

# wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2021 – 01:04 pm BST

PDB ID : 6ZA2

Title : Crystal structure of dimeric latent PorU from Porphyromonas gingivalis

Authors: Gomis-Ruth, F.X.; Goulas, T.; Guevara, T.; Rodriguez-Banqueri, A.;

Potempa, J.

Deposited on : 2020-06-04

Resolution : 3.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

 $\begin{array}{cccc} & EDS & : & 2.23.2 \\ buster-report & : & 1.1.7 \ (2018) \end{array}$ 

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$ 

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

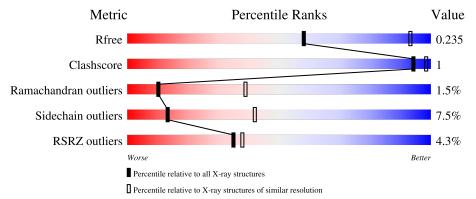
Validation Pipeline (wwPDB-VP) : 2.23.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 3.35 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 >=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 <=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	1156	83%	10%	6%
1	В	1156	5% 85%	9%	• 6%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31870 atoms, of which 15484 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 Por secretion system protein por U.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	1081	Total 16048	C 5189	H 7821	N 1406	O 1598	S 34	7821	0	0
1	В	1083	Total 15814	C 5128	H 7663	N 1395	O 1595	S 33	7663	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP B2RGP6
A	4	SER	-	expression tag	UNP B2RGP6
A	5	SER	-	expression tag	UNP B2RGP6
A	6	HIS	-	expression tag	UNP B2RGP6
A	7	HIS	-	expression tag	UNP B2RGP6
A	8	HIS	-	expression tag	UNP B2RGP6
A	9	HIS	-	expression tag	UNP B2RGP6
A	10	HIS	-	expression tag	UNP B2RGP6
A	11	HIS	-	expression tag	UNP B2RGP6
A	12	SER	-	expression tag	UNP B2RGP6
A	13	GLN	-	expression tag	UNP B2RGP6
A	14	ASP	-	expression tag	UNP B2RGP6
A	15	PRO	-	expression tag	UNP B2RGP6
A	16	ASN	-	expression tag	UNP B2RGP6
A	17	SER	-	expression tag	UNP B2RGP6
A	18	SER	-	expression tag	UNP B2RGP6
A	19	SER	-	expression tag	UNP B2RGP6
A	20	ALA	-	expression tag	UNP B2RGP6
A	21	ARG	-	expression tag	UNP B2RGP6
A	22	LEU	-	expression tag	UNP B2RGP6
A	23	GLN	-	expression tag	UNP B2RGP6
В	-21	GLY	-	expression tag	UNP B2RGP6
В	-20	SER	-	expression tag	UNP B2RGP6
В	-19	SER	-	expression tag	UNP B2RGP6
В	-18	HIS	-	expression tag	UNP B2RGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-17	HIS	-	expression tag	UNP B2RGP6
В	-16	HIS	-	expression tag	UNP B2RGP6
В	-15	HIS	-	expression tag	UNP B2RGP6
В	-14	HIS	-	expression tag	UNP B2RGP6
В	-13	HIS	-	expression tag	UNP B2RGP6
В	-12	SER	_	expression tag	UNP B2RGP6
В	-11	GLN	-	expression tag	UNP B2RGP6
В	-10	ASP	-	expression tag	UNP B2RGP6
В	-9	PRO	-	expression tag	UNP B2RGP6
В	-8	ASN	-	expression tag	UNP B2RGP6
В	-7	SER	-	expression tag	UNP B2RGP6
В	-6	SER	-	expression tag	UNP B2RGP6
В	-5	SER	-	expression tag	UNP B2RGP6
В	-4	ALA	-	expression tag	UNP B2RGP6
В	-3	ARG		expression tag	UNP B2RGP6
В	-2	LEU	-	expression tag	UNP B2RGP6
В	-1	GLN	-	expression tag	UNP B2RGP6

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	В	2	Total Ca 2 2	0	0

• Molecule 3 is water.

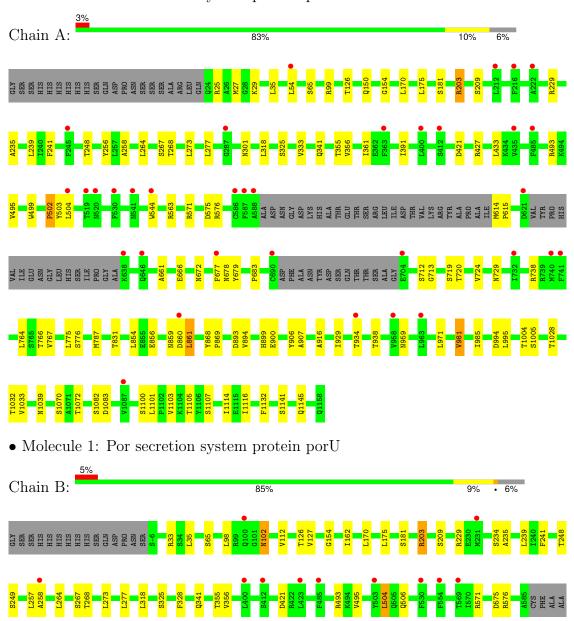
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	В	2	Total O 2 2	0	0



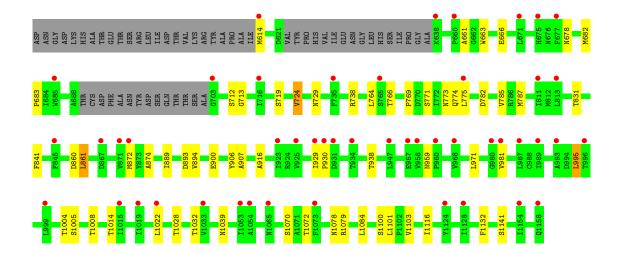
## 3 Residue-property plots (i)

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: Por secretion system protein por U









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	171.70Å 171.70Å 440.40Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	88.48 - 3.35	Depositor
resolution (A)	88.48 - 3.35	EDS
% Data completeness	100.0 (88.48-3.35)	Depositor
(in resolution range)	100.0 (88.48-3.35)	EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.14 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.202 , 0.243	Depositor
$R, R_{free}$	0.206 , $0.235$	DCC
$R_{free}$ test set	836 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$  <  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31870	wwPDB-VP
Average B, all atoms $(Å^2)$	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CA

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.52	0/8404	0.70	1/11434~(0.0%)
1	В	0.51	0/8323	0.71	1/11338 (0.0%)
All	All	0.52	0/16727	0.70	$2/22772 \ (0.0\%)$

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	В	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	571	ARG	CD-NE-CZ	11.93	140.31	123.60
1	A	571	ARG	CD-NE-CZ	6.36	132.50	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	MET	Mainchain
1	A	929	ILE	Mainchain
1	В	614	MET	Mainchain
1	В	929	ILE	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	A	8227	7821	7821	24	0
1	В	8151	7663	7665	23	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
3	A	2	0	0	0	0
3	В	2	0	0	0	0
All	All	16386	15484	15486	42	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 1.

The worst 5 of 42 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:A:861:LEU:HD11	1:B:738:ARG:HG2	1.73	0.69	
1:A:985:ILE:HG23	1:A:1033:VAL:HG12	1.77	0.65	
1:A:738:ARG:HG2	1:B:861:LEU:HD11	1.80	0.62	
1:B:504:LEU:C	1:B:504:LEU:HD22	2.24	0.57	
1:A:333:VAL:HG21	1:A:361:ILE:HG12	1.87	0.57	

There are no symmetry-related clashes.

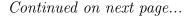
#### 5.3 Torsion angles (i)

#### 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	1073/1156 (93%)	993 (92%)	64 (6%)	16 (2%)	10 39	





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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	Percentiles	
1	В	1075/1156 (93%)	1004 (93%)	55 (5%)	16 (2%)	10	39	
All	All	2148/2312 (93%)	1997 (93%)	119 (6%)	32 (2%)	10	39	

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	SER
1	A	894	VAL
1	A	981	VAL
1	В	258	ALA
1	В	712	SER

#### 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	Rotameric Outliers		Percentiles		
1	A	859/978 (88%)	793 (92%)	66 (8%)		13	41	
1	В	839/978 (86%)	778 (93%)	61 (7%)		14	43	
All	All	1698/1956 (87%)	1571 (92%)	127 (8%)		13	42	

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1082	SER
1	В	995	LEU
1	В	126	THR
1	В	971	LEU
1	В	1070	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	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 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,  $95^{th}$  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	1081/1156 (93%)	0.35	34 (3%)	49	52	85, 127, 218, 290	0
1	В	1083/1156 (93%)	0.40	59 (5%)	25	28	85, 134, 257, 289	0
All	All	2164/2312 (93%)	0.38	93 (4%)	35	38	85, 130, 250, 290	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	CYS	11.3
1	В	703	GLY	9.9
1	A	621	ASP	5.6
1	A	704	GLU	5.1
1	В	981	VAL	4.9

### 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.

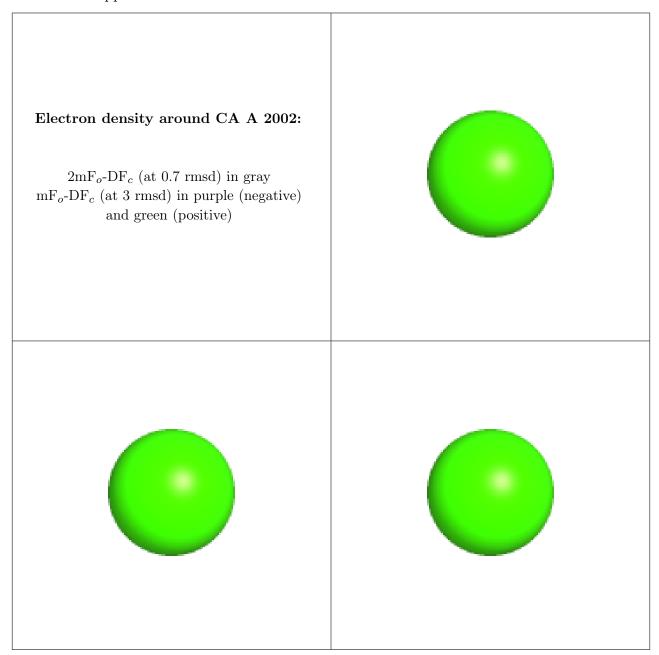
#### 6.4 Ligands (i)

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,  $95^{th}$  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.

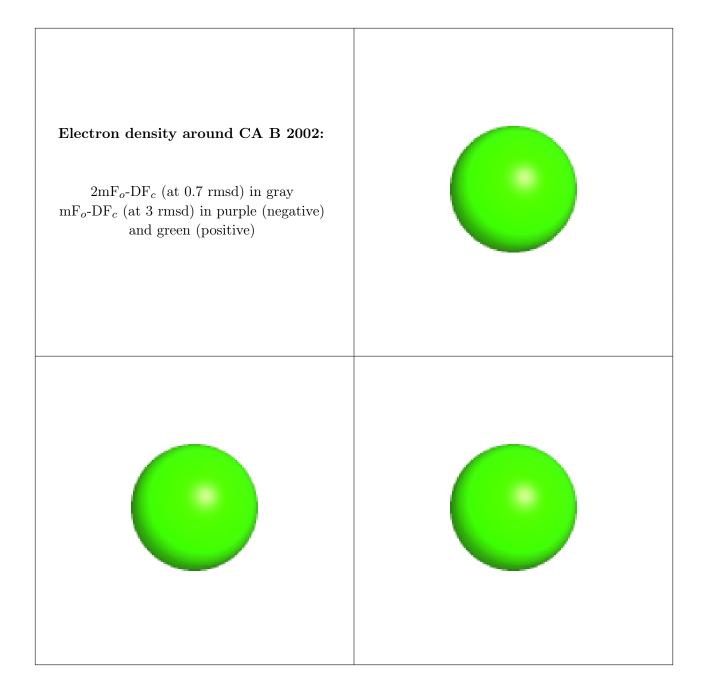


Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
2	CA	A	2002	1/1	0.63	0.11	169,169,169,169	0
2	CA	В	2002	1/1	0.76	0.10	213,213,213,213	0
2	CA	A	2001	1/1	0.97	0.21	106,106,106,106	0
2	CA	В	2001	1/1	0.98	0.23	103,103,103,103	0

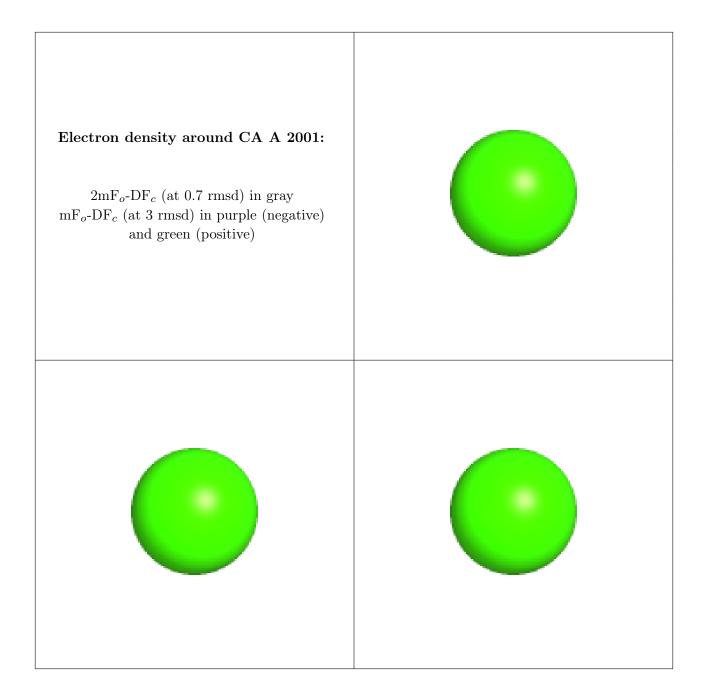
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



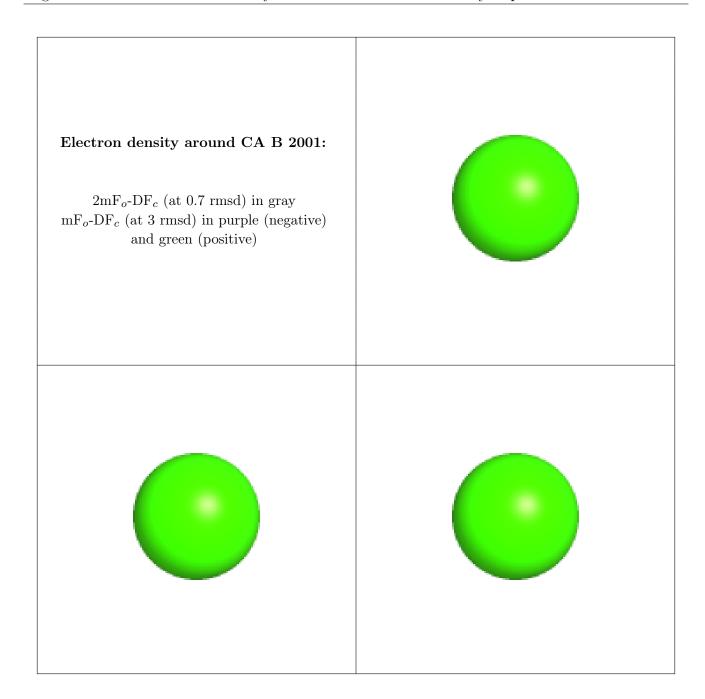












## 6.5 Other polymers (i)

There are no such residues in this entry.

