



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2022 – 04:15 am BST

PDB ID : 8A28  
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 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)

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<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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

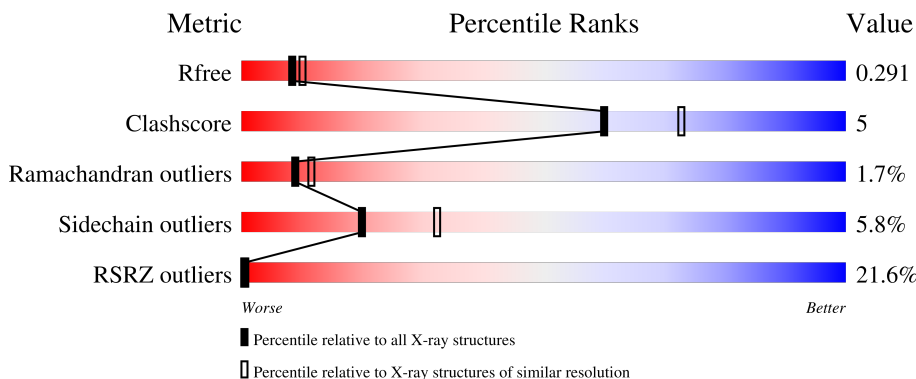
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 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	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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

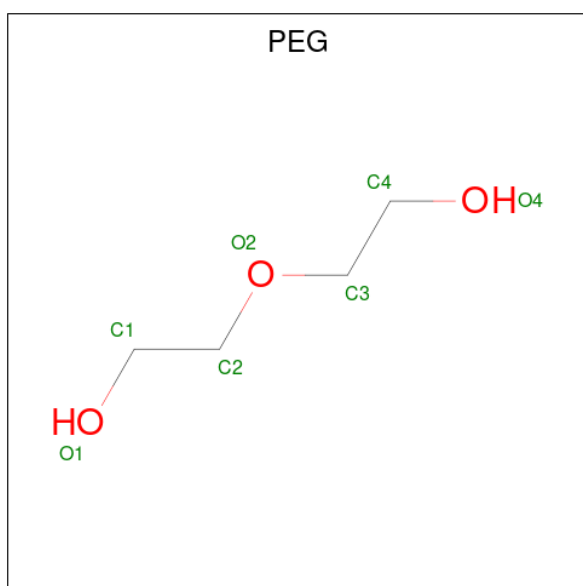
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (three-letter code: 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 (three-letter code: 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, $\alpha$ , $\beta$ , $\gamma$	115.83Å 47.57Å 236.40Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	46.73 – 2.40 76.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.73-2.40) 99.7 (76.81-2.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	48.4	Xtrriage
Anisotropy	0.570	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>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<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: PEG, GOL, PGE, ZN, MG

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	0.71	0/3063	0.78	0/4161
1	B	0.75	0/1869	0.83	1/2532 (0.0%)
All	All	0.72	0/4932	0.80	1/6693 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ILE	C-N-CA	5.16	134.60	121.70

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	24	0
1	B	1818	0	1728	20	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	43	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.

All (43) 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
1:A:129:TYR:OH	1:B:105:ARG:NH2	2.23	0.71
1:B:109:TYR:HB3	5:B:502:PEG:H12	1.74	0.70
1:B:167:ILE:CG1	1:B:211:THR:HB	2.21	0.69
1:B:113:TRP:NE1	5:B:502:PEG:H11	2.11	0.66
1:B:223:PRO:HB2	1:B:225:TRP:CD1	2.35	0.62
1:A:180:PRO:O	1:A:181:TRP:HB3	1.99	0.61
1:A:107:ASN:HB2	7:A:625:HOH:O	2.00	0.60
1:B:168:LEU:HD12	1:B:171:MET:HG3	1.85	0.58
1:A:333:PRO:HG2	1:A:387:GLY:HA3	1.89	0.55
1:A:116:VAL:HG11	1:A:148:TRP:CE2	2.42	0.54
1:B:161:GLU:OE2	6:B:503:PGE:H4	2.07	0.54
1:B:110:ASP:HB2	5:B:502:PEG:H31	1.89	0.54
1:A:150:GLU:HB3	1:A:197:LEU:HB2	1.91	0.53
1:A:271:ASN:HD21	1:A:279:PHE:N	2.09	0.51
1:A:226:LYS:NZ	7:A:601:HOH:O	2.40	0.50
1:A:39:ILE:HG23	1:A:116:VAL:HG23	1.94	0.50
1:B:150:GLU:HB3	1:B:197:LEU:HB2	1.95	0.48
1:B:226:LYS:NZ	7:B:601:HOH:O	2.42	0.48
1:A:272:GLN:HB3	1:A:275:MET:HG3	1.96	0.48
1:A:271:ASN:HD21	1:A:279:PHE:H	1.63	0.47
1:A:26:ASP:O	1:A:29:LEU:HB2	2.14	0.47
1:B:171:MET:O	1:B:174:ASN:HB2	2.15	0.47
1:A:309:LEU:HB2	1:A:378:ILE:HB	1.99	0.45
1:B:109:TYR:CB	5:B:502:PEG:H12	2.43	0.45
1:A:149:HIS:HB3	1:A:151:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:HIS:CE1	1:A:196:MET:CE	3.01	0.44
1:A:73:SER:CA	5:B:502:PEG:H42	2.44	0.44
1:A:167:ILE:HG12	1:A:211:THR:HB	1.99	0.43
1:A:179:GLU:O	1:A:180:PRO:O	2.36	0.43
1:B:63:VAL:HG21	1:B:145:VAL:HG12	1.99	0.43
1:B:167:ILE:HG12	1:B:211:THR:CB	2.37	0.42
1:B:164:TRP:HA	1:B:167:ILE:HD12	2.02	0.42
1:B:64:TYR:HA	1:B:94:LYS:O	2.20	0.41
1:A:342:ARG:HG3	1:A:374:MET:HG2	2.02	0.41
1:A:223:PRO:HB2	1:A:225:TRP:CD1	2.57	0.40
1:B:133:TRP:HB2	1:B:136:LEU:HD12	2.03	0.40
1:A:195:VAL:HG12	1:A:234:ASP:OD2	2.21	0.40
1:A:48:LYS:O	1:A:52:VAL:HG23	2.21	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	380/382 (100%)	342 (90%)	29 (8%)	9 (2%)	<b>6</b> <b>6</b>
1	B	223/382 (58%)	208 (93%)	14 (6%)	1 (0%)	34 48
All	All	603/764 (79%)	550 (91%)	43 (7%)	10 (2%)	<b>9</b> <b>11</b>

All (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

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Mol	Chain	Res	Type
1	A	180	PRO
1	A	187	ASN
1	A	247	GLU
1	A	395	ASN
1	A	322	VAL

### 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%)	288 (94%)	20 (6%)	17	27
1	B	190/327 (58%)	181 (95%)	9 (5%)	26	42
All	All	498/654 (76%)	469 (94%)	29 (6%)	20	32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	43	SER
1	A	156	ARG
1	A	181	TRP
1	A	182	GLU
1	A	186	LEU
1	A	188	GLU
1	A	243	GLU
1	A	263	GLU
1	A	265	ASN
1	A	275	MET
1	A	279	PHE
1	A	293	PHE
1	A	300	SER
1	A	311	THR
1	A	323	CYS
1	A	324	MET
1	A	361	VAL

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Mol	Chain	Res	Type
1	A	393	VAL
1	A	403	CYS
1	B	44	PRO
1	B	112	CYS
1	B	134	LYS
1	B	156	ARG
1	B	182	GLU
1	B	188	GLU
1	B	194	SER
1	B	233	SER
1	B	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	280	GLN

### 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 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	0.27	0	5,5,5	0.27	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	0.46	0
5	PEG	B	502	-	6,6,6	0.31	0	5,5,5	0.29	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
6	PGE	B	503	-	-	3/7/7/7	-
5	PEG	B	502	-	-	1/4/4/4	-

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
6	B	503	PGE	1	0
5	B	502	PEG	8	0

## 5.7 Other polymers [i](#)

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	382/382 (100%)	1.89	107 (28%) <b>0</b>   <b>0</b>	39, 70, 140, 163	159 (41%)
1	B	225/382 (58%)	1.13	24 (10%) <b>6</b>   <b>5</b>	45, 68, 105, 130	0
All	All	607/764 (79%)	1.61	131 (21%) <b>0</b>   <b>0</b>	39, 70, 136, 163	159 (26%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	9.6
1	A	403	CYS	9.5
1	A	367	LEU	8.9
1	A	369	ALA	8.9
1	A	293	PHE	8.0
1	A	288	GLY	8.0
1	A	292	TYR	7.5
1	A	268	GLY	7.4
1	A	368	LYS	7.4
1	A	365	PHE	7.2
1	A	283	TYR	7.2
1	A	398	PHE	7.2
1	A	265	ASN	6.9
1	A	258	PHE	6.8
1	A	290	THR	6.6
1	A	314	PHE	6.4
1	A	346	ASN	6.1
1	A	366	ASN	6.1
1	A	347	THR	6.1
1	A	273	VAL	6.0
1	A	350	ILE	5.8
1	A	370	GLY	5.8
1	A	343	GLN	5.7
1	A	364	ASN	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	267	CYS	5.6
1	A	357	SER	5.6
1	A	324	MET	5.6
1	A	294	MET	5.5
1	A	259	ILE	5.5
1	A	315	GLY	5.3
1	A	402	PRO	5.3
1	A	371	ARG	5.2
1	A	266	ASP	5.1
1	A	344	ASP	5.0
1	A	322	VAL	4.9
1	A	396	LEU	4.8
1	A	274	GLY	4.6
1	A	256	PRO	4.6
1	B	183	ASN	4.6
1	A	305	ALA	4.6
1	A	320	GLN	4.6
1	A	264	SER	4.5
1	A	328	VAL	4.5
1	A	345	SER	4.4
1	B	184	ASN	4.4
1	A	279	PHE	4.4
1	A	295	VAL	4.4
1	A	280	GLN	4.4
1	A	282	LYS	4.3
1	A	399	LYS	4.3
1	A	342	ARG	4.3
1	A	251	PRO	4.2
1	A	147	PHE	4.2
1	B	181	TRP	4.2
1	A	262	PHE	4.2
1	B	98	ALA	4.2
1	A	257	ASP	4.1
1	A	374	MET	4.1
1	B	100	VAL	4.1
1	B	245	PHE	4.1
1	B	246	GLY	4.1
1	A	391	VAL	4.0
1	A	245	PHE	4.0
1	A	393	VAL	4.0
1	A	253	PRO	3.9
1	B	244	CYS	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	301	SER	3.9
1	A	261	ASP	3.8
1	B	129	TYR	3.8
1	A	310	ILE	3.7
1	A	254	LYS	3.7
1	A	377	PHE	3.7
1	A	186	LEU	3.6
1	A	271	ASN	3.6
1	B	185	TYR	3.5
1	A	248	VAL	3.5
1	A	361	VAL	3.4
1	A	252	PRO	3.3
1	A	269	LEU	3.3
1	A	323	CYS	3.3
1	A	373	ASP	3.3
1	A	185	TYR	3.3
1	A	181	TRP	3.1
1	A	321	ASP	3.1
1	A	255	ILE	3.1
1	A	358	ASN	3.1
1	A	353	TYR	3.1
1	A	312	PRO	3.1
1	A	372	GLU	3.0
1	A	340	ILE	3.0
1	A	281	ARG	3.0
1	B	62	ILE	3.0
1	B	240	ARG	2.9
1	B	99	GLY	2.9
1	A	187	ASN	2.9
1	A	348	GLU	2.9
1	A	62	ILE	2.9
1	A	129	TYR	2.9
1	B	91	ILE	2.8
1	A	349	SER	2.7
1	B	187	ASN	2.7
1	A	300	SER	2.7
1	A	317	TYR	2.6
1	A	401	LYS	2.6
1	B	112	CYS	2.6
1	B	61	GLY	2.5
1	A	302	GLY	2.5
1	A	136	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	287	GLY	2.4
1	A	352	LYS	2.4
1	A	375	ARG	2.4
1	B	104	ILE	2.4
1	A	42	VAL	2.3
1	A	395	ASN	2.3
1	B	64	TYR	2.3
1	A	296	LEU	2.3
1	B	199	GLY	2.3
1	B	45	TYR	2.2
1	B	96	ARG	2.2
1	A	359	SER	2.2
1	A	207	GLY	2.2
1	A	318	GLY	2.2
1	A	289	ARG	2.1
1	A	286	LEU	2.1
1	B	136	LEU	2.1
1	B	147	PHE	2.1
1	A	98	ALA	2.1
1	A	285	THR	2.1
1	A	351	GLY	2.1
1	A	356	VAL	2.1
1	A	337	ASP	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](#)

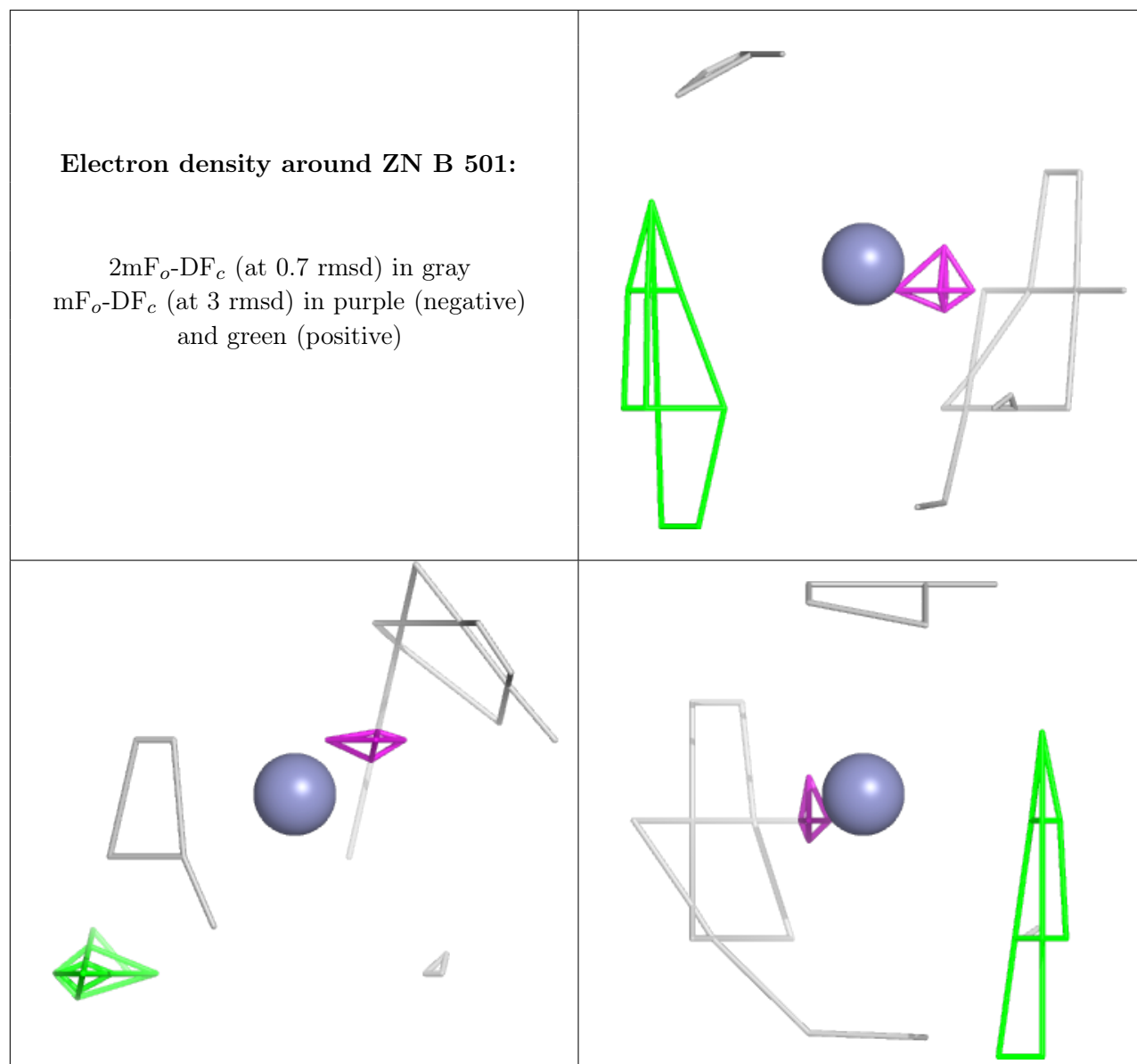
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

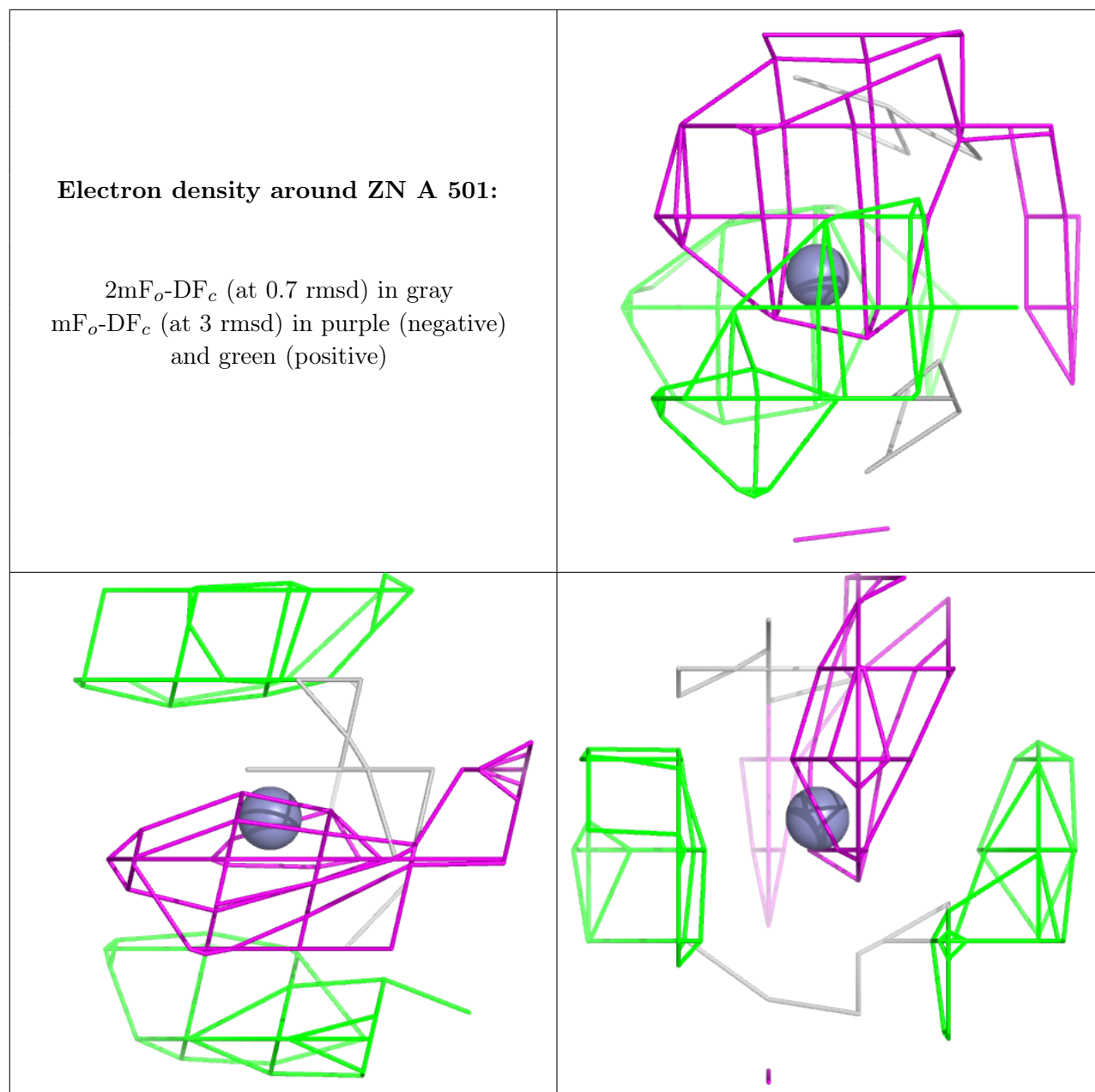
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	503	6/6	0.49	0.38	90,90,90,90	0
6	PGE	B	503	10/10	0.65	0.32	78,80,82,83	0
4	GOL	B	504	6/6	0.66	0.27	73,74,74,75	0
5	PEG	B	502	7/7	0.85	0.22	56,57,60,61	0
3	MG	A	502	1/1	0.94	0.20	47,47,47,47	0
2	ZN	B	501	1/1	0.98	0.18	51,51,51,51	0
2	ZN	A	501	1/1	0.99	0.16	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.





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.