



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 8A28 / pdb_00008a28
Title : Structure of the astacin zymogen of LAST-MAM from *Limulus polyphemus*
Authors : Guevara, T.; Rodriguez Banqueri, A.
Deposited on : 2022-06-02
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

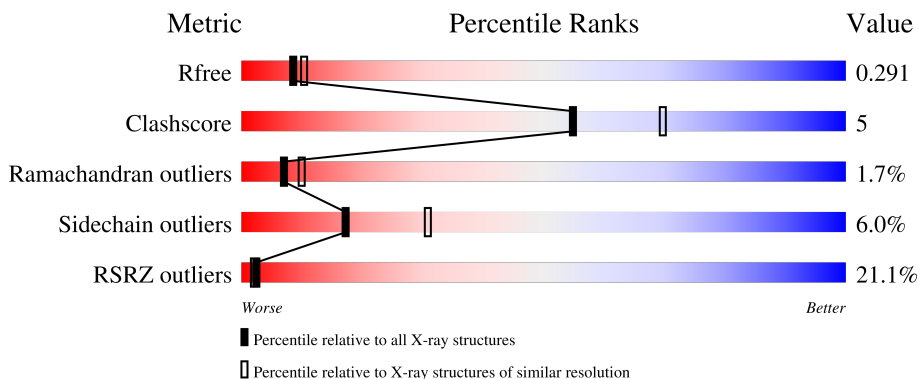
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	A	382	
1	B	382	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	B	502	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5062 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 Metalloendopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2983	1891	503	570	19	0	0	0
1	B	225	1818	1160	312	336	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	GLU	engineered mutation	UNP B4F320
B	140	ALA	GLU	engineered mutation	UNP B4F320

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

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			10	6 4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	129	Total	O	0	0
			129	129		
7	B	100	Total	O	0	0
			100	100		

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.83Å 47.57Å 236.40Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	46.73 – 2.40 46.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.73-2.40) 99.7 (46.73-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.40Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.253 , 0.289 0.258 , 0.291	Depositor DCC
R_{free} test set	741 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtrriage
Anisotropy	0.570	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5062	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ZN, PGE, PEG

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	1.16	7/3063 (0.2%)	1.30	20/4161 (0.5%)
1	B	1.18	7/1869 (0.4%)	1.44	22/2532 (0.9%)
All	All	1.17	14/4932 (0.3%)	1.35	42/6693 (0.6%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	ILE	CA-C	-7.25	1.46	1.52
1	B	112	CYS	CA-C	-6.53	1.44	1.52
1	A	163	ILE	CA-C	-6.38	1.47	1.52
1	B	67	LEU	CA-C	-6.23	1.45	1.52
1	A	149	HIS	C-N	6.16	1.42	1.34

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ILE	CA-C-N	8.25	134.60	123.05
1	B	160	ILE	C-N-CA	8.25	134.60	123.05
1	B	38	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	134	LYS	CA-C-N	7.08	127.66	119.94
1	B	134	LYS	C-N-CA	7.08	127.66	119.94

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	2983	0	2753	25	0
1	B	1818	0	1728	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	B	7	0	10	8	0
6	B	10	0	14	1	0
7	A	129	0	0	2	0
7	B	100	0	0	1	0
All	All	5062	0	4521	45	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 45 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:167:ILE:HG12	1:B:211:THR:HB	1.53	0.90
1:B:113:TRP:HE1	5:B:502:PEG:H11	1.45	0.79
1:B:113:TRP:HE1	5:B:502:PEG:C1	2.02	0.73
1:A:329:TYR:HB3	1:A:392:ALA:HB3	1.71	0.72
1:A:73:SER:HA	5:B:502:PEG:H42	1.71	0.71

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	380/382 (100%)	342 (90%)	29 (8%)	9 (2%)	4 5
1	B	223/382 (58%)	208 (93%)	14 (6%)	1 (0%)	30 43
All	All	603/764 (79%)	550 (91%)	43 (7%)	10 (2%)	7 10

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	371	ARG
1	B	186	LEU
1	A	181	TRP
1	A	319	ASN

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	308/327 (94%)	285 (92%)	23 (8%)	12 21
1	B	190/327 (58%)	183 (96%)	7 (4%)	30 51
All	All	498/654 (76%)	468 (94%)	30 (6%)	17 31

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	PHE
1	B	188	GLU
1	A	340	ILE
1	B	233	SER
1	B	112	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	GLN

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Mol	Chain	Res	Type
1	B	176	ASN
1	B	184	ASN
1	A	280	GLN
1	A	33	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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.26	0
5	PEG	B	502	-	6,6,6	0.31	0	5,5,5	0.29	0
4	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.36	0
6	PGE	B	503	-	9,9,9	0.18	0	8,8,8	0.45	0

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
4	GOL	B	504	-	-	0/4/4/4	-
5	PEG	B	502	-	-	1/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
6	PGE	B	503	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	503	PGE	O2-C3-C4-O3
6	B	503	PGE	C3-C4-O3-C5
5	B	502	PEG	C4-C3-O2-C2
6	B	503	PGE	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	PEG	8	0
6	B	503	PGE	1	0

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, 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	A	382/382 (100%)	1.30	102 (26%) 1 1	39, 67, 122, 141	158 (41%)
1	B	225/382 (58%)	1.01	26 (11%) 9 7	45, 68, 105, 130	0
All	All	607/764 (79%)	1.19	128 (21%) 2 2	39, 68, 120, 141	158 (26%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	6.5
1	B	246	GLY	6.0
1	A	245	PHE	6.0
1	B	245	PHE	4.7
1	A	353	TYR	4.7

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](#)

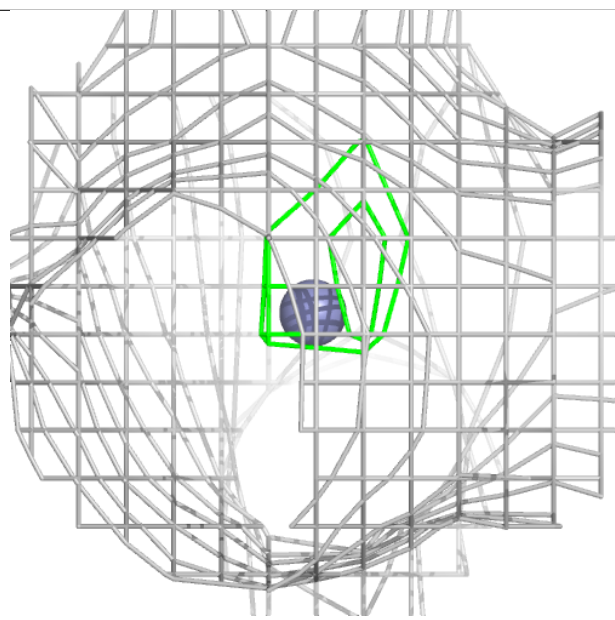
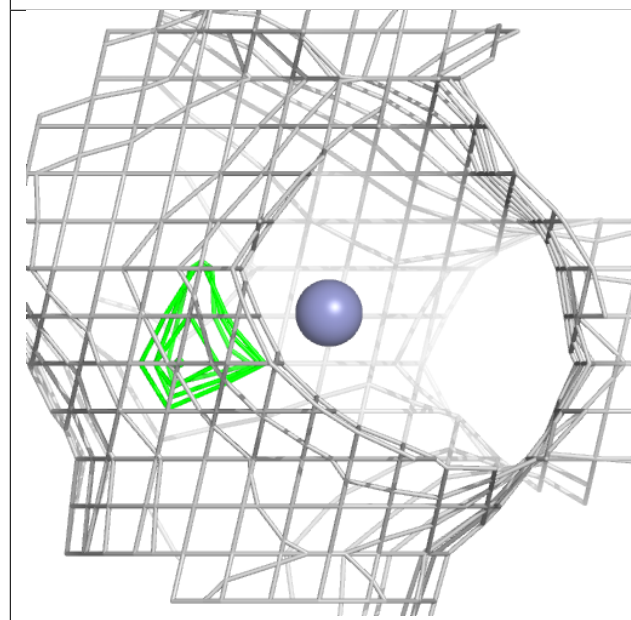
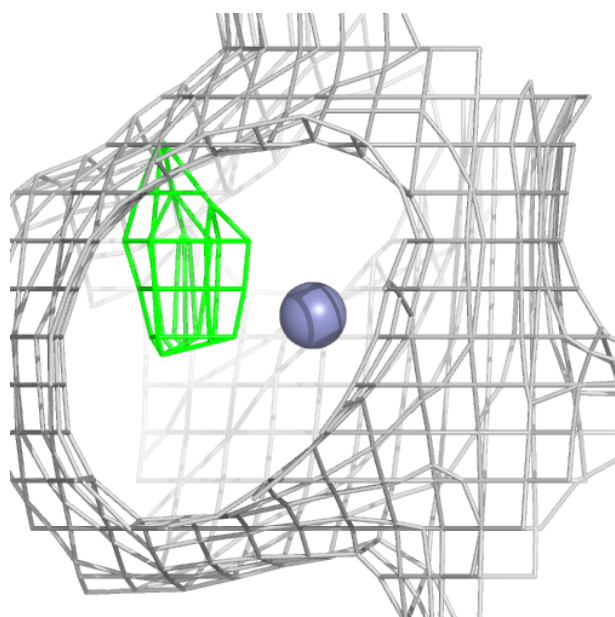
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

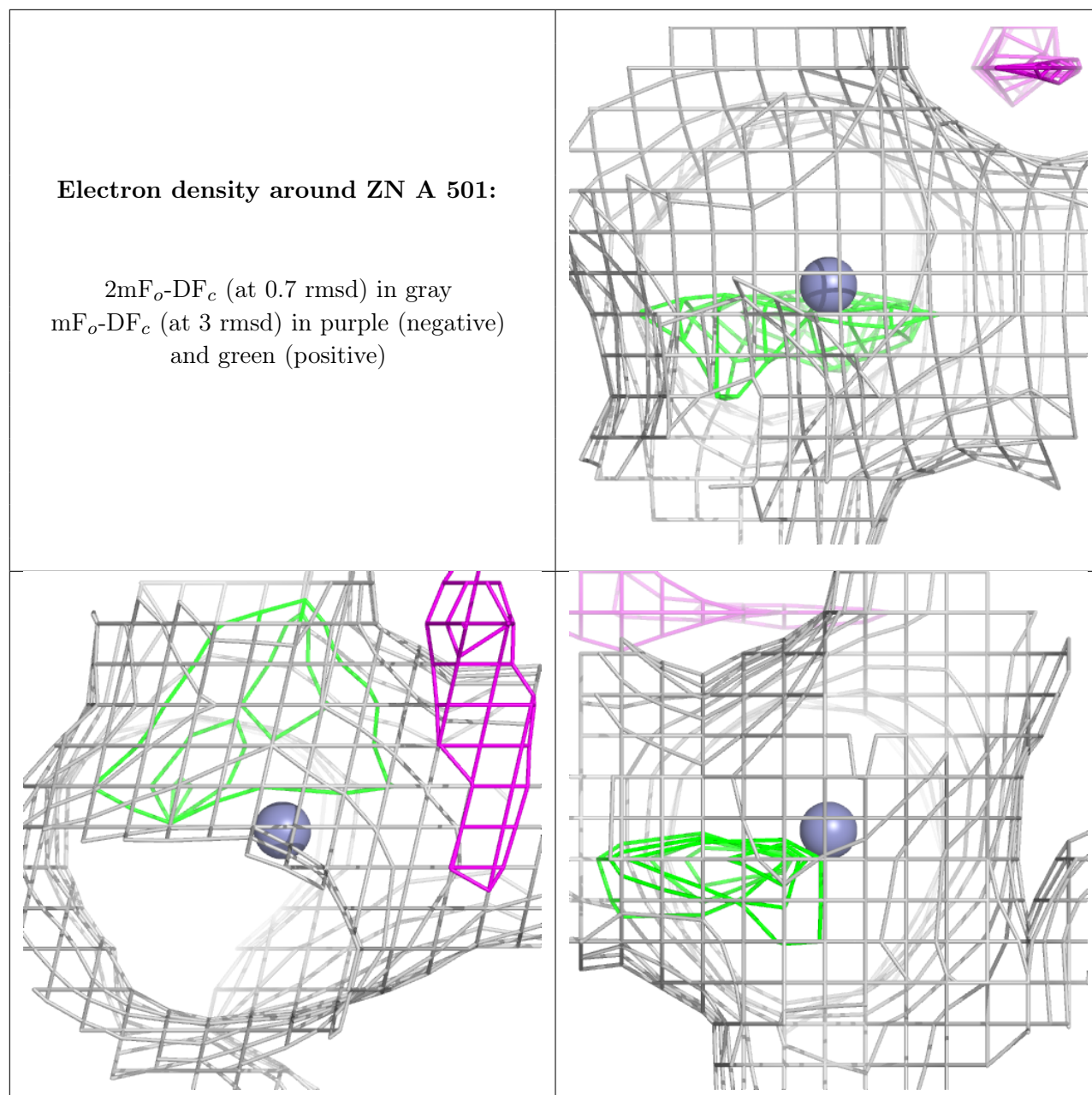
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PGE	B	503	10/10	0.76	0.22	78,80,82,83	0
4	GOL	A	503	6/6	0.79	0.19	90,90,90,90	0
4	GOL	B	504	6/6	0.82	0.17	73,74,74,75	0
5	PEG	B	502	7/7	0.91	0.14	56,57,60,61	0
3	MG	A	502	1/1	0.96	0.15	47,47,47,47	0
2	ZN	B	501	1/1	0.99	0.04	51,51,51,51	0
2	ZN	A	501	1/1	0.99	0.04	44,44,44,44	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 [i](#)

There are no such residues in this entry.