



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2022 – 03:03 pm GMT

PDB ID : 7NQB  
Title : X.ray structure of the oxaliplatin/beta-lactoglobulin adduct  
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Deposited on : 2021-03-01  
Resolution : 2.01 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 : 2.27  
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) : 2.27

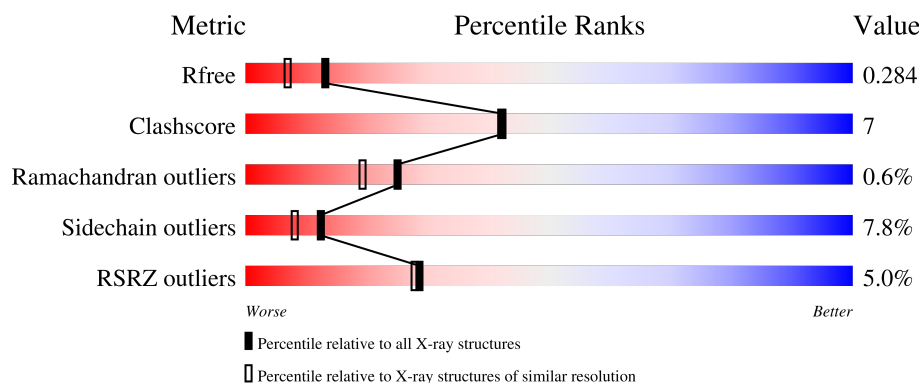
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	162	 5% 72% 25% ..
1	BBB	162	 5% 81% 15% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2592 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 Beta-lactoglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	160	Total	C	N	O	S	0	1	0
			1270	808	205	248	9			
1	BBB	159	Total	C	N	O	S	0	0	0
			1257	800	203	245	9			

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Pt	0	0
			1	1		

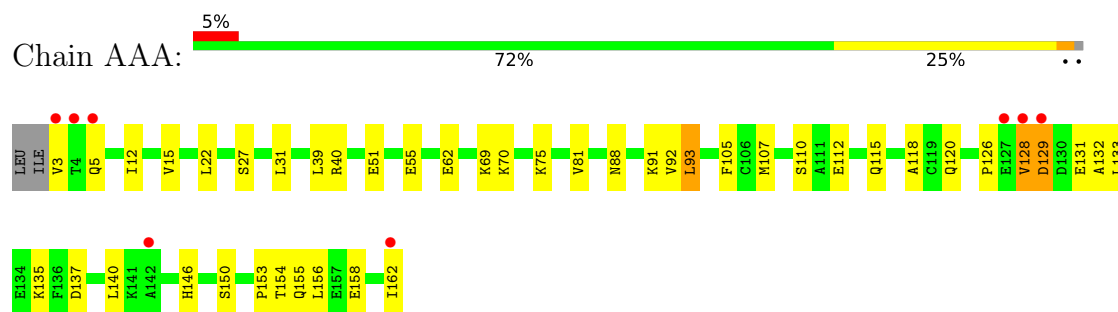
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	39	Total	O	0	0
			39	39		
3	BBB	25	Total	O	0	0
			25	25		

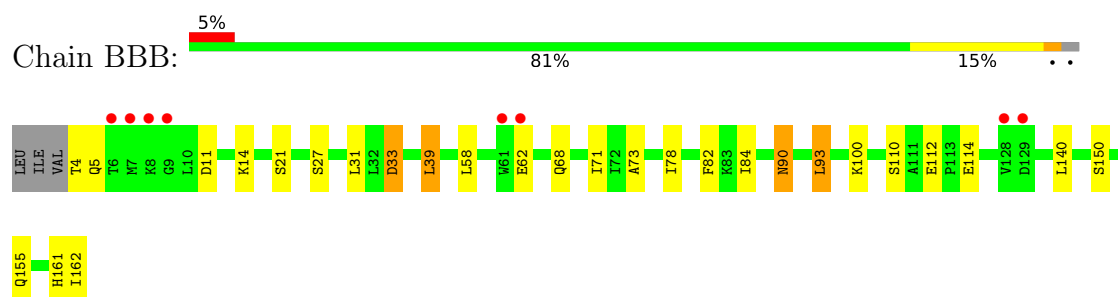
### 3 Residue-property plots [i](#)

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: Beta-lactoglobulin



- Molecule 1: Beta-lactoglobulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.87Å 112.58Å 38.08Å 90.00° 117.64° 90.00°	Depositor
Resolution (Å)	56.30 – 2.01 56.29 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.30-2.01) 97.6 (56.29-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.212 , 0.284 0.218 , 0.284	Depositor DCC
$R_{free}$ test set	772 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.057	Xtriage
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>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2592	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PT

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	0.66	0/1291	0.85	0/1746
1	BBB	0.65	0/1278	0.83	0/1728
All	All	0.66	0/2569	0.84	0/3474

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	1270	0	1283	23	0
1	BBB	1257	0	1270	12	0
2	AAA	1	0	0	0	0
3	AAA	39	0	0	2	0
3	BBB	25	0	0	0	0
All	All	2592	0	2553	35	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 7.

All (35) 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:BBB:161:HIS:O	1:BBB:162:ILE:HG12	1.75	0.86
1:AAA:112:GLU:HG3	1:AAA:115:GLN:HB3	1.73	0.69
1:BBB:21:SER:O	1:BBB:161:HIS:HE1	1.78	0.65
1:AAA:128:VAL:HG23	1:AAA:153:PRO:HG3	1.80	0.64
1:BBB:161:HIS:O	1:BBB:162:ILE:CG1	2.46	0.62
1:AAA:31:LEU:HD22	1:AAA:39:LEU:HD22	1.83	0.60
1:AAA:88:ASN:ND2	3:AAA:302:HOH:O	2.33	0.60
1:AAA:154:THR:O	1:AAA:158:GLU:HG3	2.02	0.59
1:AAA:92:VAL:HG22	1:AAA:107:MET:HG2	1.89	0.53
1:AAA:126:PRO:HA	1:AAA:156:LEU:HD12	1.92	0.52
1:AAA:91:LYS:HD2	1:AAA:110:SER:HB3	1.91	0.52
1:BBB:11:ASP:HB3	1:BBB:14:LYS:HE3	1.92	0.52
1:BBB:84:ILE:O	1:BBB:90:ASN:HA	2.11	0.51
1:AAA:158:GLU:OE2	1:AAA:162:ILE:HG22	2.10	0.50
1:BBB:58:LEU:HD21	1:BBB:71:ILE:HD12	1.93	0.50
1:AAA:55:GLU:OE1	1:AAA:70:LYS:HE2	2.11	0.50
1:AAA:39:LEU:HD23	1:AAA:118:ALA:HB2	1.97	0.47
1:AAA:154:THR:HG22	1:AAA:158:GLU:OE1	2.14	0.46
1:AAA:131:GLU:O	1:AAA:135:LYS:HG2	2.15	0.46
1:AAA:81:VAL:HG22	1:AAA:93:LEU:HD12	1.98	0.45
1:AAA:128:VAL:CG2	1:AAA:153:PRO:HD3	2.47	0.45
1:BBB:93:LEU:HD22	1:BBB:93:LEU:N	2.31	0.45
1:BBB:90:ASN:HD21	1:BBB:110:SER:H	1.63	0.45
1:AAA:12:ILE:O	1:AAA:15:VAL:HG22	2.17	0.44
1:AAA:51:GLU:O	1:AAA:75:LYS:NZ	2.30	0.44
1:BBB:73:ALA:HB1	1:BBB:82:PHE:HB3	1.99	0.44
1:AAA:129:ASP:HB3	1:AAA:132:ALA:HB3	2.01	0.43
1:AAA:105:PHE:CE1	1:AAA:120:GLN:HB2	2.54	0.43
1:BBB:31:LEU:HD13	1:BBB:39:LEU:HD22	2.01	0.42
1:AAA:27:SER:O	1:AAA:146:HIS:HD2	2.02	0.42
1:AAA:5:GLN:NE2	3:AAA:306:HOH:O	2.52	0.42
1:AAA:22:LEU:HG	1:AAA:133:LEU:HD21	2.02	0.41
1:BBB:27:SER:OG	1:BBB:114:GLU:O	2.29	0.41
1:AAA:155:GLN:HE21	1:AAA:162:ILE:HG12	1.86	0.41
1:BBB:155:GLN:HG2	1:BBB:162:ILE:HG23	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	159/162 (98%)	147 (92%)	11 (7%)	1 (1%)	25	19
1	BBB	157/162 (97%)	147 (94%)	9 (6%)	1 (1%)	25	19
All	All	316/324 (98%)	294 (93%)	20 (6%)	2 (1%)	25	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	128	VAL
1	BBB	33	ASP

### 5.3.2 Protein sidechains

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	142/143 (99%)	133 (94%)	9 (6%)	18	13
1	BBB	140/143 (98%)	127 (91%)	13 (9%)	9	5
All	All	282/286 (99%)	260 (92%)	22 (8%)	12	8

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	3	VAL
1	AAA	40	ARG
1	AAA	62	GLU
1	AAA	69	LYS

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Mol	Chain	Res	Type
1	AAA	93	LEU
1	AAA	129	ASP
1	AAA	137	ASP
1	AAA	140	LEU
1	AAA	150	SER
1	BBB	4	THR
1	BBB	5	GLN
1	BBB	33	ASP
1	BBB	39	LEU
1	BBB	62	GLU
1	BBB	68	GLN
1	BBB	78	ILE
1	BBB	90	ASN
1	BBB	93	LEU
1	BBB	100	LYS
1	BBB	112	GLU
1	BBB	140	LEU
1	BBB	150	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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, 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	160/162 (98%)	0.07	8 (5%) 28 28	11, 23, 48, 66	0
1	BBB	159/162 (98%)	0.11	8 (5%) 28 28	11, 25, 45, 63	0
All	All	319/324 (98%)	0.09	16 (5%) 28 28	11, 24, 47, 66	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	128	VAL	7.5
1	AAA	142	ALA	3.3
1	BBB	9	GLY	3.2
1	BBB	62	GLU	3.1
1	AAA	129	ASP	2.7
1	AAA	162	ILE	2.6
1	AAA	5	GLN	2.6
1	AAA	4	THR	2.5
1	BBB	7	MET	2.5
1	AAA	127	GLU	2.4
1	BBB	128	VAL	2.2
1	AAA	3	VAL	2.2
1	BBB	8	LYS	2.2
1	BBB	61	TRP	2.1
1	BBB	129	ASP	2.1
1	BBB	6	THR	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

There are no monosaccharides in this entry.

### 6.4 Ligands

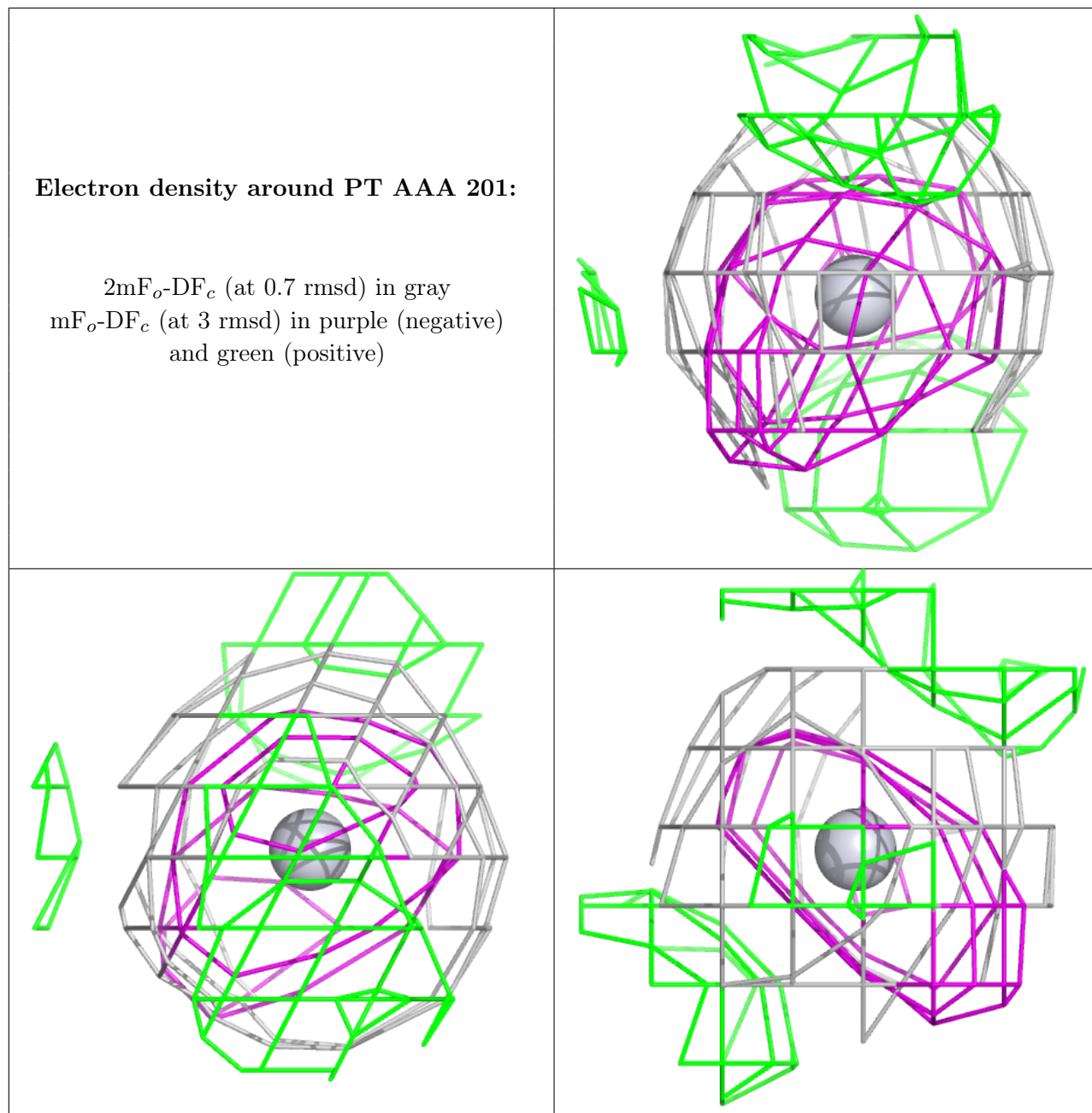
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	PT	AAA	201	1/1	0.99	0.03	29,29,29,29	1

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 PT 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.