-	expression tag	UNP O14965
A	110	PRO	-	expression tag	UNP O14965
A	111	THR	-	expression tag	UNP O14965
A	112	THR	-	expression tag	UNP O14965
A	113	GLU	-	expression tag	UNP O14965
A	114	ASN	-	expression tag	UNP O14965
A	115	LEU	-	expression tag	UNP O14965
A	116	TYR	-	expression tag	UNP O14965
A	117	PHE	-	expression tag	UNP O14965
A	118	GLN	- expression tag		UNP O14965
A	119	GLY	- expression tag		UNP O14965
A	120	ALA	- expression tag		UNP O14965
A	121	MET	-	expression tag	UNP O14965

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Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	CYS	engineered mutation	UNP O14965
A	339	CYS	LYS	engineered mutation	UNP O14965
A	393	ALA	CYS	engineered mutation	UNP O14965

• Molecule 2 is a protein called N-myc proto-oncogene protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	D	10	Total	С	N	О	S	0	0	0
	Б	18	147	97	21	28	1	U		0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	85	LYS	ASN	engineered mutation	UNP P04198

• Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

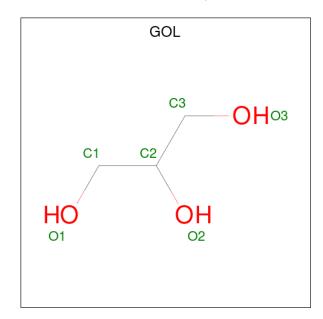
Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
3	Δ	1	Total	С	N	О	Р	0	0
9	A	1	27	10	5	10	2		

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

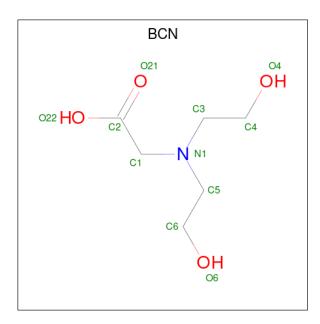
 $\bullet$  Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 



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

 $\bullet$  Molecule 6 is BICINE (three-letter code: BCN) (formula:  $\mathrm{C_6H_{13}NO_4}).$ 



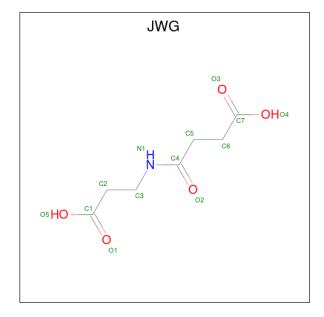


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 11	C 6	N 1	O 4	0	0

• Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

• Molecule 8 is 4-(3-hydroxy-3-oxopropylamino)-4-oxidanylidene-butanoic acid (three-letter code: JWG) (formula:  $C_7H_{11}NO_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total C N O 12 7 1 4	0	0

## $\bullet\,$ Molecule 9 is water.

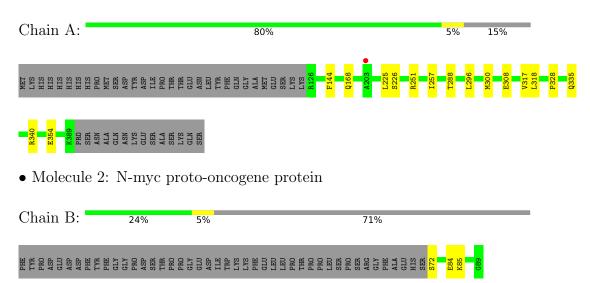
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	196	Total O 198 198	0	2
9	В	12	Total O 12 12	0	0



# 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: Aurora kinase A





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	86.61Å 86.61Å 91.79Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	39.17 - 1.90	Depositor
Resolution (A)	39.17 - 1.90	EDS
% Data completeness	100.0 (39.17-1.90)	Depositor
(in resolution range)	99.9 (39.17-1.90)	EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.24 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D.D.	0.163 , 0.193	Depositor
$R, R_{free}$	0.163 , $0.193$	DCC
$R_{free}$ test set	1594 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 52.7	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: ADP, JWG, TPO, GOL, BCN, NA, MG

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.41	0/2215	0.62	0/2998	
2	В	0.39	0/152	0.51	0/206	
All	All	0.41	0/2367	0.61	0/3204	

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	2161	0	2132	9	0
2	В	147	0	137	2	0
3	A	27	0	12	0	0
4	A	2	0	0	0	0
5	A	18	0	24	0	0
6	A	11	0	10	1	0
7	A	1	0	0	0	0
8	В	12	0	0	0	0
9	A	198	0	0	1	2
9	В	12	0	0	0	1
All	All	2589	0	2315	10	2



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 2.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:335:GLN:HG3	2:B:84:GLU:OE1	2.06	0.55
1:A:335:GLN:HE21	2:B:85:LYS:NZ	2.05	0.55
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.91	0.53
1:A:296:LEU:HD22	1:A:300[A]:MET:HG2	1.92	0.51
1:A:251[B]:ARG:NH2	1:A:308:GLU:OE2	2.41	0.51
1:A:144:PHE:HD1	1:A:168:GLN:HB3	1.81	0.46
1:A:225:LEU:O	1:A:226:SER:HB2	2.17	0.44
6:A:506:BCN:H41	6:A:506:BCN:H52	1.82	0.43
1:A:340:ARG:NE	9:A:609:HOH:O	2.51	0.42
1:A:257[A]:ILE:O	1:A:318:LEU:HD11	2.20	0.42

All (2) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
9:A:771:HOH:O	9:A:775:HOH:O[5_565]	2.15	0.05
9:A:663:HOH:O	9:B:208:HOH:O[2_564]	2.17	0.03

## 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	267/309 (86%)	259 (97%)	8 (3%)	0	100	100	
2	В	16/62~(26%)	16 (100%)	0	0	100	100	
All	All	283/371 (76%)	275 (97%)	8 (3%)	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	224/272 (82%)	222 (99%)	2 (1%)	78 79		
2	В	16/56 (29%)	15 (94%)	1 (6%)	18 8		
All	All	240/328 (73%)	237 (99%)	3 (1%)	78 68		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354[A]	GLU
1	A	354[B]	GLU
2	В	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	335	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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).



М	1 Typ	_	Chain	Pog	Link	B	ond leng	$_{ m gths}$	В	ond ang	les
Mol   Type	е	Chain	ain Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
1	TPO	)	A	288	1	8,10,11	1.58	1 (12%)	10,14,16	1.46	1 (10%)

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	
1	TPO	A	288	1	-	1/9/11/13	-	

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	288	TPO	P-O1P	3.10	1.60	1.50

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$	
1	A	288	TPO	P-OG1-CB	-3.33	113.16	123.21	

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	288	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	Tuno	Chain	Res	Res Link Bond lengths			ths	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	505	-	5,5,5	0.87	0	5,5,5	1.19	0
5	GOL	A	504	_	5,5,5	0.88	0	5,5,5	1.26	1 (20%)
5	GOL	A	507	-	5,5,5	0.90	0	5,5,5	0.93	0
3	ADP	A	501	4	24,29,29	1.01	1 (4%)	29,45,45	1.25	2 (6%)
6	BCN	A	506	4	10,10,10	0.70	0	11,11,11	0.97	1 (9%)
8	JWG	В	101	2,1	11,11,12	0.61	0	10,12,14	1.14	1 (10%)

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	GOL	A	505	-	-	0/4/4/4	-
5	GOL	A	504	-	-	2/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-
3	ADP	A	501	4	-	0/12/32/32	0/3/3/3
6	BCN	A	506	4	-	0/10/10/10	-
8	JWG	В	101	2,1	-	3/9/10/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	A	501	ADP	C5-C4	2.40	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
3	A	501	ADP	N3-C2-N1	-3.24	123.61	128.68
8	В	101	JWG	C3-N1-C4	2.41	127.31	122.84
6	A	506	BCN	C4-C3-N1	-2.28	105.22	113.40
3	A	501	ADP	C2-N1-C6	2.12	122.38	118.75
5	A	504	GOL	C3-C2-C1	-2.08	103.60	111.70

There are no chirality outliers.



All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	GOL	O2-C2-C3-O3
5	A	504	GOL	C1-C2-C3-O3
5	A	507	GOL	C1-C2-C3-O3
5	A	507	GOL	O2-C2-C3-O3
8	В	101	JWG	C2-C3-N1-C4
8	В	101	JWG	C5-C6-C7-O3
8	В	101	JWG	C5-C6-C7-O4

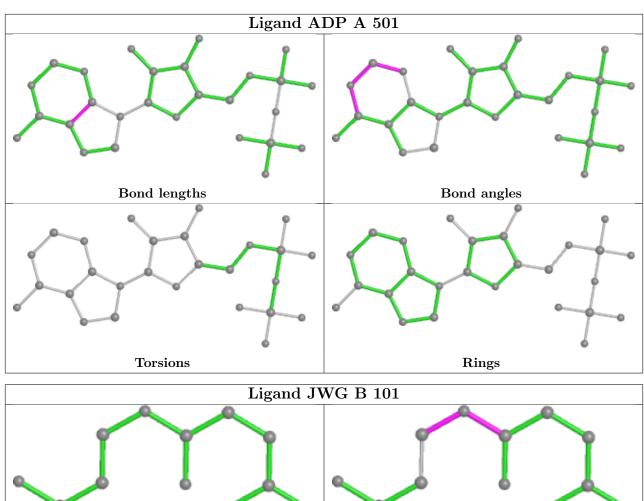
There are no ring outliers.

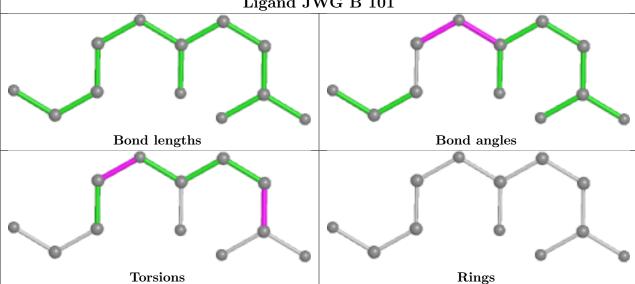
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	506	BCN	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 then 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	263/309~(85%)	-0.30	1 (0%) 92 93	29, 42, 60, 91	1 (0%)
2	В	18/62 (29%)	-0.23	0 100 100	40, 51, 91, 105	0
All	All	281/371 (75%)	-0.29	1 (0%) 92 93	29, 43, 63, 105	1 (0%)

#### All (1) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	203	ALA	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	TPO	A	288	11/12	0.95	0.10	48,54,56,59	0

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

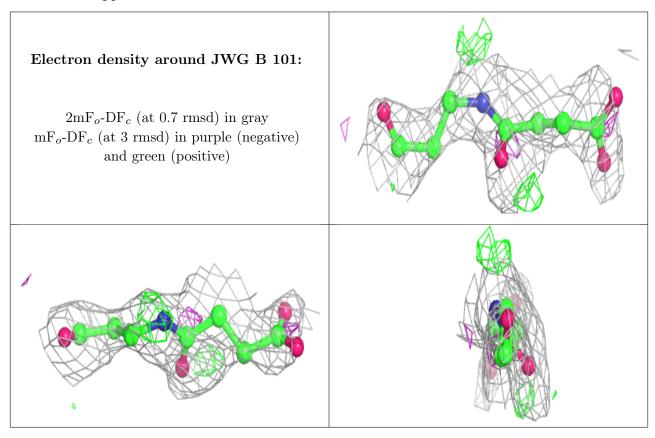
## 6.4 Ligands (i)

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,  $95^{th}$  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.

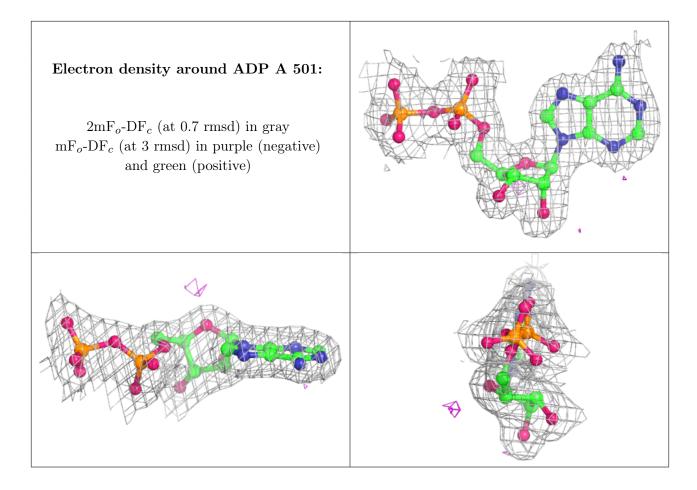


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
8	JWG	В	101	12/13	0.83	0.26	66,71,74,75	0
5	GOL	A	507	6/6	0.84	0.22	60,68,71,75	0
5	GOL	A	504	6/6	0.91	0.12	47,48,57,58	0
5	GOL	A	505	6/6	0.93	0.23	46,56,60,61	0
7	NA	A	508	1/1	0.97	0.04	55,55,55,55	0
6	BCN	A	506	11/11	0.97	0.11	29,30,34,35	0
3	ADP	A	501	27/27	0.99	0.09	27,30,34,35	0
4	MG	A	503	1/1	0.99	0.10	28,28,28,28	0
4	MG	A	502	1/1	1.00	0.07	32,32,32,32	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.







# 6.5 Other polymers (i)

There are no such residues in this entry.

