



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 12:03 pm GMT

PDB ID : 7OS3  
Title : Crystal structure of Rhizobium etli inducible L-asparaginase ReAV solved by S-SAD (orthorhombic form START)  
Authors : Gilski, M.; Loch, J.I.; Imiolczyk, B.; Jaskolski, M.  
Deposited on : 2021-06-07  
Resolution : 2.18 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 : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

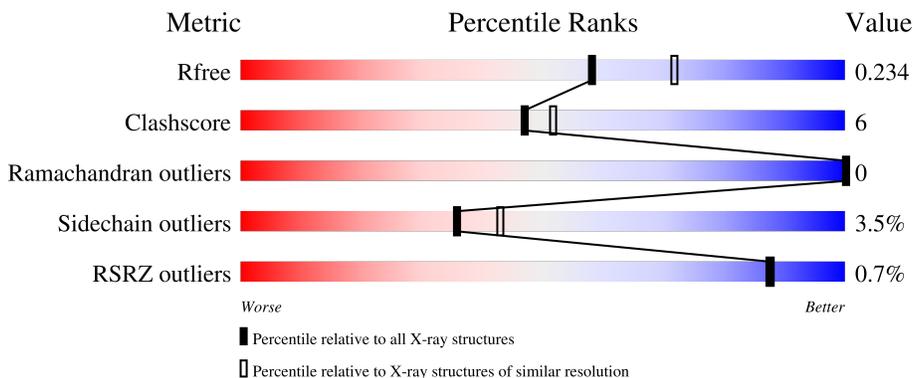
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	AAA	373	 88% 11% ..
1	BBB	373	 82% 11% • 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5639 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 L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	369	2736	1688	505	522	21	0	0	0
1	BBB	349	2585	1595	478	492	20	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	GLY	-	expression tag	UNP Q2K0Z2
AAA	-4	ILE	-	expression tag	UNP Q2K0Z2
AAA	-3	ASP	-	expression tag	UNP Q2K0Z2
AAA	-2	PRO	-	expression tag	UNP Q2K0Z2
AAA	-1	PHE	-	expression tag	UNP Q2K0Z2
AAA	0	THR	-	expression tag	UNP Q2K0Z2
BBB	-5	GLY	-	expression tag	UNP Q2K0Z2
BBB	-4	ILE	-	expression tag	UNP Q2K0Z2
BBB	-3	ASP	-	expression tag	UNP Q2K0Z2
BBB	-2	PRO	-	expression tag	UNP Q2K0Z2
BBB	-1	PHE	-	expression tag	UNP Q2K0Z2
BBB	0	THR	-	expression tag	UNP Q2K0Z2

- 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	AAA	1	Total	Zn	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	Total Cl 2 2	0	0

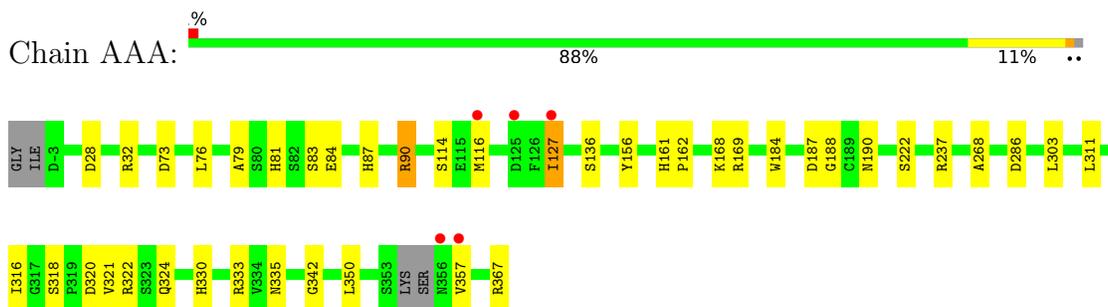
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	159	Total O 159 159	0	0
4	BBB	155	Total O 155 155	0	0

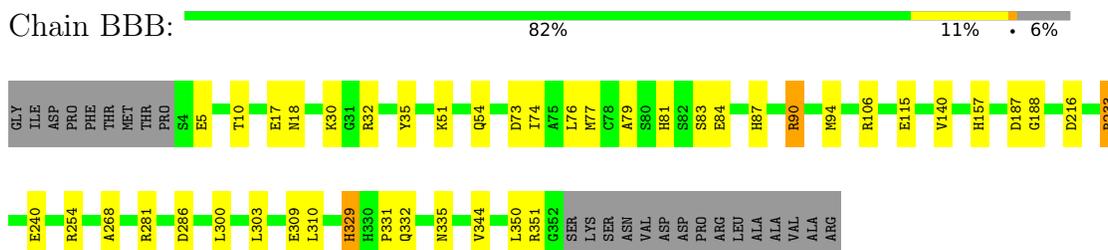
### 3 Residue-property plots [i](#)

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: L-asparaginase II protein



- Molecule 1: L-asparaginase II protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.15Å 91.05Å 105.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.02 – 2.18 69.02 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (69.02-2.18) 98.6 (69.02-2.18)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.168 , 0.224 0.177 , 0.234	Depositor DCC
$R_{free}$ test set	1000 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtrriage
Anisotropy	0.798	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.05 % 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 3.3610e-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: ZN, CL

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	AAA	0.70	0/2783	0.79	0/3763
1	BBB	0.69	0/2629	0.76	0/3552
All	All	0.70	0/5412	0.77	0/7315

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	AAA	0	1
1	BBB	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	79	ALA	Peptide
1	BBB	79	ALA	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	AAA	2736	0	2699	30	0
1	BBB	2585	0	2551	38	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	2	0	0	0	0
4	AAA	159	0	0	7	0
4	BBB	155	0	0	4	0
All	All	5639	0	5250	65	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 6.

All (65) 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:AAA:237:ARG:HD2	4:AAA:552:HOH:O	1.72	0.88
1:BBB:5:GLU:O	1:BBB:5:GLU:HG2	1.73	0.85
1:BBB:300:LEU:HB3	4:BBB:595:HOH:O	1.77	0.84
1:BBB:76:LEU:HD22	1:BBB:90:ARG:HG2	1.60	0.83
1:BBB:81:HIS:HD2	1:BBB:83:SER:H	1.28	0.79
1:AAA:81:HIS:HD2	1:AAA:83:SER:H	1.35	0.75
1:BBB:84:GLU:H	1:BBB:87:HIS:HD2	1.34	0.74
1:BBB:10:THR:HG23	1:BBB:17:GLU:HB3	1.71	0.73
1:BBB:240:GLU:CG	1:BBB:254:ARG:HH21	2.03	0.71
1:AAA:318:SER:OG	1:AAA:321:VAL:HG23	1.97	0.65
1:BBB:81:HIS:HD2	1:BBB:83:SER:N	1.96	0.63
1:BBB:73:ASP:OD1	1:BBB:90:ARG:HD3	2.00	0.60
1:BBB:81:HIS:CD2	1:BBB:83:SER:H	2.17	0.59
1:BBB:240:GLU:HG3	1:BBB:254:ARG:HH21	1.68	0.59
1:AAA:76:LEU:HD22	1:AAA:90:ARG:HG2	1.84	0.59
1:BBB:51:LYS:HA	1:BBB:54:GLN:HE21	1.69	0.58
1:AAA:84:GLU:H	1:AAA:87:HIS:HD2	1.51	0.57
1:AAA:81:HIS:HD2	1:AAA:83:SER:N	2.03	0.56
1:BBB:30:LYS:HD2	1:BBB:32:ARG:NH2	2.22	0.55
1:AAA:322:ARG:HD2	4:AAA:637:HOH:O	2.07	0.54
1:BBB:106:ARG:HG3	1:BBB:157:HIS:CE1	2.43	0.54
1:BBB:309:GLU:OE1	1:BBB:329:HIS:HE1	1.91	0.53
1:BBB:76:LEU:HD22	1:BBB:90:ARG:CG	2.38	0.52
1:AAA:81:HIS:CD2	1:AAA:83:SER:H	2.23	0.52
1:AAA:76:LEU:HD22	1:AAA:90:ARG:CG	2.40	0.51
1:AAA:190:ASN:ND2	4:AAA:510:HOH:O	2.44	0.51
1:AAA:311:LEU:HB2	4:AAA:637:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:222:SER:HB2	4:AAA:621:HOH:O	2.10	0.51
1:AAA:333:ARG:HB2	1:AAA:342:GLY:O	2.11	0.51
1:BBB:240:GLU:CG	1:BBB:254:ARG:NH2	2.72	0.49
1:BBB:331:PRO:HD2	1:BBB:344:VAL:HG21	1.93	0.49
1:BBB:30:LYS:HD2	1:BBB:32:ARG:HH21	1.78	0.48
1:BBB:309:GLU:OE1	1:BBB:329:HIS:CE1	2.66	0.48
1:AAA:161:HIS:CG	1:AAA:162:PRO:HD2	2.49	0.48
1:AAA:330:HIS:HD2	4:AAA:626:HOH:O	1.96	0.47
1:AAA:28:ASP:OD2	1:AAA:32:ARG:NH1	2.47	0.47
1:BBB:87:HIS:HE1	1:BBB:240:GLU:O	1.98	0.47
1:AAA:335:ASN:HB2	1:BBB:188:GLY:HA2	1.97	0.47
1:BBB:10:THR:HG22	1:BBB:18:ASN:H	1.81	0.46
1:BBB:281:ARG:HD2	4:BBB:529:HOH:O	2.15	0.46
1:BBB:240:GLU:HG2	1:BBB:254:ARG:HH21	1.80	0.45
1:AAA:81:HIS:HE1	1:AAA:136:SER:OG	1.99	0.45
1:AAA:190:ASN:HD22	1:BBB:335:ASN:HD21	1.64	0.45
1:AAA:333:ARG:HD3	1:AAA:333:ARG:HA	1.87	0.43
1:AAA:316:ILE:N	1:AAA:316:ILE:HD13	2.34	0.43
1:AAA:156:TYR:HA	1:AAA:161:HIS:CD2	2.53	0.43
1:AAA:268:ALA:HA	1:AAA:303:LEU:HD22	2.00	0.43
1:AAA:350:LEU:HD12	1:AAA:350:LEU:HA	1.88	0.43
1:BBB:10:THR:CG2	1:BBB:18:ASN:H	2.31	0.43
1:BBB:268:ALA:HA	1:BBB:303:LEU:HD22	2.01	0.43
1:AAA:73:ASP:OD1	1:AAA:90:ARG:HD3	2.18	0.43
1:BBB:74:ILE:O	1:BBB:77:MET:HB2	2.19	0.42
1:AAA:321:VAL:O	1:AAA:324:GLN:OE1	2.38	0.42
1:AAA:127:ILE:HD12	1:AAA:127:ILE:O	2.20	0.42
1:BBB:300:LEU:CB	4:BBB:595:HOH:O	2.52	0.42
1:BBB:84:GLU:HB2	1:BBB:87:HIS:CD2	2.55	0.42
1:BBB:240:GLU:OE2	1:BBB:254:ARG:NH2	2.52	0.42
1:BBB:240:GLU:HG2	1:BBB:254:ARG:NH2	2.34	0.42
1:BBB:94:MET:HB3	1:BBB:140:VAL:HG11	2.01	0.41
1:BBB:310:LEU:HA	1:BBB:310:LEU:HD23	1.81	0.41
1:AAA:188:GLY:HA2	1:BBB:335:ASN:HB2	2.03	0.41
1:BBB:233:ARG:HG2	4:BBB:609:HOH:O	2.21	0.41
1:BBB:35:TYR:HA	1:BBB:351:ARG:O	2.21	0.40
1:AAA:127:ILE:CD1	4:AAA:647:HOH:O	2.70	0.40
1:AAA:168:LYS:HG3	1:AAA:184:TRP:CZ2	2.56	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	AAA	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	BBB	347/373 (93%)	334 (96%)	13 (4%)	0	100	100
All	All	712/746 (95%)	687 (96%)	25 (4%)	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	AAA	280/283 (99%)	270 (96%)	10 (4%)	35	42
1	BBB	263/283 (93%)	254 (97%)	9 (3%)	37	44
All	All	543/566 (96%)	524 (96%)	19 (4%)	36	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	90	ARG
1	AAA	114	SER
1	AAA	116	MET
1	AAA	127	ILE
1	AAA	169	ARG
1	AAA	187	ASP
1	AAA	286	ASP
1	AAA	320	ASP

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Mol	Chain	Res	Type
1	AAA	357	VAL
1	AAA	367	ARG
1	BBB	90	ARG
1	BBB	115	GLU
1	BBB	187	ASP
1	BBB	216	ASP
1	BBB	233	ARG
1	BBB	286	ASP
1	BBB	329	HIS
1	BBB	332	GLN
1	BBB	350	LEU

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

### 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 monosaccharides in this entry.

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

Of 4 ligands modelled in this entry, 4 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 [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	AAA	369/373 (98%)	-0.17	5 (1%) 75 75	23, 33, 58, 91	0
1	BBB	349/373 (93%)	-0.24	0 100 100	24, 34, 54, 85	0
All	All	718/746 (96%)	-0.21	5 (0%) 87 88	23, 34, 57, 91	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	356	ASN	3.9
1	AAA	357	VAL	3.7
1	AAA	116	MET	2.4
1	AAA	127	ILE	2.2
1	AAA	125	ASP	2.1

### 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](#)

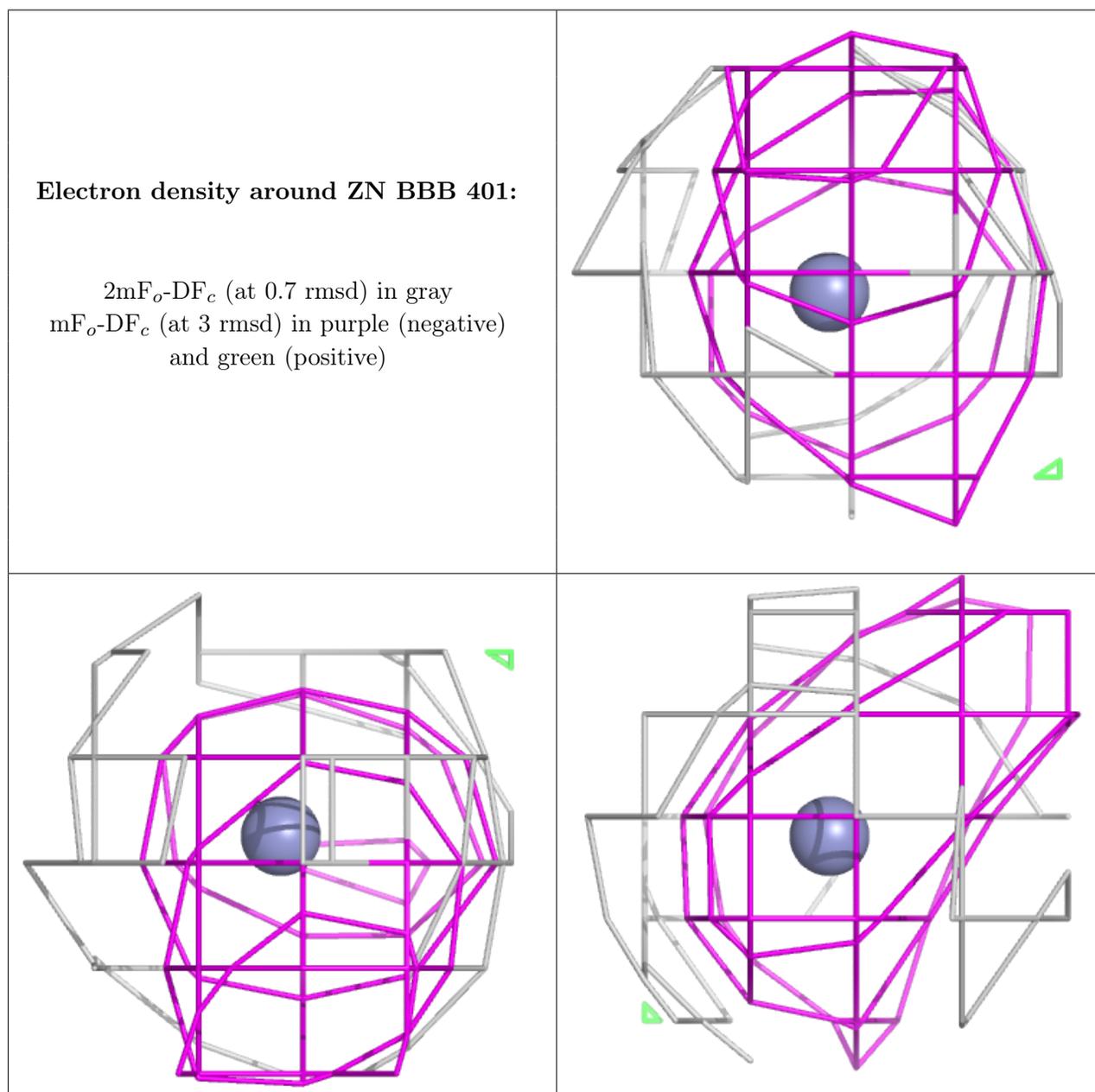
There are no monosaccharides in this entry.

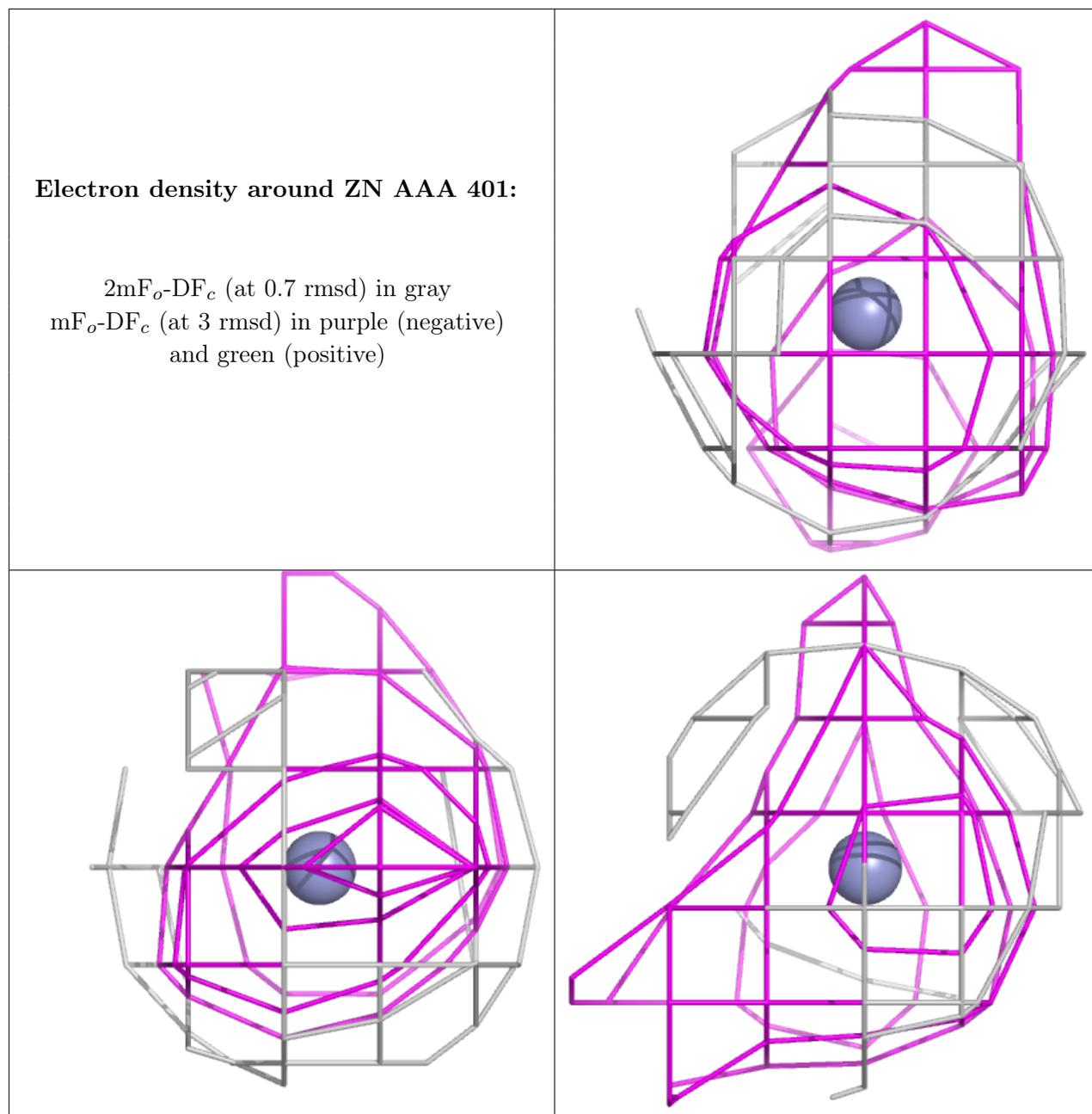
### 6.4 Ligands [i](#)

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
3	CL	AAA	402	1/1	0.86	0.13	64,64,64,64	0
3	CL	AAA	403	1/1	0.95	0.20	56,56,56,56	0
2	ZN	BBB	401	1/1	0.98	0.05	46,46,46,46	0
2	ZN	AAA	401	1/1	0.99	0.04	47,47,47,47	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.