



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2021 – 11:06 am GMT

PDB ID : 7BGO
Title : The crystal structure of gene product PA4063 from *Pseudomonas aeruginosa* in complex with Zn (space group P65)
Authors : Fiorillo, A.; Ilari, A.
Deposited on : 2021-01-08
Resolution : 3.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

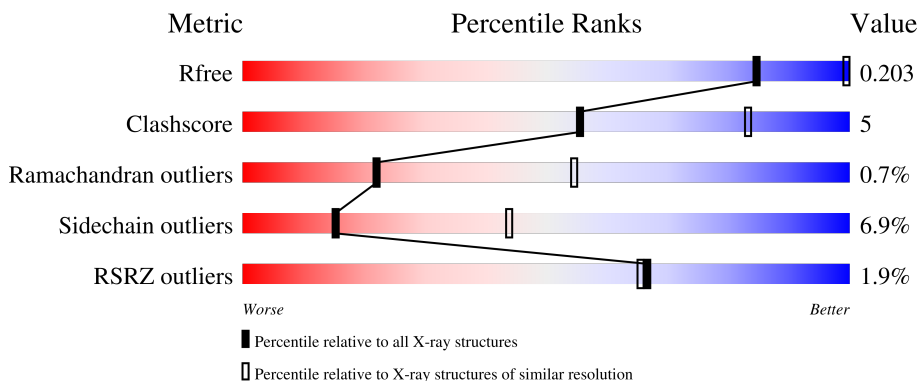
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. 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	179	<div> <div>2%</div> <div>65% 12% 22%</div> </div>
1	BBB	179	<div> <div>69% 11% 20%</div> </div>
1	CCC	179	<div> <div>2% 62% 16% 21%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6435 atoms, of which 3231 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 DUF2796 domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	140	Total	C	H	N	O	S	19	0	0
			2126	671	1070	180	202	3			
1	CCC	141	Total	C	H	N	O	S	21	0	0
			2139	675	1077	183	201	3			
1	BBB	143	Total	C	H	N	O	S	21	0	0
			2158	681	1084	185	205	3			

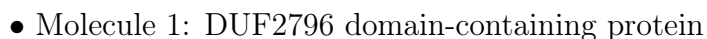
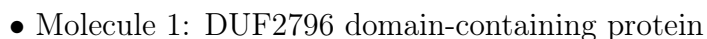
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Zn	0	0
			2	2		
2	CCC	2	Total	Zn	0	0
			2	2		
2	BBB	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	2	Total	O	0	0
			2	2		
3	CCC	2	Total	O	0	0
			2	2		
3	BBB	2	Total	O	0	0
			2	2		

- Molecule 1: DUF2796 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	122.00Å 122.00Å 102.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.94 – 3.30 46.94 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.94-3.30) 95.8 (46.94-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.211 0.181 , 0.203	Depositor DCC
R_{free} test set	550 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	123.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6435	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	AAA	0.70	0/1074	0.90	0/1451
1	BBB	0.71	0/1093	0.92	0/1476
1	CCC	0.70	0/1081	0.90	0/1460
All	All	0.70	0/3248	0.91	0/4387

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

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	1056	1070	1067	11	0
1	BBB	1074	1084	1080	8	0
1	CCC	1062	1077	1073	15	0
2	AAA	2	0	0	0	0
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
3	AAA	2	0	0	0	0
3	BBB	2	0	0	0	0
3	CCC	2	0	0	0	0
All	All	3204	3231	3220	33	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 5.

The worst 5 of 33 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:158:GLN:HE21	1:AAA:165:GLN:HE22	1.25	0.82
1:BBB:67:GLU:HA	1:BBB:86:GLN:HE22	1.54	0.71
1:CCC:16:HIS:CE1	1:CCC:120:HIS:HB3	2.29	0.68
1:CCC:128:GLN:HE22	1:BBB:77:VAL:HG11	1.59	0.67
1:AAA:37:ASP:OD1	1:AAA:124:HIS:ND1	2.28	0.63

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	136/179 (76%)	127 (93%)	8 (6%)	1 (1%)	22	54
1	BBB	139/179 (78%)	127 (91%)	11 (8%)	1 (1%)	22	54
1	CCC	137/179 (76%)	127 (93%)	9 (7%)	1 (1%)	22	54
All	All	412/537 (77%)	381 (92%)	28 (7%)	3 (1%)	22	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	168	ALA
1	BBB	168	ALA
1	CCC	168	ALA

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	110/140 (79%)	102 (93%)	8 (7%)	14	41
1	BBB	111/140 (79%)	105 (95%)	6 (5%)	22	53
1	CCC	110/140 (79%)	101 (92%)	9 (8%)	11	36
All	All	331/420 (79%)	308 (93%)	23 (7%)	15	44

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	152	THR
1	BBB	42	ASN
1	CCC	178	LYS
1	BBB	52	THR
1	AAA	152	THR

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

Of 6 ligands modelled in this entry, 6 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 [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, 95th 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 ²)	Q<0.9
1	AAA	140/179 (78%)	0.15	2 (1%) 75 75	101, 141, 171, 189	0
1	BBB	143/179 (79%)	0.05	2 (1%) 75 75	104, 138, 168, 182	0
1	CCC	141/179 (78%)	0.21	4 (2%) 53 51	107, 149, 196, 216	0
All	All	424/537 (78%)	0.14	8 (1%) 66 65	101, 142, 177, 216	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	51	SER	3.6
1	CCC	44	VAL	3.6
1	CCC	50	ALA	3.4
1	AAA	50	ALA	3.3
1	BBB	50	ALA	2.9

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 monosaccharides in this entry.

6.4 Ligands [i](#)

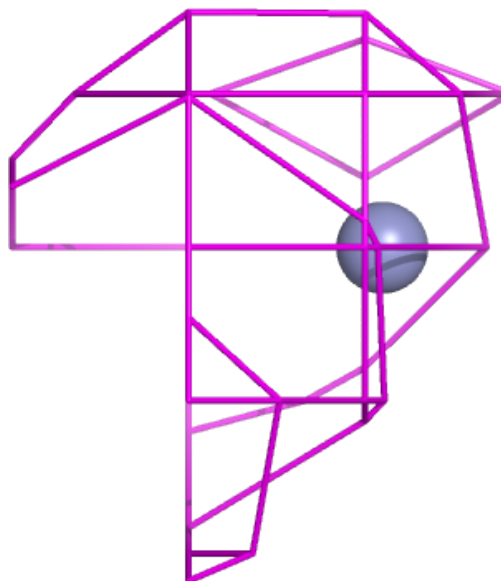
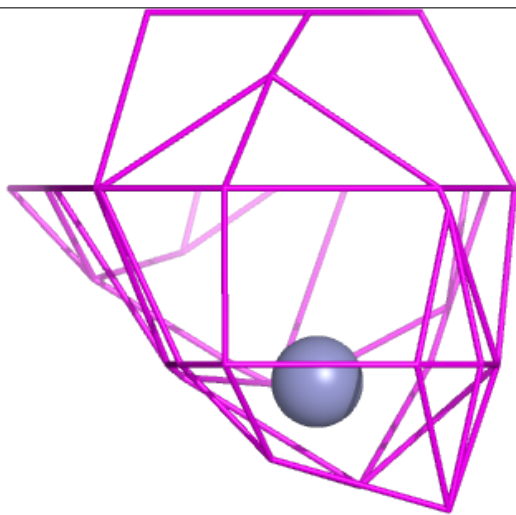
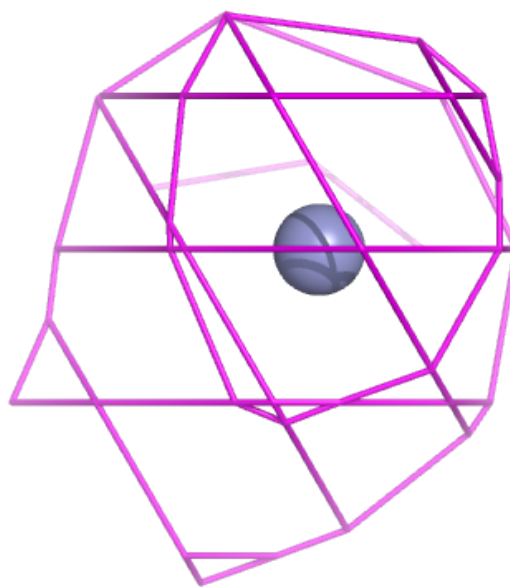
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	BBB	201	1/1	0.87	0.06	134,134,134,134	0
2	ZN	AAA	202	1/1	0.92	0.04	147,147,147,147	0
2	ZN	AAA	201	1/1	0.92	0.10	158,158,158,158	0
2	ZN	BBB	202	1/1	0.95	0.09	134,134,134,134	0
2	ZN	CCC	201	1/1	0.97	0.07	185,185,185,185	0
2	ZN	CCC	202	1/1	0.99	0.11	176,176,176,176	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.

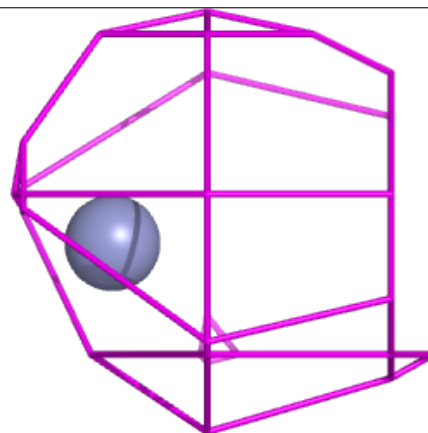
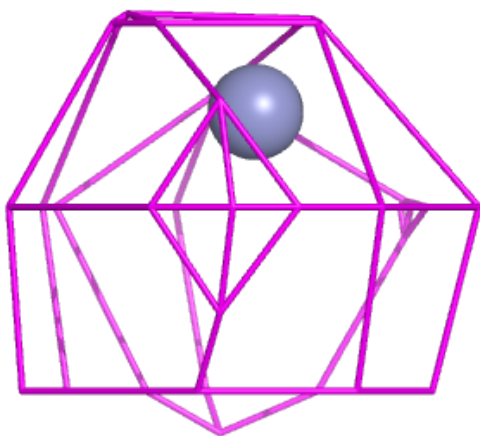
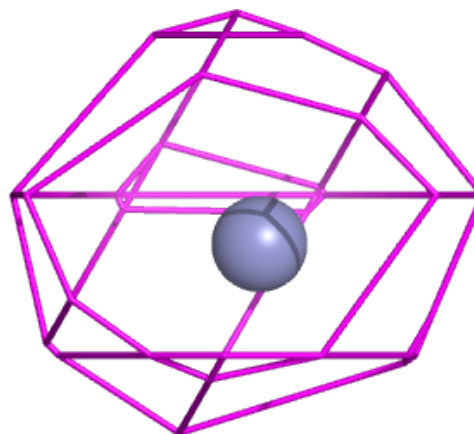
Electron density around ZN BBB 201:

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



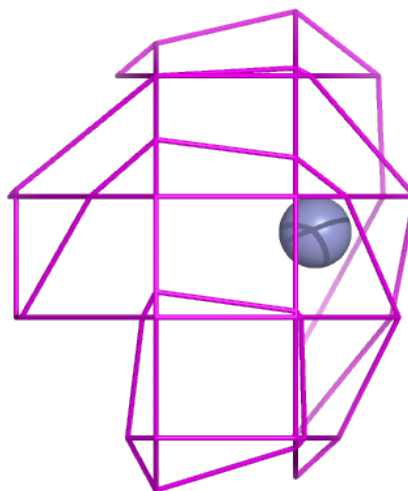
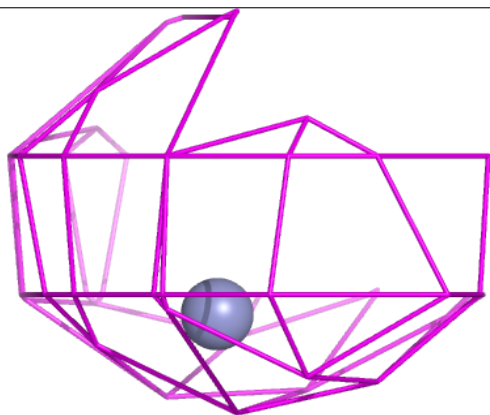
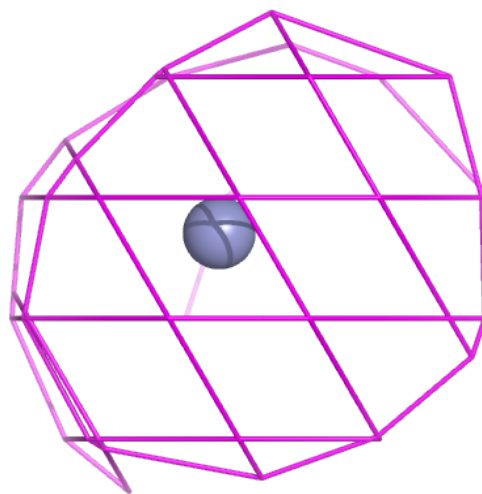
Electron density around ZN AAA 202:

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



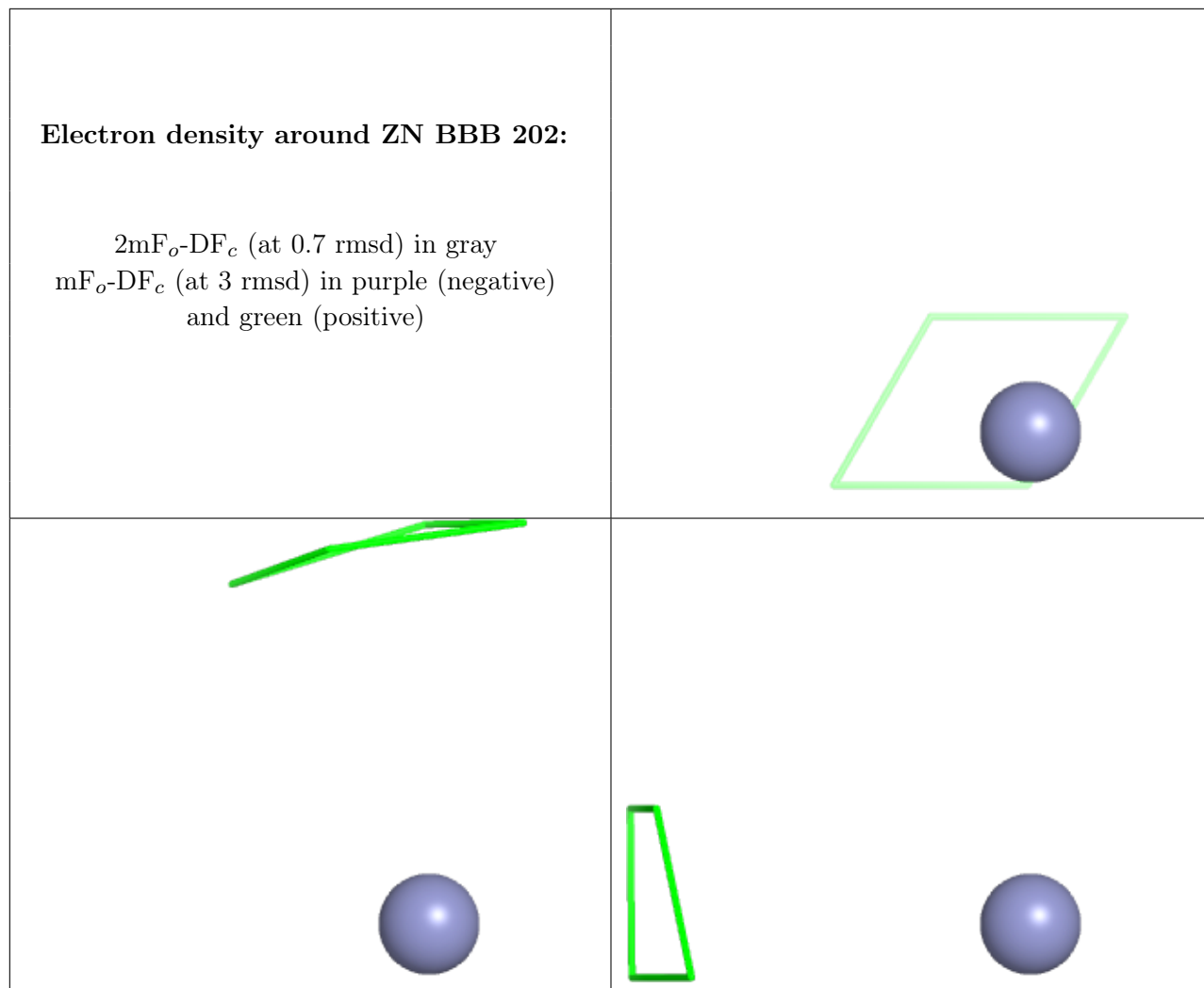
Electron density around ZN AAA 201:

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



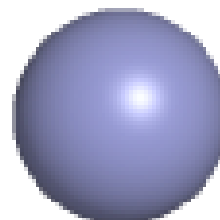
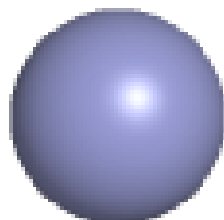
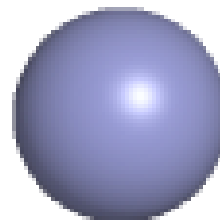
Electron density around ZN BBB 202:

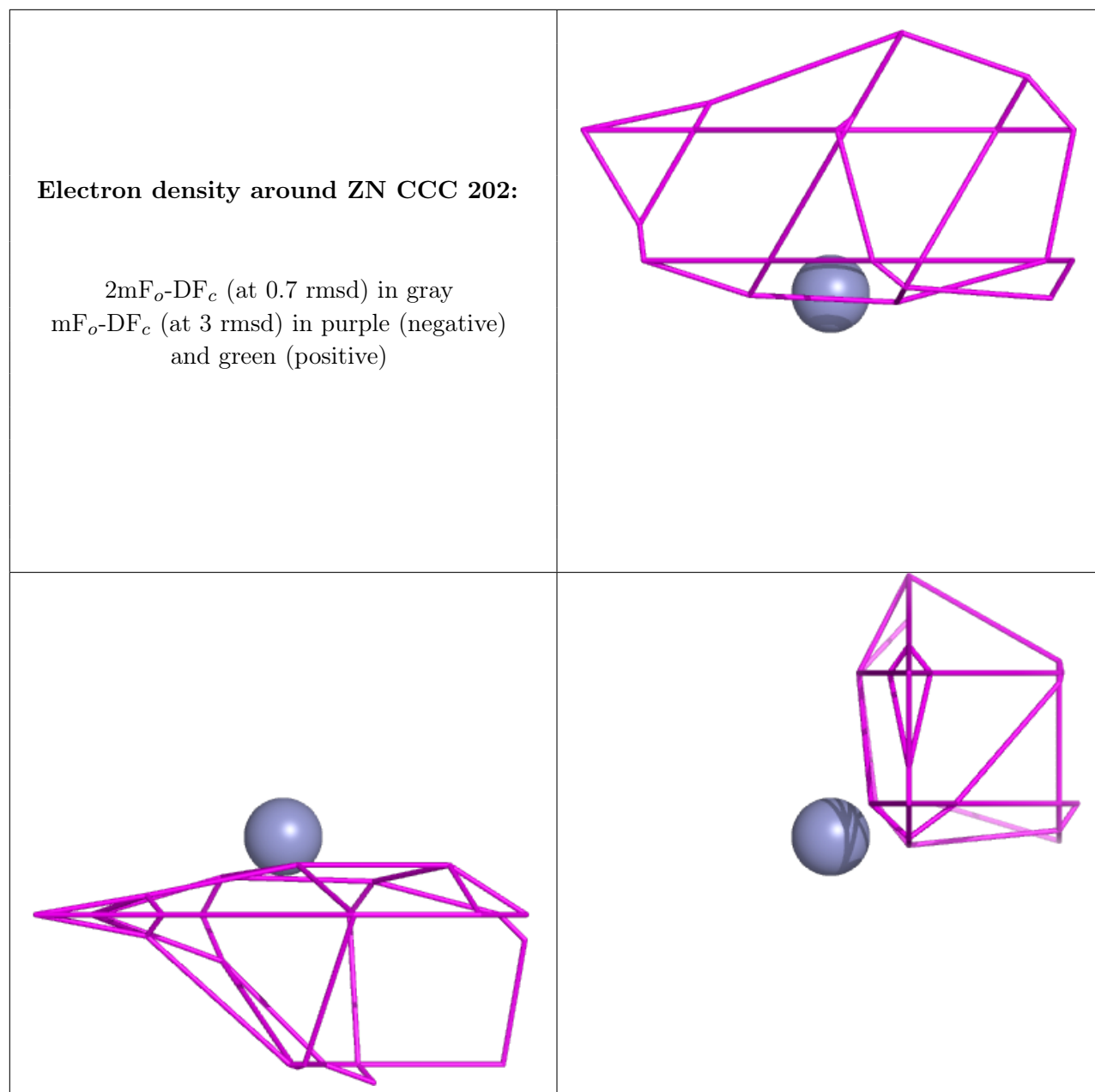
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN CCC 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.