



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 02:06 PM EDT

PDB ID : 7SOJ
Title : Structure of V750A Soybean Lipoxygenase at 277K
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Deposited on : 2021-10-31
Resolution : 1.85 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

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 : 4.02b-467
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 : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

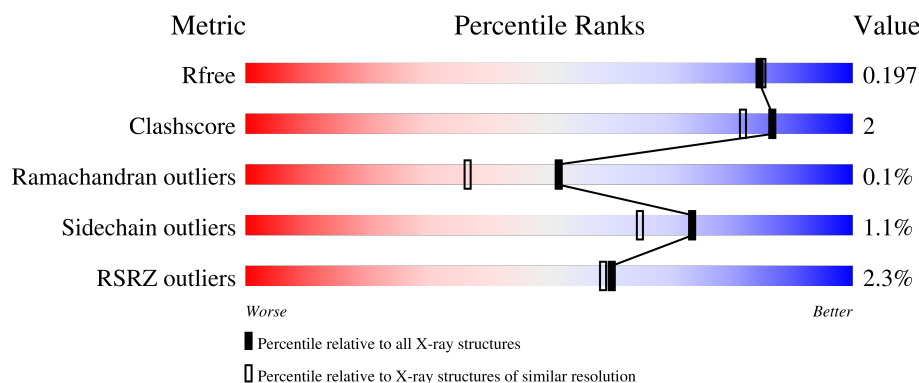
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	839	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	B	839	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28088 atoms, of which 13599 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 Lipoyxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	818	Total	C	H	N	O	S	0	102	0
			13533	4314	6786	1147	1267	19			
1	B	820	Total	C	H	N	O	S	0	97	0
			13619	4350	6813	1151	1285	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	750	ALA	VAL	engineered mutation	UNP B3TDK4
B	750	ALA	VAL	engineered mutation	UNP B3TDK4

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

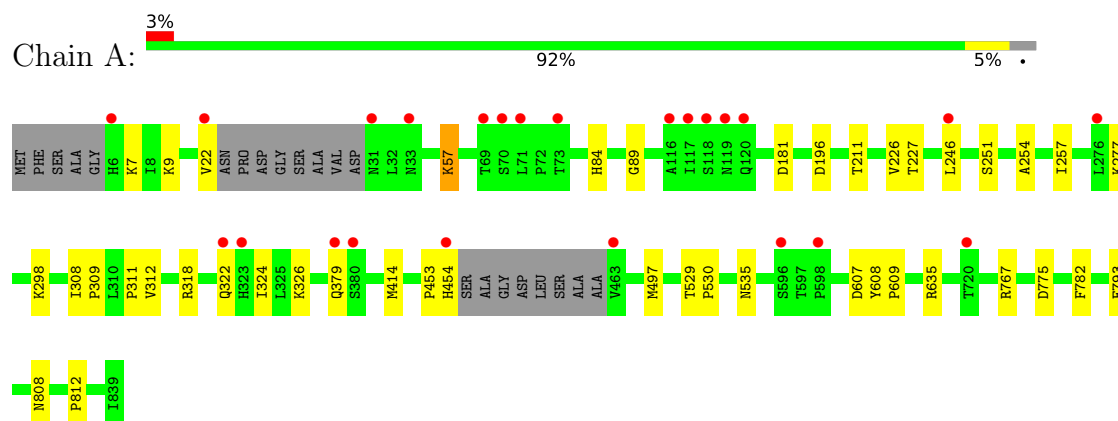
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	480	Total	O	0	0
			480	480		
3	B	454	Total	O	0	0
			454	454		

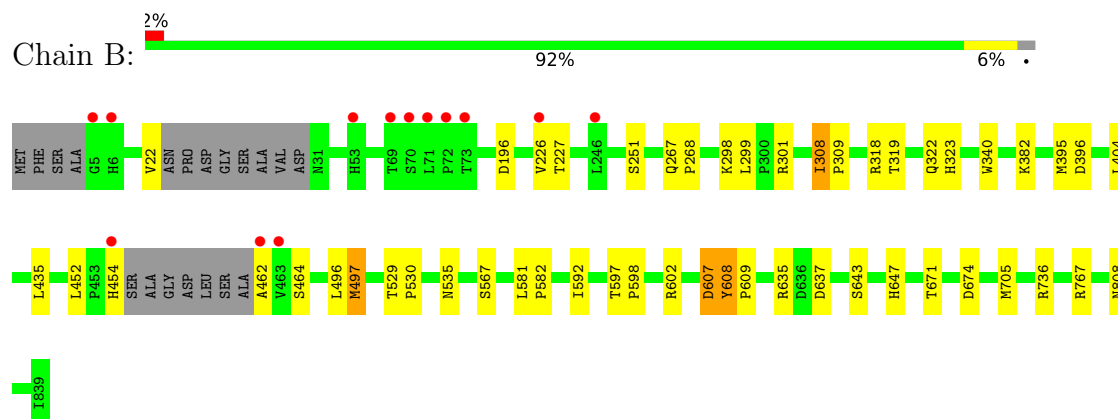
3 Residue-property plots [i](#)

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: Lipoxxygenase



• Molecule 1: Lipoxxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.54Å 92.69Å 100.27Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	46.35 – 1.85 46.35 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.35-1.85) 98.9 (46.35-1.85)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.169 , 0.198 0.168 , 0.197	Depositor DCC
R_{free} test set	6993 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28088	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7202e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FE

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	0.31	0/7456	0.58	0/10117
1	B	0.31	0/7454	0.58	0/10121
All	All	0.31	0/14910	0.58	0/20238

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	607[B]	ASP	Mainchain

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5.2 Torsion angles [i](#)

5.2.1 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	912/839 (109%)	882 (97%)	30 (3%)	0	100	100
1	B	907/839 (108%)	879 (97%)	27 (3%)	1 (0%)	51	36
All	All	1819/1678 (108%)	1761 (97%)	57 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	608	TYR

5.2.2 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	A	788/729 (108%)	781 (99%)	7 (1%)	78	72
1	B	792/729 (109%)	782 (99%)	10 (1%)	69	58
All	All	1580/1458 (108%)	1563 (99%)	17 (1%)	73	65

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	57	LYS
1	A	277	LYS
1	A	414	MET
1	A	497	MET
1	A	535	ASN
1	A	608	TYR
1	B	308	ILE
1	B	382	LYS
1	B	435	LEU
1	B	454	HIS
1	B	464	SER

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Mol	Chain	Res	Type
1	B	497[A]	MET
1	B	497[B]	MET
1	B	535	ASN
1	B	608	TYR
1	B	736	ARG

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

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.5 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.

5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 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, 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	818/839 (97%)	-0.00	24 (2%) 51 50	17, 28, 56, 102	0
1	B	820/839 (97%)	-0.05	13 (1%) 72 72	17, 28, 53, 89	0
All	All	1638/1678 (97%)	-0.03	37 (2%) 60 59	17, 28, 55, 102	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	VAL	6.5
1	A	69	THR	5.5
1	B	462	ALA	5.2
1	A	120	GLN	4.7
1	B	73	THR	4.5
1	A	117	ILE	4.5
1	A	118	SER	4.1
1	B	70	SER	4.1
1	B	5	GLY	4.0
1	A	116[A]	ALA	3.6
1	A	598	PRO	3.4
1	B	226	VAL	3.3
1	B	463	VAL	3.3
1	B	246[A]	LEU	3.2
1	A	22	VAL	3.2
1	A	31	ASN	3.0
1	A	119	ASN	2.9
1	A	6	HIS	2.7
1	A	379	GLN	2.6
1	B	71	LEU	2.6
1	A	70	SER	2.6
1	A	380	SER	2.6
1	A	454	HIS	2.5
1	B	72	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	71[A]	LEU	2.5
1	B	6	HIS	2.5
1	A	323	HIS	2.4
1	A	596	SER	2.4
1	A	720	THR	2.4
1	B	454	HIS	2.4
1	B	53	HIS	2.3
1	A	33[A]	ASN	2.2
1	B	69[A]	THR	2.2
1	A	276	LEU	2.1
1	A	73	THR	2.1
1	A	246[A]	LEU	2.1
1	A	322	GLN	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 [i](#)

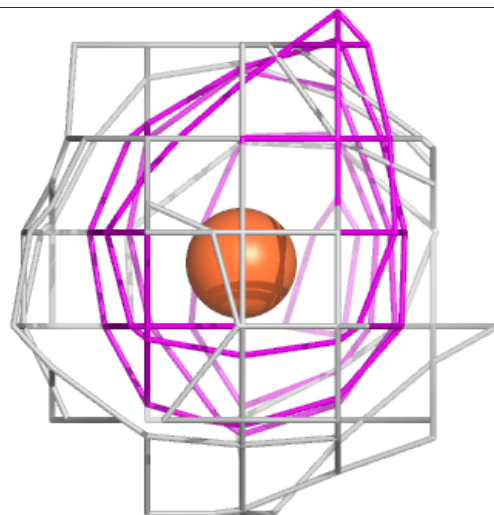
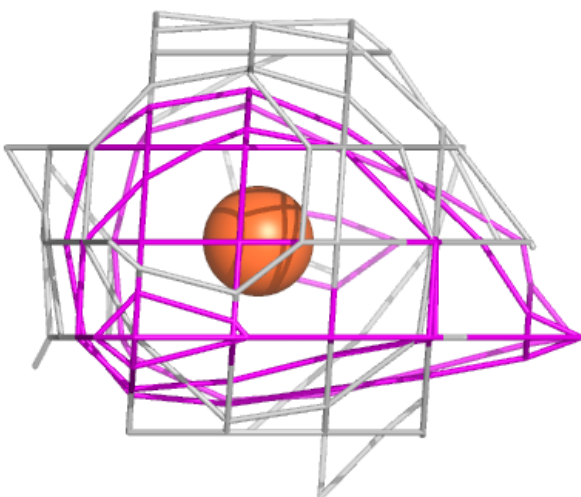
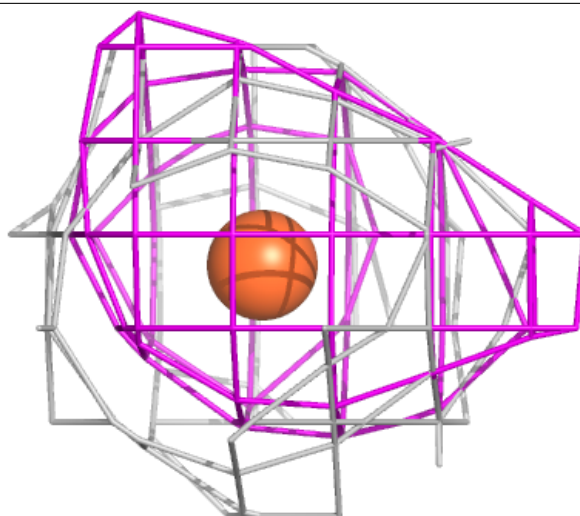
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

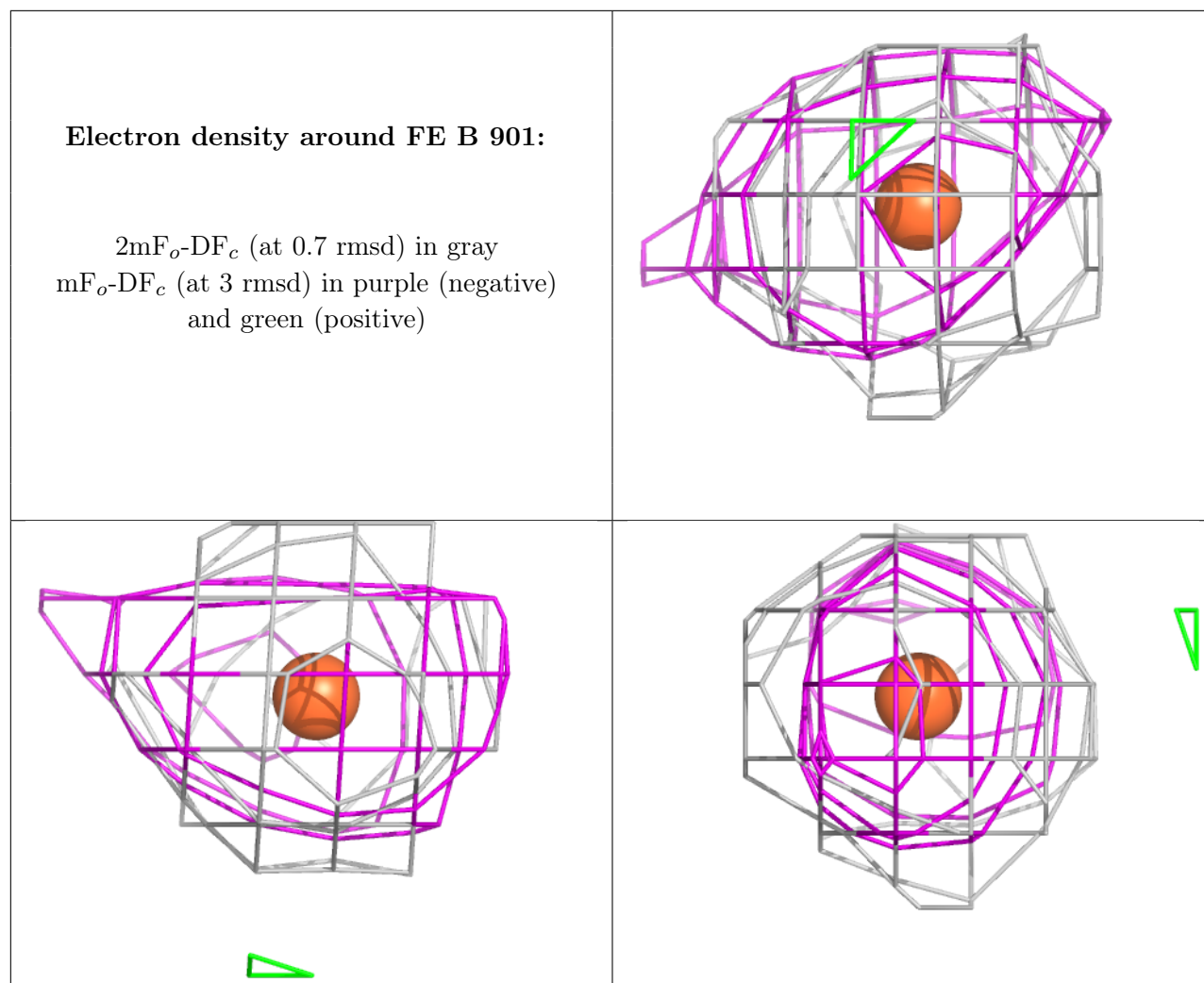
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	901	1/1	1.00	0.04	32,32,32,32	0
2	FE	B	901	1/1	1.00	0.04	32,32,32,32	0

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 FE A 901:

$2mF_o-DF_c$ (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.