



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 2OLV / pdb\_00002olv  
Title : Structural Insight Into the Transglycosylation Step Of Bacterial Cell Wall Biosynthesis : Donor Ligand Complex  
Authors : Lovering, A.L.; De Castro, L.; Lim, D.; Strynadka, N.C.J.  
Deposited on : 2007-01-19  
Resolution : 2.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

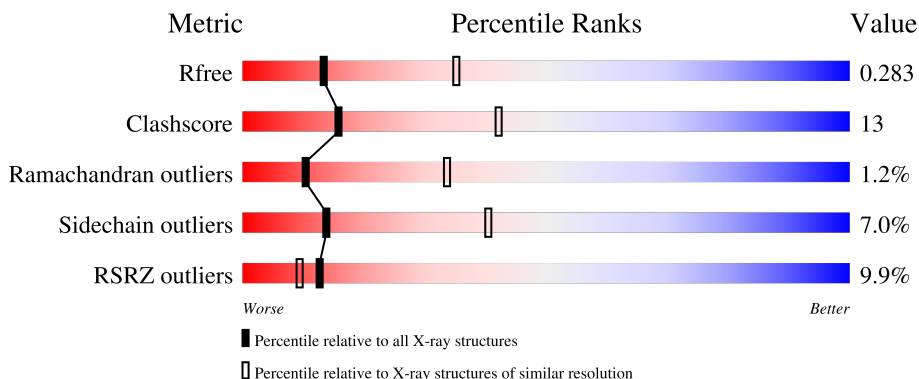
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	669	
1	B	669	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9878 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	617	4851	3038	837	964	12	0	0	0
1	B	618	4859	3042	839	966	12	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

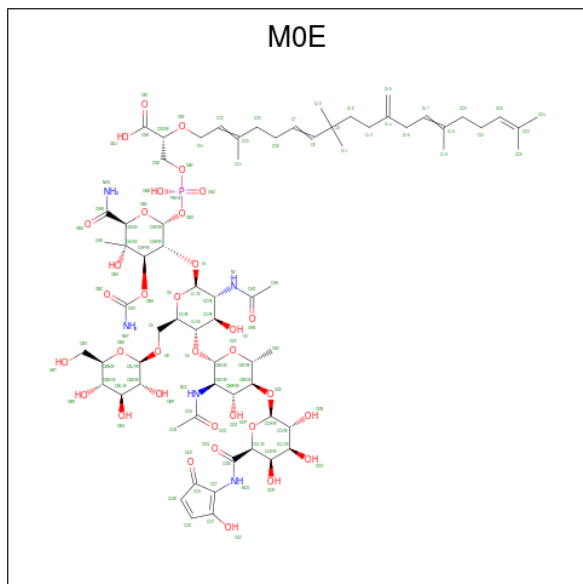
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MSE	-	SEE REMARK 999	UNP Q2YY56
A	106	MSE	MET	modified residue	UNP Q2YY56
A	257	MSE	MET	modified residue	UNP Q2YY56
A	285	PRO	ALA	variant	UNP Q2YY56
A	311	MSE	MET	modified residue	UNP Q2YY56
A	335	MSE	MET	modified residue	UNP Q2YY56
A	413	MSE	MET	modified residue	UNP Q2YY56
A	439	THR	VAL	variant	UNP Q2YY56
A	548	MSE	MET	modified residue	UNP Q2YY56
A	555	MSE	MET	modified residue	UNP Q2YY56
A	559	MSE	MET	modified residue	UNP Q2YY56
A	580	MSE	MET	modified residue	UNP Q2YY56
A	618	MSE	MET	modified residue	UNP Q2YY56
A	622	MSE	MET	modified residue	UNP Q2YY56
A	652	MSE	MET	modified residue	UNP Q2YY56
B	59	MSE	-	SEE REMARK 999	UNP Q2YY56
B	106	MSE	MET	modified residue	UNP Q2YY56
B	257	MSE	MET	modified residue	UNP Q2YY56
B	285	PRO	ALA	variant	UNP Q2YY56
B	311	MSE	MET	modified residue	UNP Q2YY56
B	335	MSE	MET	modified residue	UNP Q2YY56
B	413	MSE	MET	modified residue	UNP Q2YY56
B	439	THR	VAL	variant	UNP Q2YY56
B	548	MSE	MET	modified residue	UNP Q2YY56
B	555	MSE	MET	modified residue	UNP Q2YY56

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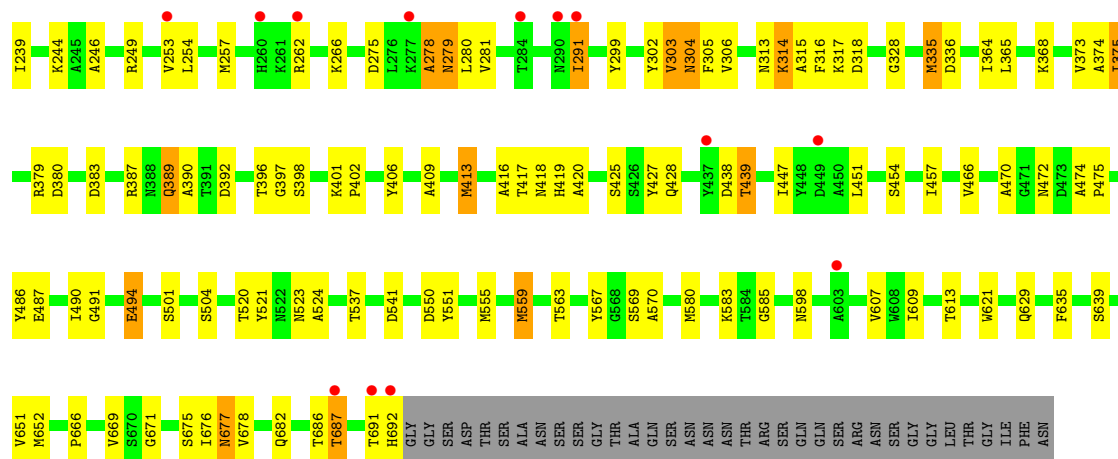
Chain	Residue	Modelled	Actual	Comment	Reference
B	559	MSE	MET	modified residue	UNP Q2YY56
B	580	MSE	MET	modified residue	UNP Q2YY56
B	618	MSE	MET	modified residue	UNP Q2YY56
B	622	MSE	MET	modified residue	UNP Q2YY56
B	652	MSE	MET	modified residue	UNP Q2YY56

- Molecule 2 is MOENOMYCIN (CCD ID: M0E) (formula:  $C_{69}H_{106}N_5O_{34}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
2	A	1	Total	84	44	5	34	1	0	0
2	B	1	Total	84	44	5	34	1	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.56Å 212.21Å 91.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 2.80 44.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-2.80) 99.9 (44.15-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.81Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.231 , 0.280 0.237 , 0.283	Depositor DCC
$R_{free}$ test set	1955 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% 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: M0E

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	0.72	1/4943 (0.0%)	0.87	5/6662 (0.1%)
1	B	0.69	0/4951	0.89	1/6673 (0.0%)
All	All	0.71	1/9894 (0.0%)	0.88	6/13335 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	VAL	CA-CB	5.32	1.62	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	THR	N-CA-C	5.77	118.62	110.14
1	A	302	TYR	N-CA-C	-5.73	105.12	111.71
1	A	385	VAL	CB-CA-C	-5.25	105.20	112.24
1	B	303	VAL	CB-CA-C	-5.11	105.17	112.22
1	A	303	VAL	CB-CA-C	-5.06	105.24	112.22

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLU	Peptide
1	A	608	TRP	Peptide
1	B	120	GLU	Peptide

## 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	4851	0	4666	131	1
1	B	4859	0	4672	117	0
2	A	84	0	62	6	0
2	B	84	0	62	5	0
All	All	9878	0	9462	257	1

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 13.

The worst 5 of 257 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:253:VAL:HG12	1:A:257:MSE:HE2	1.18	1.14
1:A:254:LEU:HA	1:A:257:MSE:HE3	1.45	0.97
1:B:253:VAL:HG12	1:B:257:MSE:HE2	1.52	0.89
1:B:254:LEU:HA	1:B:257:MSE:HE3	1.56	0.88
1:A:551:TYR:HB2	1:A:555:MSE:HE3	1.55	0.87

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:OH	1:A:126:TYR:OH[2_465]	2.15	0.05

## 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	613/669 (92%)	538 (88%)	67 (11%)	8 (1%)	9	31
1	B	614/669 (92%)	554 (90%)	53 (9%)	7 (1%)	11	36
All	All	1227/1338 (92%)	1092 (89%)	120 (10%)	15 (1%)	10	34

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	PHE
1	A	278	ALA
1	A	317	LYS
1	A	337	LYS
1	A	439	THR

### 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	520/546 (95%)	487 (94%)	33 (6%)	16	45
1	B	521/546 (95%)	481 (92%)	40 (8%)	12	36
All	All	1041/1092 (95%)	968 (93%)	73 (7%)	14	40

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	428	GLN

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Mol	Chain	Res	Type
1	B	682	GLN
1	B	487	GLU
1	B	550	ASP
1	A	537	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	GLN
1	B	334	ASN
1	B	692	HIS
1	B	638	HIS
1	B	282	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 oligosaccharides 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
2	M0E	B	901	-	87,89,114	1.57	8 (9%)	118,134,166	1.68	28 (23%)
2	M0E	A	901	-	87,89,114	1.60	9 (10%)	118,134,166	1.57	25 (21%)

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	M0E	B	901	-	-	22/56/175/206	0/6/6/6
2	M0E	A	901	-	-	19/56/175/206	0/6/6/6

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	M0E	CCX-CCW	8.43	1.54	1.35
2	A	901	M0E	CCX-CCW	8.33	1.53	1.35
2	A	901	M0E	OCQ-CCM	6.99	1.36	1.23
2	B	901	M0E	OCQ-CCM	6.80	1.36	1.23
2	B	901	M0E	CCT-CCU	-3.75	1.39	1.50

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	M0E	CCW-CCX-CCY	-5.96	103.45	108.28
2	A	901	M0E	CCW-CCX-CCY	-5.49	103.82	108.28
2	B	901	M0E	OCP-CCH-CCI	-4.83	100.44	110.37
2	B	901	M0E	OBH-CAV-NAT	4.79	118.34	110.92
2	A	901	M0E	OBH-CAV-NAT	4.43	117.78	110.92

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

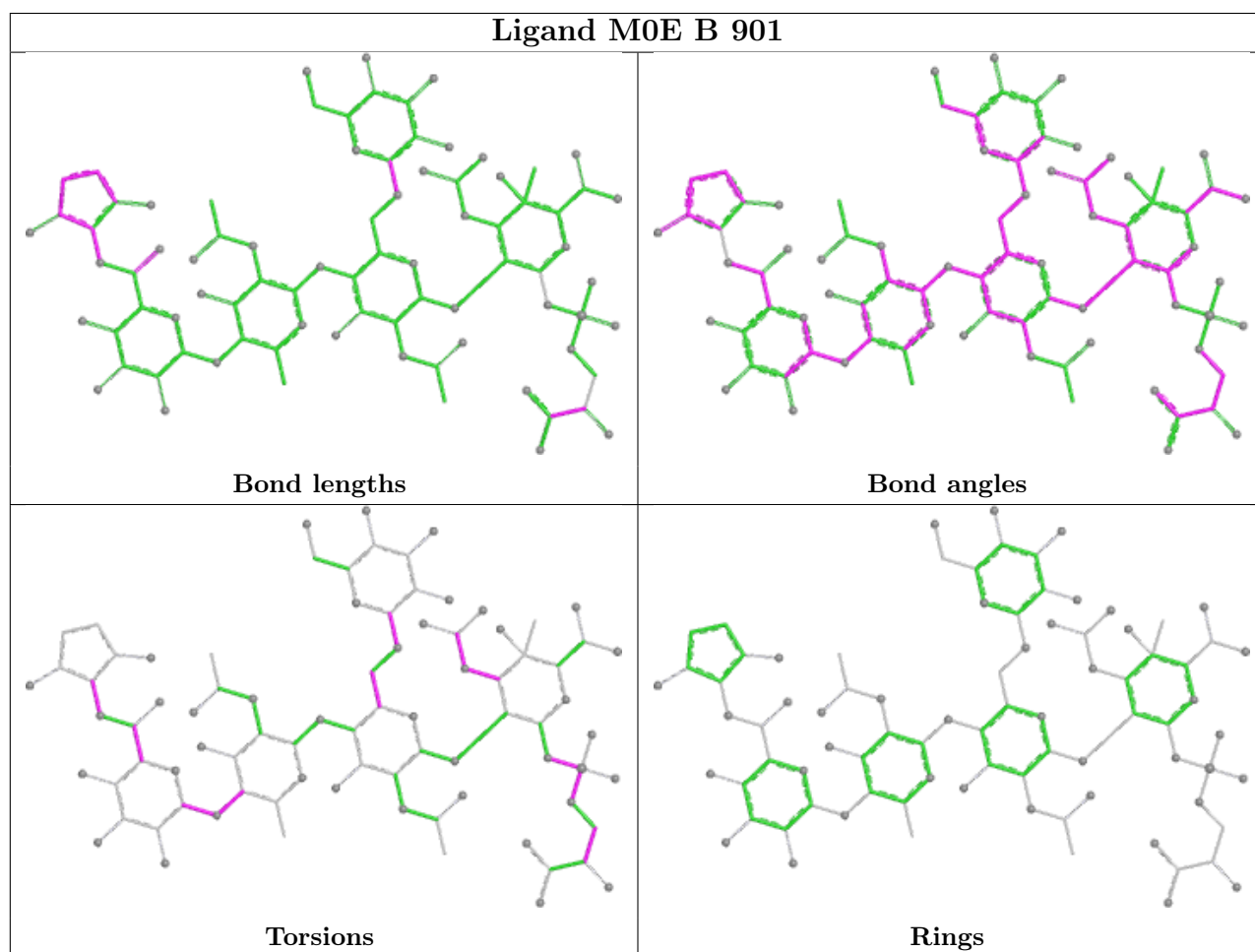
Mol	Chain	Res	Type	Atoms
2	A	901	M0E	ODF-CDG-CDK-OBF
2	A	901	M0E	CDH-CDG-CDK-OBF
2	A	901	M0E	OBE-CAQ-CAW-NAU
2	A	901	M0E	OBC-CAV-OBH-CAP
2	A	901	M0E	NAT-CAV-OBH-CAP

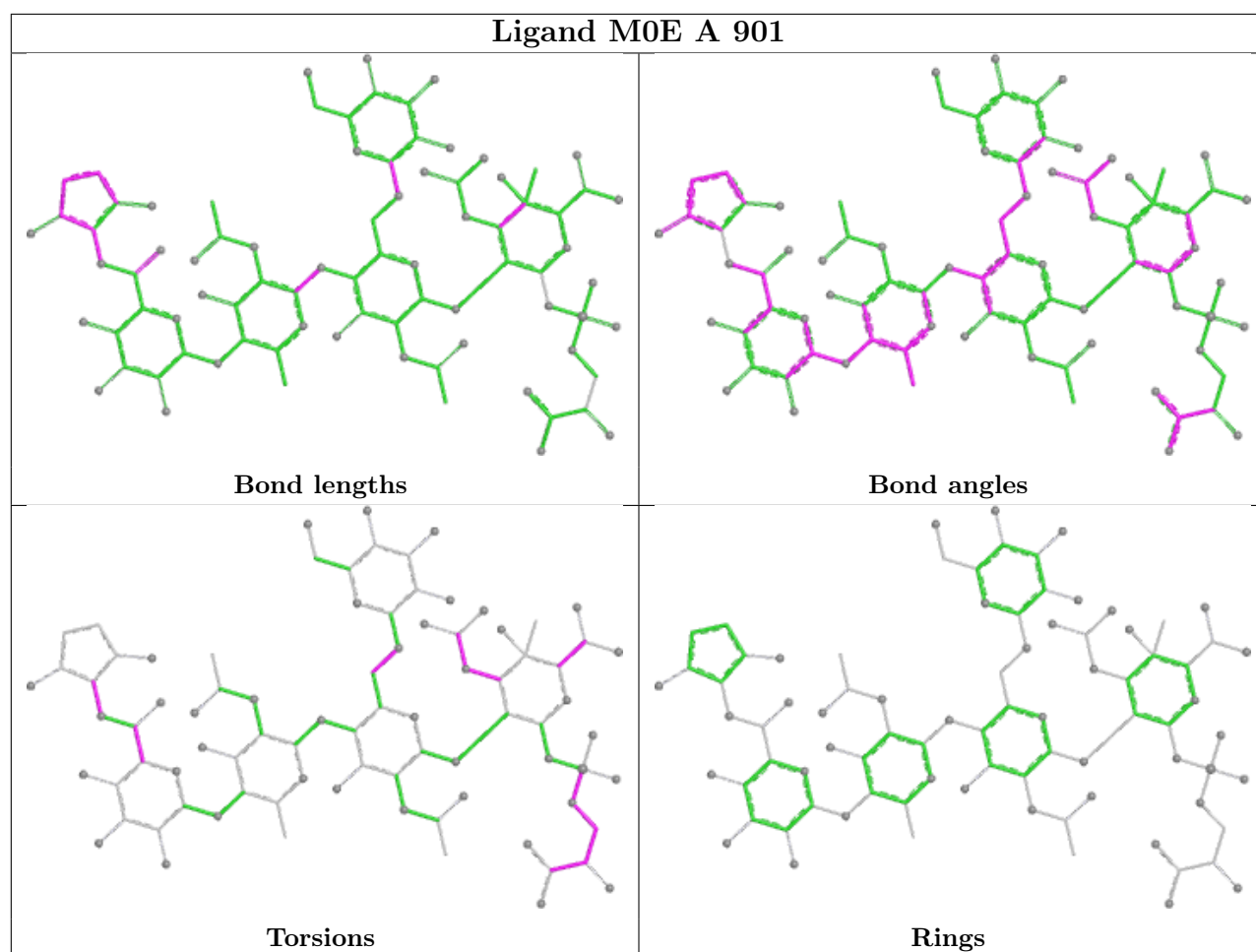
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	M0E	5	0
2	A	901	M0E	6	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	605/669 (90%)	0.91	66 (10%) 10 8	31, 71, 107, 127	0
1	B	606/669 (90%)	0.70	54 (8%) 15 11	33, 72, 108, 127	0
All	All	1211/1338 (90%)	0.81	120 (9%) 13 9	31, 72, 108, 127	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	TYR	5.5
1	A	162	HIS	5.1
1	A	133	ILE	4.6
1	A	165	ILE	4.2
1	B	149	LEU	3.9

### 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](#)

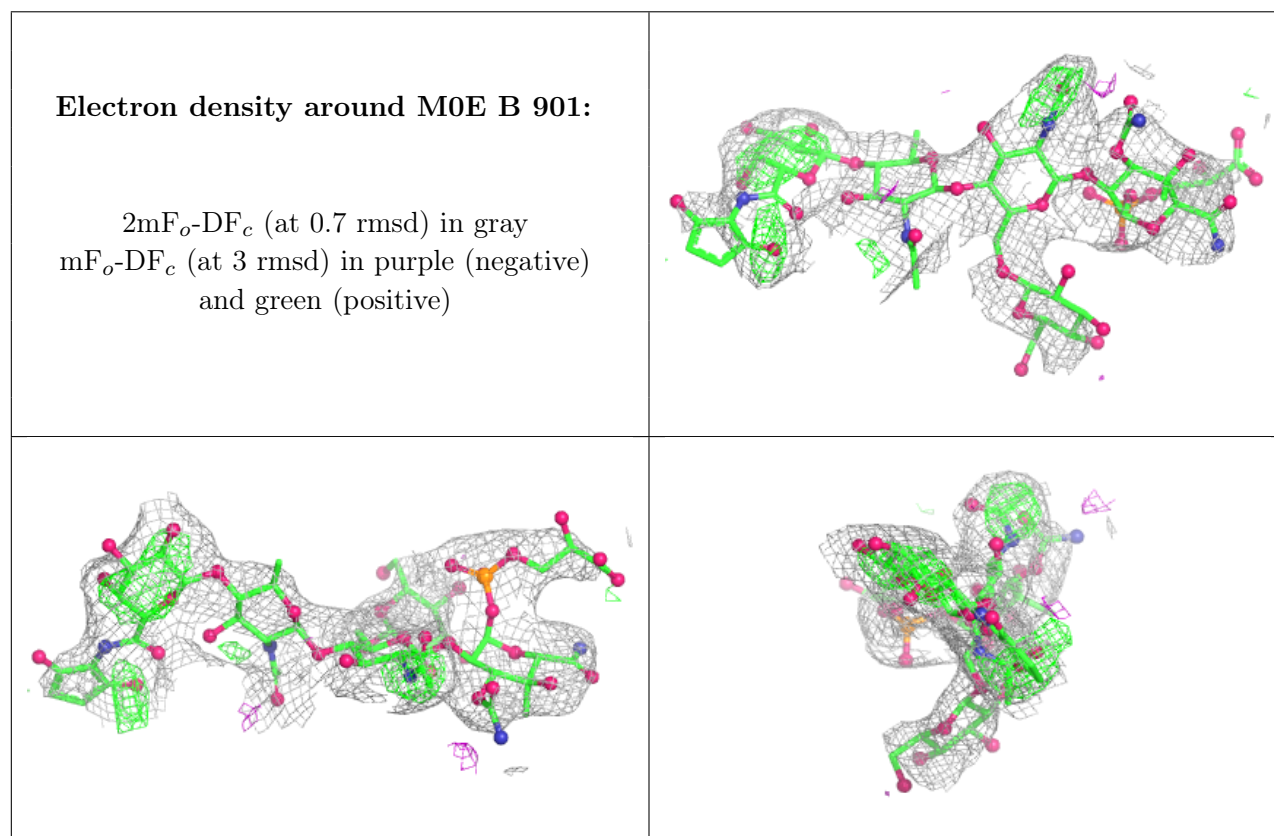
There are no oligosaccharides in this entry.

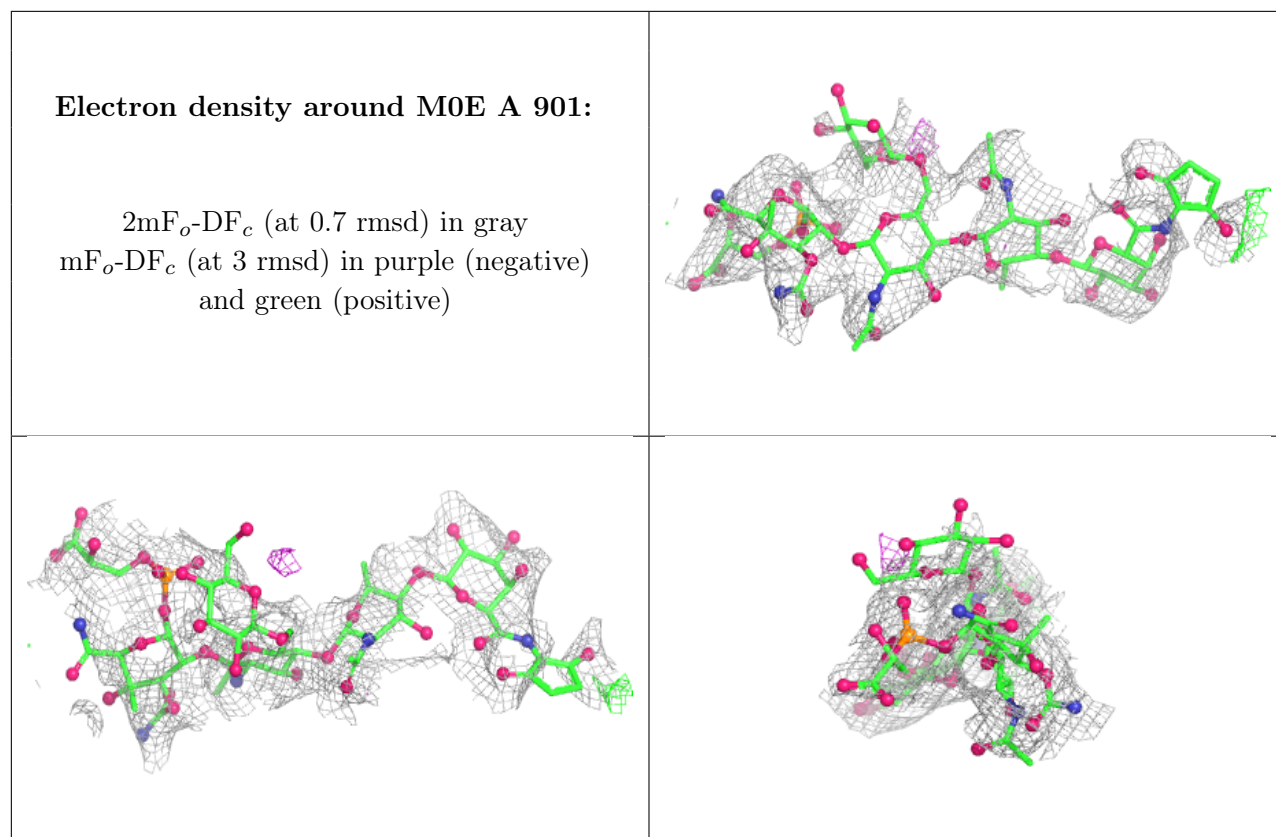
### 6.4 Ligands [i](#)

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	M0E	B	901	84/109	0.65	0.23	113,116,124,124	0
2	M0E	A	901	84/109	0.66	0.17	113,116,124,125	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.