



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2023 – 10:35 pm BST

PDB ID : 8A6U  
Title : PcIDS1 in complex with Mg<sup>2+</sup>  
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Deposited on : 2022-06-20  
Resolution : 1.65 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.

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  
Xtriage (Phenix) : 1.13  
EDS : 2.33  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

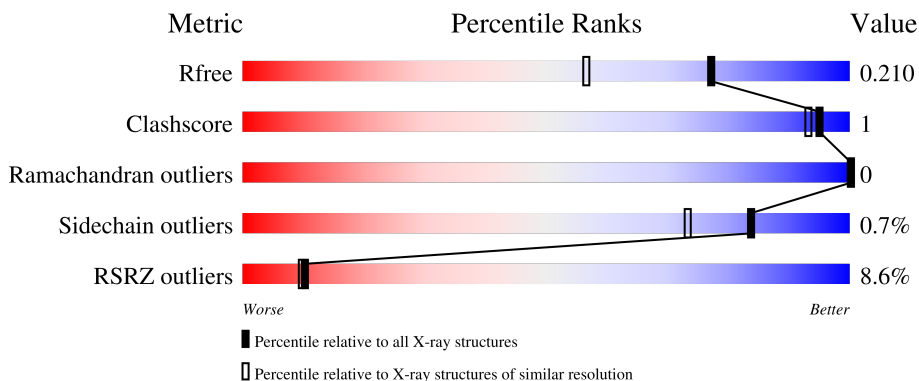
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	346	 9% 87% 5% 8%
1	B	346	 7% 90% 7% 7%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5786 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 Isoprenyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2572	1659	425	471	17	0	0	0
1	B	323	2618	1688	432	481	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP M1JS91
A	85	SER	-	expression tag	UNP M1JS91
B	84	GLY	-	expression tag	UNP M1JS91
B	85	SER	-	expression tag	UNP M1JS91

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

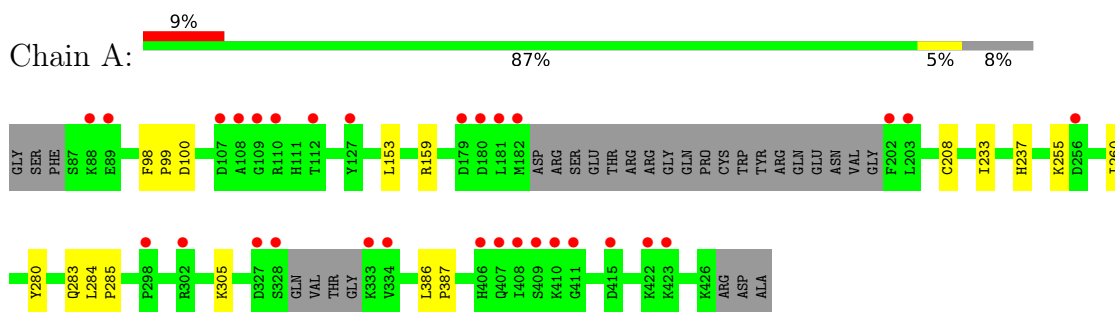
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total 245	O 245	0	0
3	B	349	Total 349	O 349	0	0

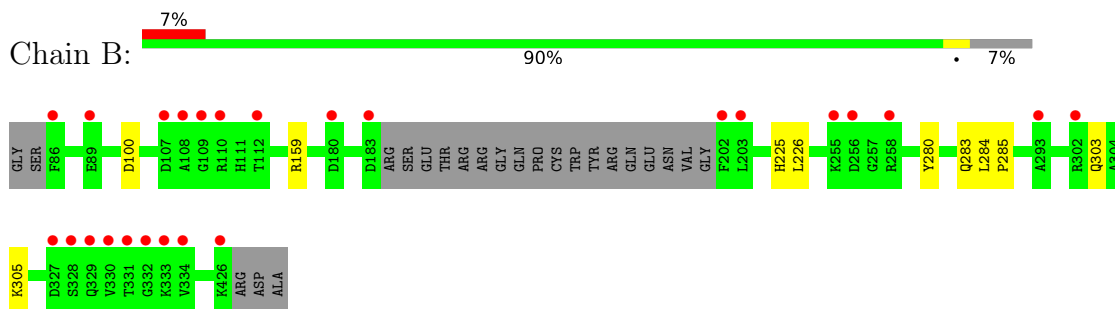
### 3 Residue-property plots [i](#)

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: Isoprenyl diphosphate synthase



- Molecule 1: Isoprenyl diphosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.16Å 78.33Å 89.61Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	15.00 – 1.65 14.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-1.65) 98.0 (14.98-1.65)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.155 , 0.195 0.166 , 0.210	Depositor DCC
$R_{free}$ test set	4712 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtrriage
Anisotropy	1.064	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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: 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	0.66	0/2629	0.67	0/3547
1	B	0.76	0/2677	0.69	0/3614
All	All	0.71	0/5306	0.68	0/7161

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	A	2572	0	2585	8	0
1	B	2618	0	2626	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	245	0	0	0	0
3	B	349	0	0	0	0
All	All	5786	0	5211	12	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.

All (12) 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:284:LEU:HB3	1:B:285:PRO:HD3	1.90	0.52
1:A:283:GLN:OE1	1:A:305:LYS:HA	2.11	0.51
1:A:100:ASP:OD2	1:A:159:ARG:NH2	2.46	0.48
1:A:284:LEU:HB3	1:A:285:PRO:HD3	1.96	0.47
1:B:283:GLN:OE1	1:B:305:LYS:HA	2.17	0.44
1:B:225:HIS:CE1	1:B:226:LEU:HG	2.54	0.43
1:A:255:LYS:HB2	1:A:260:ILE:HD11	2.00	0.42
1:B:100:ASP:OD2	1:B:159:ARG:NH1	2.51	0.42
1:A:98:PHE:HB3	1:A:99:PRO:HD3	2.01	0.42
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.93	0.41
1:A:386:LEU:N	1:A:387:PRO:CD	2.84	0.41
1:A:233:ILE:HG22	1:A:237:HIS:CE1	2.57	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	311/346 (90%)	304 (98%)	7 (2%)	0	100	100
1	B	319/346 (92%)	313 (98%)	6 (2%)	0	100	100
All	All	630/692 (91%)	617 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	286/310 (92%)	284 (99%)	2 (1%)	84	73
1	B	291/310 (94%)	289 (99%)	2 (1%)	84	73
All	All	577/620 (93%)	573 (99%)	4 (1%)	84	73

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	CYS
1	A	280	TYR
1	B	280	TYR
1	B	303	GLN

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 [i](#)

Of 2 ligands modelled in this entry, 2 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

### 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	317/346 (91%)	0.44	30 (9%) <b>8</b> <b>7</b>	24, 38, 65, 90	0
1	B	323/346 (93%)	0.54	25 (7%) <b>13</b> <b>13</b>	22, 32, 60, 95	0
All	All	640/692 (92%)	0.49	55 (8%) <b>10</b> <b>10</b>	22, 35, 63, 95	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	PHE	11.6
1	B	330	VAL	7.6
1	A	333	LYS	6.7
1	B	333	LYS	6.7
1	B	329	GLN	6.5
1	A	108	ALA	6.2
1	B	332	GLY	6.2
1	A	256	ASP	5.7
1	A	109	GLY	5.6
1	B	331	THR	5.4
1	A	334	VAL	5.3
1	B	328	SER	5.2
1	B	334	VAL	5.1
1	B	203	LEU	5.1
1	B	256	ASP	4.9
1	A	202	PHE	4.7
1	B	110	ARG	4.6
1	A	409	SER	4.5
1	A	110	ARG	4.2
1	B	183	ASP	4.1
1	A	327	ASP	3.8
1	A	422	LYS	3.7
1	A	415	ASP	3.6
1	B	109	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	86	PHE	3.6
1	A	408	ILE	3.6
1	A	298	PRO	3.4
1	A	181	LEU	3.4
1	A	88	LYS	3.4
1	A	423	LYS	3.2
1	B	89	GLU	3.2
1	B	327	ASP	3.2
1	A	406	HIS	3.1
1	A	411	GLY	3.1
1	A	127	TYR	3.1
1	A	203	LEU	3.0
1	A	328	SER	2.8
1	B	108	ALA	2.8
1	B	258	ARG	2.8
1	A	107	ASP	2.7
1	B	426	LYS	2.7
1	A	302	ARG	2.7
1	B	112	THR	2.6
1	A	89	GLU	2.6
1	A	410	LYS	2.4
1	A	407	GLN	2.4
1	A	180	ASP	2.4
1	B	180	ASP	2.4
1	A	182	MET	2.3
1	B	107	ASP	2.3
1	A	112	THR	2.2
1	A	179	ASP	2.2
1	B	302	ARG	2.1
1	B	255	LYS	2.1
1	B	293	ALA	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

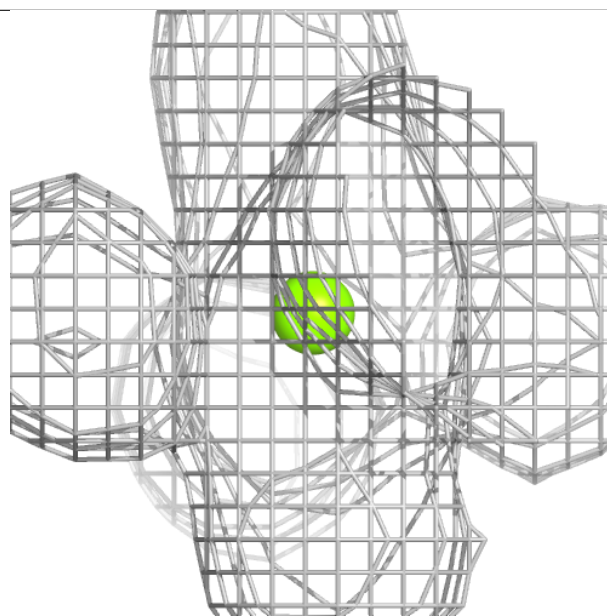
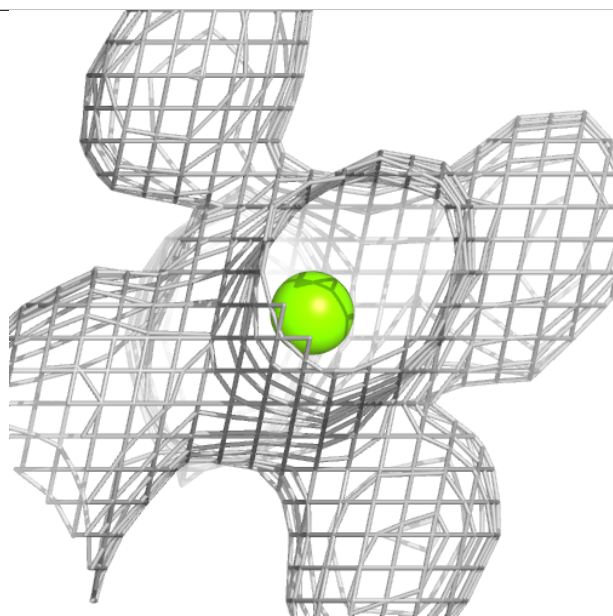
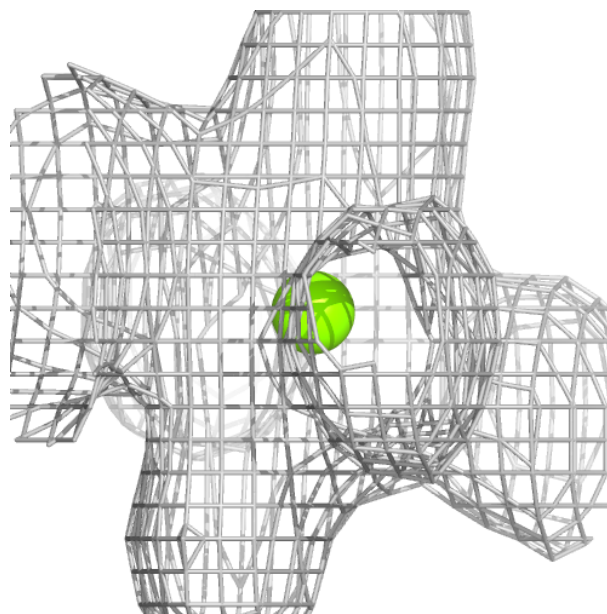
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

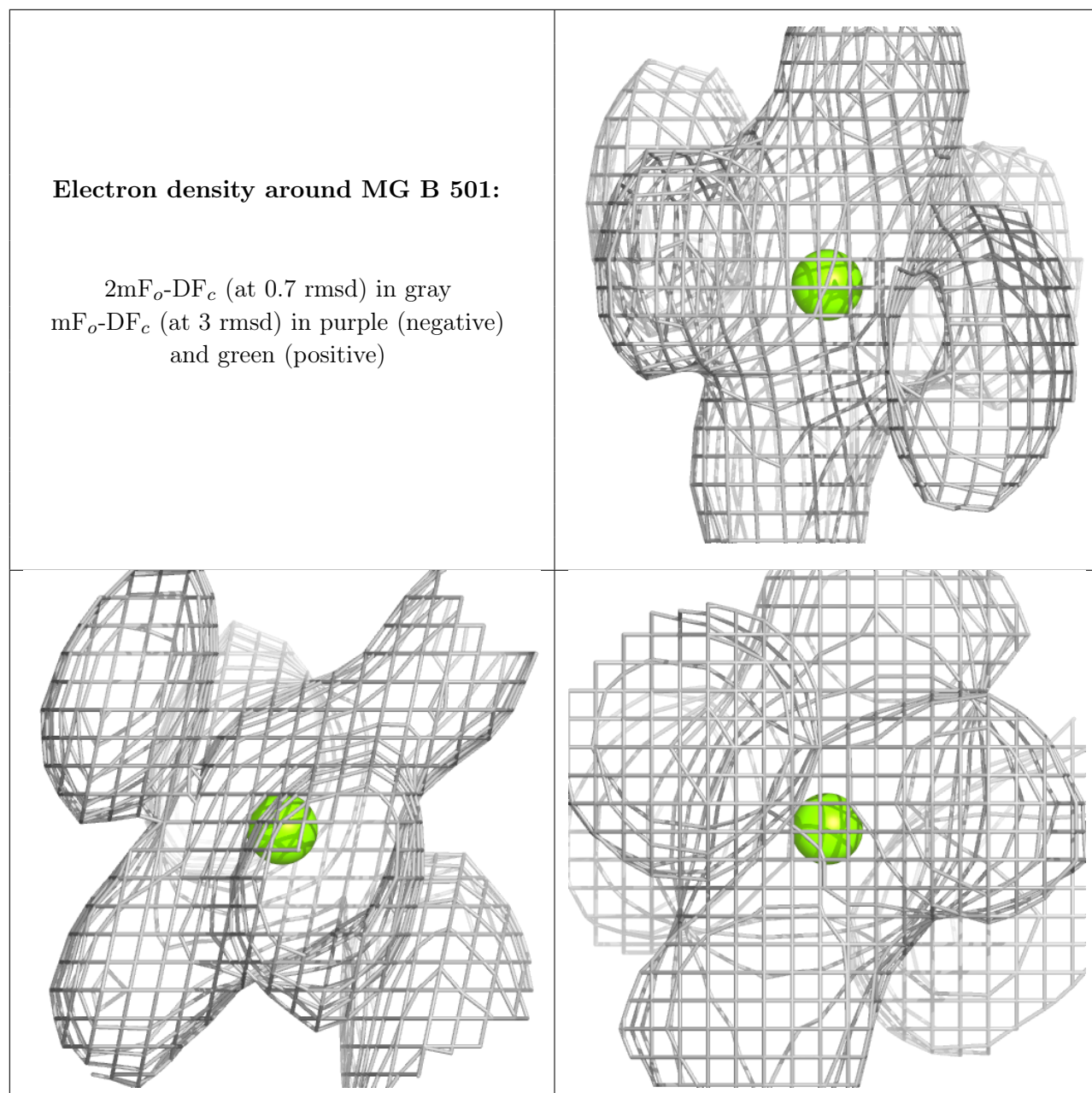
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	501	1/1	0.97	0.06	41,41,41,41	0
2	MG	B	501	1/1	0.99	0.03	34,34,34,34	0

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 MG A 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.