



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2021 – 12:39 PM JST

PDB ID : 7BVA  
Title : Crystal structure of UDP-N-acetylmuramic Acid L-alanine ligase (MurC) from Mycobacterium bovis  
Authors : Seo, P.W.; Kim, J.S.  
Deposited on : 2020-04-10  
Resolution : 2.30 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
Xtriage (Phenix)	:	1.13
EDS	:	2.18
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)	:	2.18

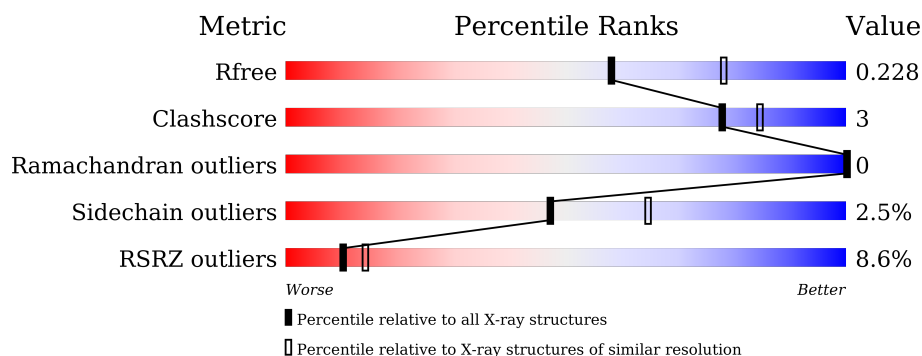
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	519	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	519	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7288 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	480	Total	C	N	O	S	0	0	0
			3497	2185	638	657	17			
1	B	479	Total	C	N	O	S	0	0	0
			3488	2180	637	654	17			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P65473
A	-23	SER	-	expression tag	UNP P65473
A	-22	TYR	-	expression tag	UNP P65473
A	-21	TYR	-	expression tag	UNP P65473
A	-20	HIS	-	expression tag	UNP P65473
A	-19	HIS	-	expression tag	UNP P65473
A	-18	HIS	-	expression tag	UNP P65473
A	-17	HIS	-	expression tag	UNP P65473
A	-16	HIS	-	expression tag	UNP P65473
A	-15	HIS	-	expression tag	UNP P65473
A	-14	ASP	-	expression tag	UNP P65473
A	-13	TYR	-	expression tag	UNP P65473
A	-12	ASP	-	expression tag	UNP P65473
A	-11	ILE	-	expression tag	UNP P65473
A	-10	PRO	-	expression tag	UNP P65473
A	-9	THR	-	expression tag	UNP P65473
A	-8	THR	-	expression tag	UNP P65473
A	-7	GLU	-	expression tag	UNP P65473
A	-6	ASN	-	expression tag	UNP P65473
A	-5	LEU	-	expression tag	UNP P65473
A	-4	TYR	-	expression tag	UNP P65473
A	-3	PHE	-	expression tag	UNP P65473
A	-2	GLN	-	expression tag	UNP P65473
A	-1	GLY	-	expression tag	UNP P65473
A	0	HIS	-	expression tag	UNP P65473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP P65473
B	-23	SER	-	expression tag	UNP P65473
B	-22	TYR	-	expression tag	UNP P65473
B	-21	TYR	-	expression tag	UNP P65473
B	-20	HIS	-	expression tag	UNP P65473
B	-19	HIS	-	expression tag	UNP P65473
B	-18	HIS	-	expression tag	UNP P65473
B	-17	HIS	-	expression tag	UNP P65473
B	-16	HIS	-	expression tag	UNP P65473
B	-15	HIS	-	expression tag	UNP P65473
B	-14	ASP	-	expression tag	UNP P65473
B	-13	TYR	-	expression tag	UNP P65473
B	-12	ASP	-	expression tag	UNP P65473
B	-11	ILE	-	expression tag	UNP P65473
B	-10	PRO	-	expression tag	UNP P65473
B	-9	THR	-	expression tag	UNP P65473
B	-8	THR	-	expression tag	UNP P65473
B	-7	GLU	-	expression tag	UNP P65473
B	-6	ASN	-	expression tag	UNP P65473
B	-5	LEU	-	expression tag	UNP P65473
B	-4	TYR	-	expression tag	UNP P65473
B	-3	PHE	-	expression tag	UNP P65473
B	-2	GLN	-	expression tag	UNP P65473
B	-1	GLY	-	expression tag	UNP P65473
B	0	HIS	-	expression tag	UNP P65473

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

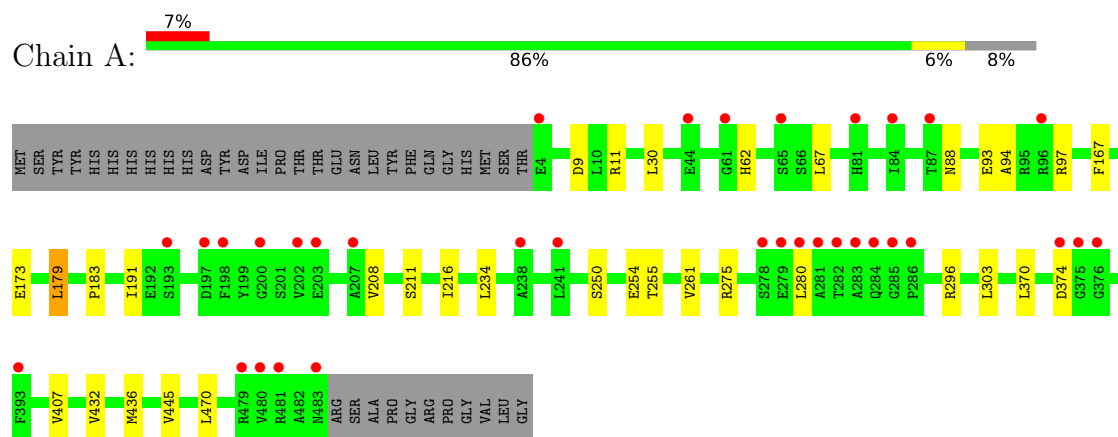
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	176	Total O 176 176	0	0
3	B	125	Total O 125 125	0	0

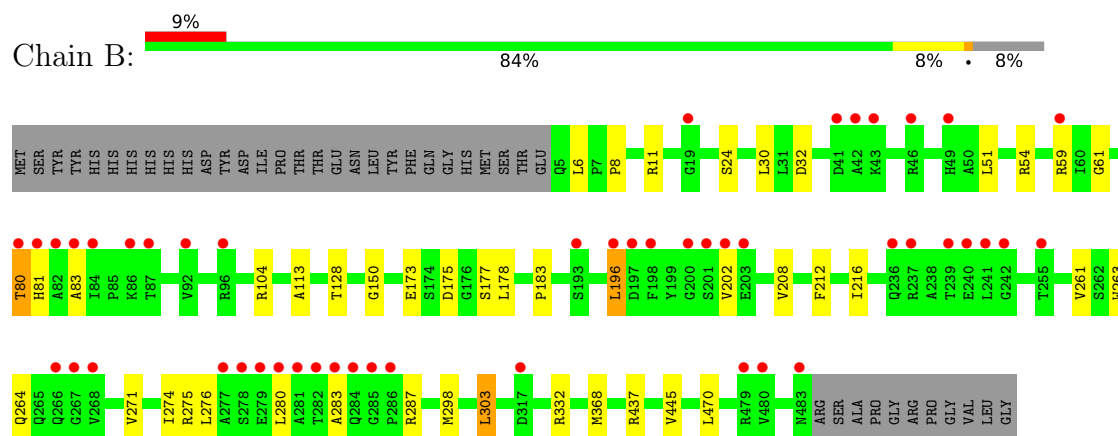
### 3 Residue-property plots [i](#)

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: UDP-N-acetylmuramate--L-alanine ligase



- Molecule 1: UDP-N-acetylmuramate--L-alanine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.30Å 76.70Å 103.96Å 90.00° 105.99° 90.00°	Depositor
Resolution (Å)	32.73 – 2.30 32.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (32.73-2.30) 98.6 (32.73-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.205 , 0.228 0.205 , 0.228	Depositor DCC
$R_{free}$ test set	2595 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: ZN

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	0.27	0/3557	0.48	0/4837
1	B	0.33	1/3548 (0.0%)	0.48	1/4825 (0.0%)
All	All	0.30	1/7105 (0.0%)	0.48	1/9662 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	GLY	C-O	-5.80	1.14	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	LEU	CA-CB-CG	5.31	127.52	115.30

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	3497	0	3516	13	0
1	B	3488	0	3510	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	176	0	0	2	0
3	B	125	0	0	4	0
All	All	7288	0	7026	40	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 3.

All (40) 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:8:PRO:HA	1:B:11:ARG:HD2	1.67	0.77
1:B:104:ARG:NH1	3:B:602:HOH:O	2.19	0.63
1:B:264:GLN:HG3	1:B:271:VAL:HG13	1.80	0.63
1:B:32:ASP:OD1	1:B:54:ARG:NH1	2.32	0.62
1:B:283:ALA:HB1	1:B:287:ARG:HH22	1.64	0.62
1:B:6:LEU:O	1:B:11:ARG:NH1	2.33	0.62
1:B:263:TRP:HH2	1:B:368:MET:HG3	1.70	0.56
1:A:250:SER:OG	1:A:296:ARG:NH2	2.39	0.56
1:B:59:ARG:NH2	1:B:61:GLY:O	2.40	0.55
1:B:113:ALA:O	3:B:601:HOH:O	2.18	0.54
1:A:94:ALA:HA	3:A:741:HOH:O	2.07	0.54
1:B:283:ALA:CB	1:B:287:ARG:HH22	2.22	0.52
1:B:175:ASP:OD1	1:B:177:SER:OG	2.25	0.51
1:B:283:ALA:HA	1:B:287:ARG:HH12	1.75	0.51
1:A:67:LEU:HD22	1:A:93:GLU:HG3	1.92	0.51
1:A:261:VAL:HG21	1:A:275:ARG:HG2	1.92	0.51
1:A:97:ARG:HB2	3:A:741:HOH:O	2.10	0.50
1:B:178:LEU:HD22	1:B:212:PHE:CD1	2.47	0.50
1:B:263:TRP:CH2	1:B:368:MET:HG3	2.48	0.48
1:B:196:LEU:HD11	1:B:202:VAL:HA	1.94	0.48
1:A:179:LEU:HD11	1:A:211:SER:HB2	1.95	0.47
1:B:437:ARG:NE	3:B:616:HOH:O	2.48	0.47
1:B:261:VAL:HG22	1:B:275:ARG:HG2	1.95	0.47
1:B:80:THR:HG22	1:B:83:ALA:H	1.80	0.46
1:B:276:LEU:HD12	1:B:276:LEU:HA	1.80	0.46
1:B:54:ARG:NH2	3:B:618:HOH:O	2.49	0.45
1:B:24:SER:HA	1:B:51:LEU:HD11	1.98	0.45
1:A:183:PRO:HG2	1:A:216:ILE:HG12	1.98	0.45
1:B:274:ILE:HG21	1:B:303:LEU:HD11	1.98	0.44
1:A:445:VAL:HG11	1:A:470:LEU:HD13	1.99	0.44
1:B:332:ARG:HD3	1:B:332:ARG:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:CG	1:A:88:ASN:HD21	2.37	0.43
1:A:407:VAL:O	1:A:436:MET:HA	2.18	0.43
1:B:183:PRO:HG2	1:B:216:ILE:HG12	2.01	0.43
1:A:9:ASP:OD1	1:A:9:ASP:N	2.49	0.41
1:A:254:GLU:HG3	1:A:255:THR:HG23	2.02	0.41
1:A:191:ILE:HD11	1:A:234:LEU:HD22	2.02	0.41
1:B:261:VAL:CG2	1:B:275:ARG:HG2	2.51	0.41
1:B:128:THR:HG21	1:B:298:MET:SD	2.61	0.40
1:B:445:VAL:HG11	1:B:470:LEU:HD13	2.03	0.40

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	478/519 (92%)	472 (99%)	6 (1%)	0	100	100
1	B	477/519 (92%)	463 (97%)	14 (3%)	0	100	100
All	All	955/1038 (92%)	935 (98%)	20 (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	355/389 (91%)	344 (97%)	11 (3%)	40	55
1	B	354/389 (91%)	347 (98%)	7 (2%)	55	72
All	All	709/778 (91%)	691 (98%)	18 (2%)	47	65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	30	LEU
1	A	167	PHE
1	A	173	GLU
1	A	179	LEU
1	A	208	VAL
1	A	280	LEU
1	A	303	LEU
1	A	370	LEU
1	A	374	ASP
1	A	432	VAL
1	B	30	LEU
1	B	80	THR
1	B	81	HIS
1	B	173	GLU
1	B	196	LEU
1	B	208	VAL
1	B	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	480/519 (92%)	0.32	34 (7%)	16 21	18, 34, 62, 99	0
1	B	479/519 (92%)	0.51	48 (10%)	7 10	23, 38, 69, 118	0
All	All	959/1038 (92%)	0.41	82 (8%)	10 14	18, 36, 67, 118	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ALA	11.4
1	B	280	LEU	6.7
1	B	282	THR	6.3
1	A	375	GLY	6.3
1	A	282	THR	5.8
1	B	278	SER	5.1
1	B	268	VAL	4.9
1	A	200	GLY	4.6
1	B	279	GLU	4.5
1	B	285	GLY	4.5
1	B	198	PHE	4.5
1	B	201	SER	4.3
1	A	374	ASP	4.3
1	A	285	GLY	4.3
1	A	279	GLU	4.2
1	A	483	ASN	4.1
1	B	83	ALA	4.0
1	B	42	ALA	4.0
1	B	277	ALA	3.9
1	A	281	ALA	3.7
1	A	81	HIS	3.6
1	B	197	ASP	3.6
1	A	278	SER	3.5
1	B	196	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	41	ASP	3.5
1	B	203	GLU	3.4
1	A	241	LEU	3.4
1	B	284	GLN	3.4
1	A	4	GLU	3.3
1	A	197	ASP	3.3
1	B	43	LYS	3.3
1	A	198	PHE	3.2
1	B	286	PRO	3.2
1	B	267	GLY	3.2
1	A	283	ALA	3.1
1	B	483	ASN	3.1
1	B	255	THR	3.1
1	A	203	GLU	3.1
1	B	81	HIS	3.0
1	B	84	ILE	3.0
1	A	280	LEU	2.9
1	B	283	ALA	2.9
1	A	87	THR	2.9
1	A	284	GLN	2.9
1	B	240	GLU	2.9
1	B	200	GLY	2.8
1	A	480	VAL	2.8
1	B	87	THR	2.7
1	B	46	ARG	2.7
1	B	80	THR	2.7
1	B	19	GLY	2.7
1	B	266	GLN	2.6
1	A	481	ARG	2.6
1	A	84	ILE	2.6
1	B	480	VAL	2.5
1	A	61	GLY	2.5
1	B	49	HIS	2.4
1	B	59	ARG	2.4
1	B	242	GLY	2.4
1	B	241	LEU	2.4
1	A	393	PHE	2.4
1	B	236	GLN	2.4
1	B	96	ARG	2.4
1	B	82	ALA	2.3
1	B	86	LYS	2.3
1	B	193	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	286	PRO	2.3
1	B	239	THR	2.3
1	B	202	VAL	2.3
1	A	479	ARG	2.2
1	A	376	GLY	2.2
1	A	44	GLU	2.2
1	A	207	ALA	2.2
1	B	479	ARG	2.1
1	B	317	ASP	2.1
1	A	202	VAL	2.1
1	B	237	ARG	2.1
1	A	238	ALA	2.1
1	A	65	SER	2.0
1	B	92	VAL	2.0
1	A	193	SER	2.0
1	A	96	ARG	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

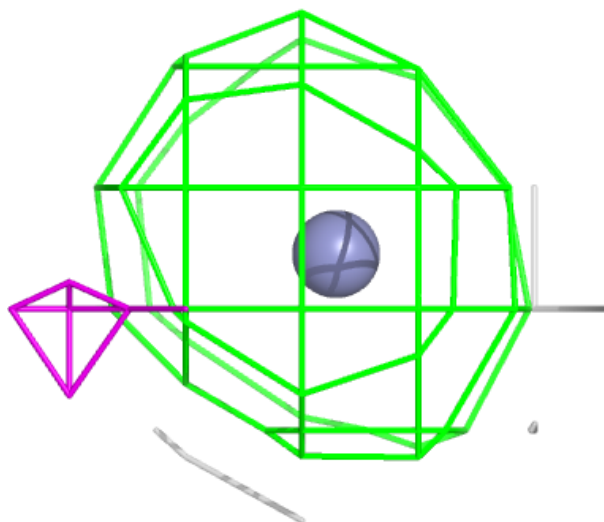
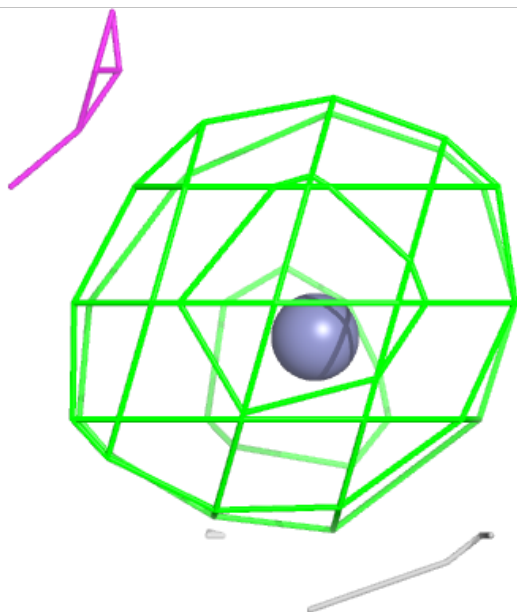
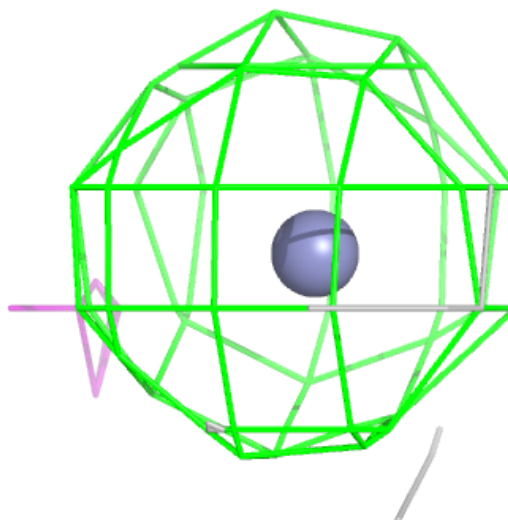
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

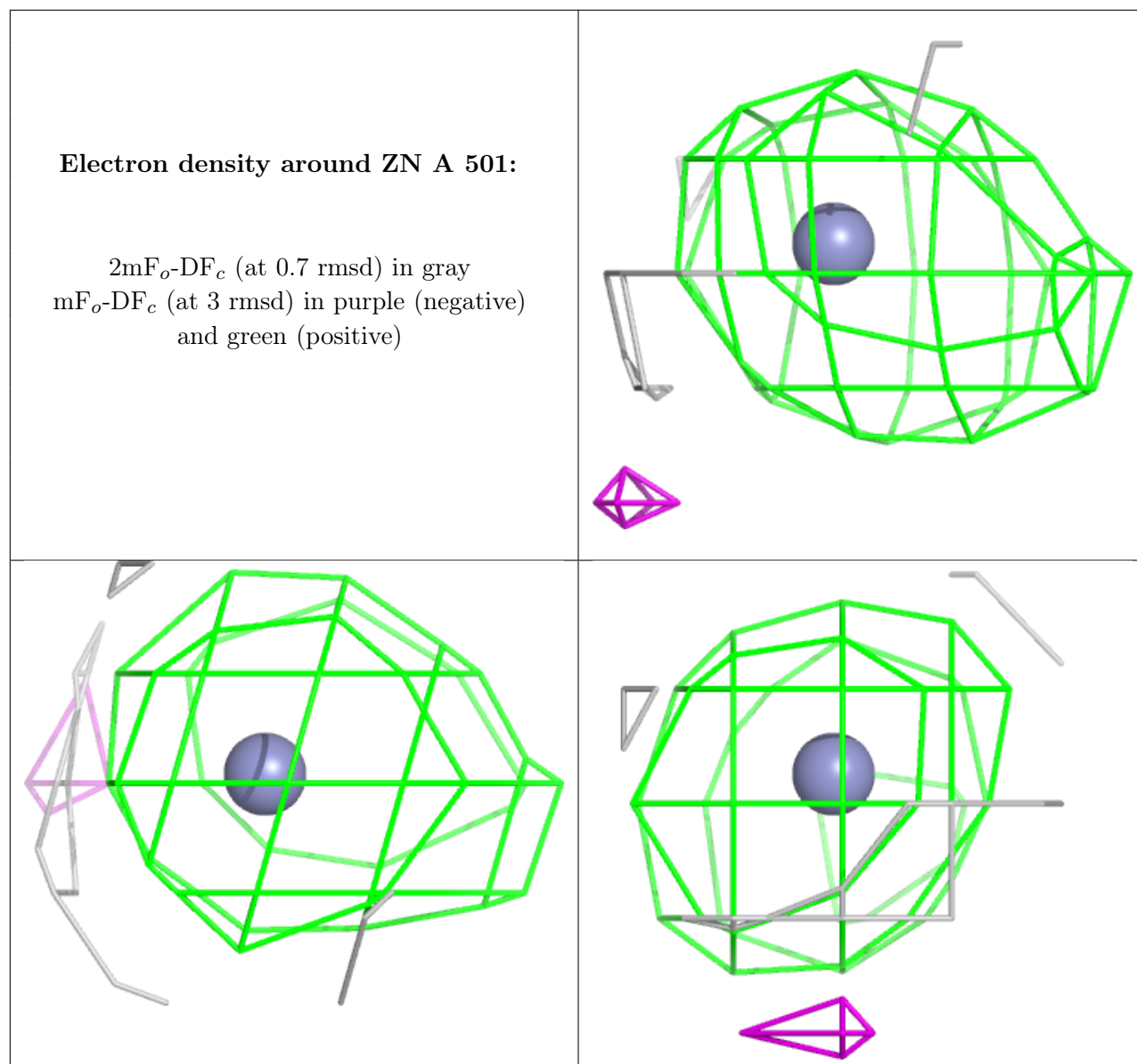
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	501	1/1	0.92	0.32	88,88,88,88	0
2	ZN	A	501	1/1	0.98	0.25	71,71,71,71	0

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 ZN 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.