



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 12:31 AM EST

PDB ID : 6ON1  
Title : A resting state structure of L-DOPA dioxygenase from *Streptomyces sclerotialus*  
Authors : Wang, Y.; Shin, I.; Fu, Y.; Colabroy, K.; Liu, A.  
Deposited on : 2019-04-19  
Resolution : 1.98 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

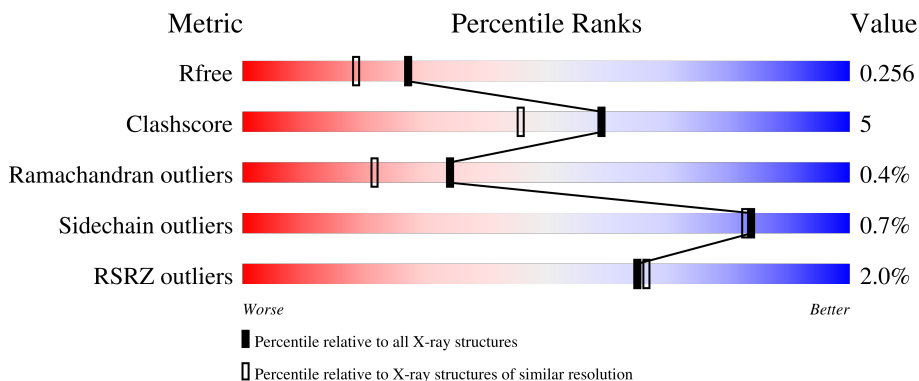
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	165	 83% 6% 11%
1	B	165	 82% 5% 12%
1	C	165	 80% 8% 11%
1	D	165	 77% 8% 14%
1	E	165	 74% 12% 14%

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Mol	Chain	Length	Quality of chain
1	F	165	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a small red segment (2%), a large green segment (72%), a yellow segment (14%), and a grey segment (14%).</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7572 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 L-DOPA dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	147	1232	785	212	232	3	0	3	0
1	B	146	1204	769	204	228	3	0	0	0
1	C	147	1216	776	208	229	3	0	1	0
1	D	142	1180	754	200	223	3	0	0	0
1	E	142	1183	757	200	223	3	0	1	0
1	F	142	1175	751	198	223	3	0	0	0

- 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 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0
2	E	1	Total 1	Fe 1	0	0
2	F	1	Total 1	Fe 1	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).

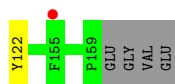


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	D	1	8	4	1	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	80	Total	O	0	0
			80	80		
4	C	40	Total	O	0	0
			40	40		
4	D	68	Total	O	0	0
			68	68		
4	E	39	Total	O	0	0
			39	39		
4	F	54	Total	O	0	0
			54	54		





- Molecule 1: L-DOPA dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.98Å 45.22Å 131.15Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	33.33 – 1.98 49.61 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.33-1.98) 91.1 (49.61-1.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.98Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.256 0.208 , 0.256	Depositor DCC
$R_{free}$ test set	2000 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtrriage
Anisotropy	1.168	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.7	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	0.95	EDS
Total number of atoms	7572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: TRS, 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	0.42	0/1272	0.60	0/1730
1	B	0.39	0/1237	0.56	0/1682
1	C	0.34	0/1253	0.55	0/1705
1	D	0.35	0/1212	0.53	0/1645
1	E	0.35	0/1219	0.51	0/1656
1	F	0.37	0/1206	0.56	0/1638
All	All	0.37	0/7399	0.55	0/10056

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 [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	1232	0	1166	10	0
1	B	1204	0	1133	9	0
1	C	1216	0	1150	12	0
1	D	1180	0	1110	10	0
1	E	1183	0	1115	16	0
1	F	1175	0	1107	22	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	D	8	0	12	1	0
4	A	87	0	0	2	0
4	B	80	0	0	0	0
4	C	40	0	0	0	0
4	D	68	0	0	0	0
4	E	39	0	0	1	0
4	F	54	0	0	0	0
All	All	7572	0	6793	66	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 (66) 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:C:54[B]:ARG:HH11	1:C:54[B]:ARG:HB3	1.45	0.81
1:C:20:ILE:HD12	1:D:95:HIS:O	1.84	0.77
1:F:63:LEU:HD23	1:F:76:PHE:HB3	1.67	0.76
1:A:62:ARG:NH2	4:A:302:HOH:O	2.20	0.73
1:C:89:GLU:OE2	1:C:89:GLU:N	2.22	0.72
1:F:37:PHE:O	1:F:112:ARG:NH2	2.23	0.72
1:C:54[B]:ARG:HB3	1:C:54[B]:ARG:NH1	2.06	0.70
1:A:137:GLU:OE1	4:A:301:HOH:O	2.11	0.68
1:C:54[B]:ARG:NH2	1:C:59:GLY:H	1.92	0.67
1:A:16:ARG:HH12	1:B:100:THR:C	2.00	0.65
1:D:138:ASP:OD1	1:D:138:ASP:N	2.30	0.63
1:D:89:GLU:OE2	1:D:89:GLU:N	2.28	0.61
1:F:65:GLU:CD	1:F:72:ARG:HD3	2.20	0.61
1:B:51:ASP:OD1	1:B:54:ARG:NH2	2.27	0.61
1:C:57:LEU:HB3	1:C:78:ARG:HD3	1.85	0.58
1:D:137:GLU:HG3	1:D:138:ASP:OD1	2.03	0.58
1:E:102:SER:OG	1:E:104:GLU:HG2	2.04	0.57
1:D:28:GLU:HB2	3:D:202:TRS:H21	1.85	0.57
1:E:96:LEU:HD13	1:F:20:ILE:HD12	1.88	0.55
1:E:48:LYS:O	4:E:301:HOH:O	2.19	0.54
1:C:54[A]:ARG:HH11	1:C:54[A]:ARG:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:GLU:OE1	1:F:121:ARG:NH1	2.36	0.53
1:E:16:ARG:NH1	1:F:101:ARG:HG2	2.25	0.52
1:E:96:LEU:HD13	1:F:20:ILE:CD1	2.41	0.51
1:F:63:LEU:CD2	1:F:76:PHE:HB3	2.39	0.50
1:A:100:THR:O	1:B:16:ARG:NH2	2.45	0.50
1:F:18:HIS:O	1:F:72:ARG:NH2	2.46	0.49
1:E:96:LEU:CD1	1:F:20:ILE:HD12	2.42	0.49
1:F:43:ASN:HB2	1:F:65:GLU:HG2	1.94	0.48
1:A:101:ARG:HG2	1:B:16:ARG:NH2	2.29	0.48
1:C:54[A]:ARG:HH11	1:C:54[A]:ARG:CG	2.25	0.48
1:F:108:GLU:O	1:F:112:ARG:HG3	2.14	0.48
1:B:40:CYS:HB3	1:B:66:LEU:HB3	1.96	0.48
1:A:130:PRO:HB3	1:A:145:VAL:HG12	1.96	0.48
1:C:141:LEU:HB2	1:C:157:TYR:HB3	1.95	0.47
1:E:35:ARG:HA	1:E:40:CYS:HB2	1.95	0.47
1:E:71:LEU:HG	1:E:73:ILE:HD11	1.96	0.47
1:F:18:HIS:CD2	1:F:72:ARG:HH22	2.33	0.46
1:A:16:ARG:NH1	1:B:100:THR:C	2.67	0.46
1:D:141:LEU:HB2	1:D:157:TYR:HB3	1.98	0.46
1:F:65:GLU:OE2	1:F:72:ARG:HD3	2.16	0.46
1:F:35:ARG:HG2	1:F:40:CYS:O	2.16	0.45
1:F:18:HIS:CE1	1:F:72:ARG:NH2	2.85	0.45
1:E:102:SER:OG	1:E:105:GLU:HG3	2.17	0.45
1:E:17:PHE:HD1	1:F:96:LEU:HD11	1.82	0.44
1:D:130:PRO:HB3	1:D:145:VAL:HG12	2.00	0.43
1:E:92:GLN:HA	1:F:151:LEU:HD21	2.00	0.43
1:E:31:LEU:O	1:E:35:ARG:HG3	2.18	0.43
1:E:101:ARG:N	1:E:101:ARG:HD2	2.33	0.43
1:A:84:PRO:HB2	1:B:90:VAL:HG12	2.01	0.43
1:B:85:ALA:HA	1:B:125:VAL:HG11	2.01	0.42
1:D:46:LEU:HD21	1:D:48:LYS:O	2.18	0.42
1:E:63:LEU:HD11	1:E:74:HIS:HB3	2.02	0.42
1:F:65:GLU:OE1	1:F:74:HIS:NE2	2.43	0.42
1:E:84:PRO:HB2	1:E:85:ALA:H	1.66	0.42
1:C:80:ALA:O	1:C:81:ASP:HB2	2.19	0.42
1:F:96:LEU:HD12	1:F:97:CYS:N	2.34	0.42
1:C:16:ARG:HE	1:C:16:ARG:HB2	1.59	0.42
1:D:107:THR:HA	1:D:133:ILE:HD11	2.02	0.41
1:D:94:GLN:OE1	1:D:95:HIS:ND1	2.49	0.41
1:A:52:LEU:HD11	1:B:131:THR:HG21	2.03	0.41
1:E:116:LEU:HD12	1:E:122:TYR:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.91	0.40
1:F:52:LEU:O	1:F:56:ARG:HG2	2.22	0.40
1:C:36:GLU:HG2	1:C:116:LEU:HD21	2.02	0.40
1:F:47:GLU:HG3	1:F:62:ARG:HG3	2.03	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	148/165 (90%)	148 (100%)	0	0	100	100
1	B	142/165 (86%)	138 (97%)	3 (2%)	1 (1%)	22	11
1	C	146/165 (88%)	140 (96%)	4 (3%)	2 (1%)	11	3
1	D	138/165 (84%)	137 (99%)	1 (1%)	0	100	100
1	E	139/165 (84%)	138 (99%)	1 (1%)	0	100	100
1	F	138/165 (84%)	137 (99%)	1 (1%)	0	100	100
All	All	851/990 (86%)	838 (98%)	10 (1%)	3 (0%)	34	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	ASP
1	B	85	ALA
1	C	79	ALA

### 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	132/142 (93%)	132 (100%)	0	100	100
1	B	129/142 (91%)	129 (100%)	0	100	100
1	C	130/142 (92%)	127 (98%)	3 (2%)	50	44
1	D	127/142 (89%)	125 (98%)	2 (2%)	62	56
1	E	128/142 (90%)	127 (99%)	1 (1%)	81	80
1	F	126/142 (89%)	126 (100%)	0	100	100
All	All	772/852 (91%)	766 (99%)	6 (1%)	84	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	54[A]	ARG
1	C	54[B]	ARG
1	C	119	SER
1	D	136	ASP
1	D	138	ASP
1	E	101	ARG

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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
3	TRS	D	202	-	7,7,7	0.18	0	9,9,9	0.55	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	D	202	-	-	0/9/9/9	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	TRS	1	0

## 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

### 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	147/165 (89%)	0.22	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	29, 38, 57, 73	0
1	B	146/165 (88%)	0.19	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">88</span>	30, 40, 57, 77	0
1	C	147/165 (89%)	0.32	6 (4%) <span style="border: 1px solid red; padding: 2px;">37</span> <span style="border: 1px solid red; padding: 2px;">39</span>	36, 48, 72, 99	0
1	D	142/165 (86%)	0.00	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	33, 43, 61, 74	0
1	E	142/165 (86%)	0.42	7 (4%) <span style="border: 1px solid red; padding: 2px;">29</span> <span style="border: 1px solid red; padding: 2px;">32</span>	37, 55, 73, 81	0
1	F	142/165 (86%)	0.22	3 (2%) <span style="border: 1px solid blue; padding: 2px;">63</span> <span style="border: 1px solid blue; padding: 2px;">65</span>	35, 46, 67, 79	0
All	All	866/990 (87%)	0.23	17 (1%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">66</span>	29, 45, 69, 99	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	ALA	6.2
1	E	85	ALA	4.8
1	C	80	ALA	4.2
1	F	85	ALA	3.3
1	E	155	PHE	3.2
1	F	16	ARG	3.1
1	C	81	ASP	3.0
1	E	68	ALA	2.9
1	B	96	LEU	2.8
1	E	71	LEU	2.7
1	E	101	ARG	2.7
1	F	17	PHE	2.5
1	E	86	PRO	2.4
1	C	85	ALA	2.2
1	C	101	ARG	2.0
1	C	16	ARG	2.0
1	E	98	LEU	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.

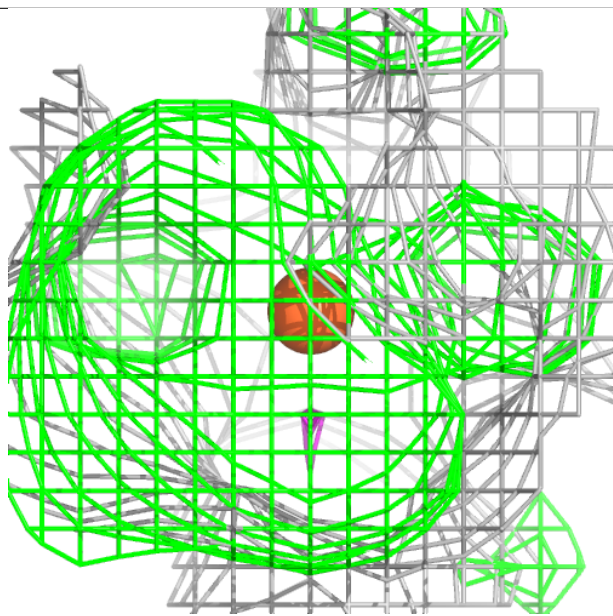
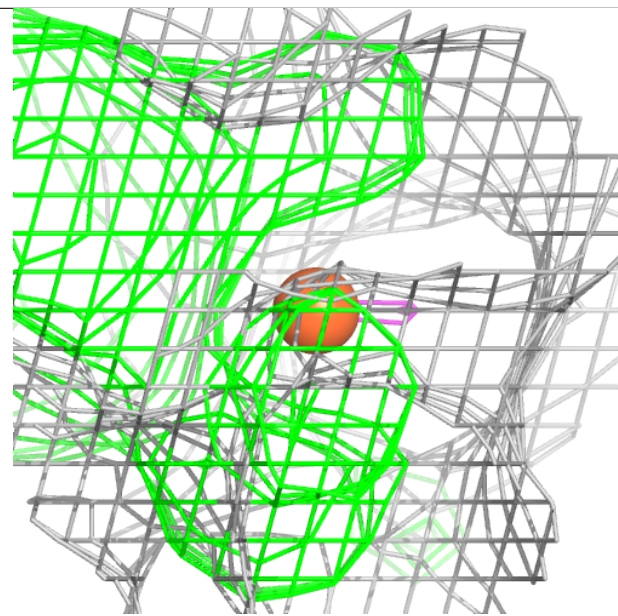
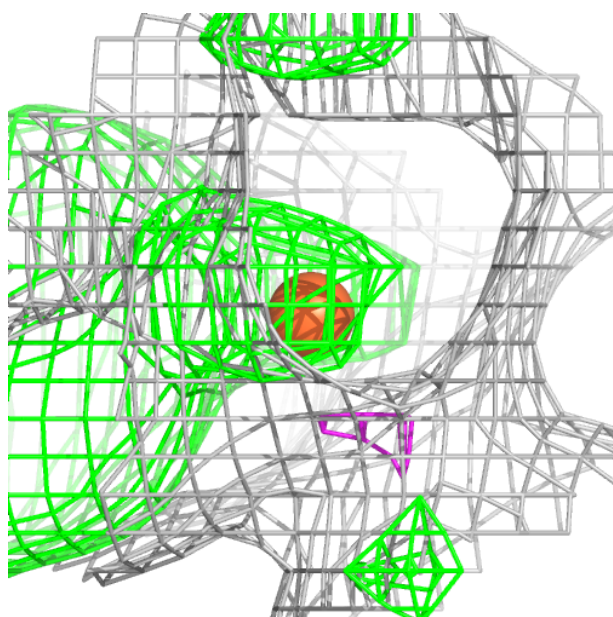
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	TRS	D	202	8/8	0.74	0.18	48,51,55,58	0
2	FE	B	201	1/1	0.98	0.18	29,29,29,29	0
2	FE	C	201	1/1	0.98	0.16	36,36,36,36	0
2	FE	D	201	1/1	0.98	0.15	34,34,34,34	0
2	FE	E	201	1/1	0.98	0.17	40,40,40,40	0
2	FE	F	201	1/1	0.98	0.17	37,37,37,37	0
2	FE	A	201	1/1	0.98	0.22	31,31,31,31	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.



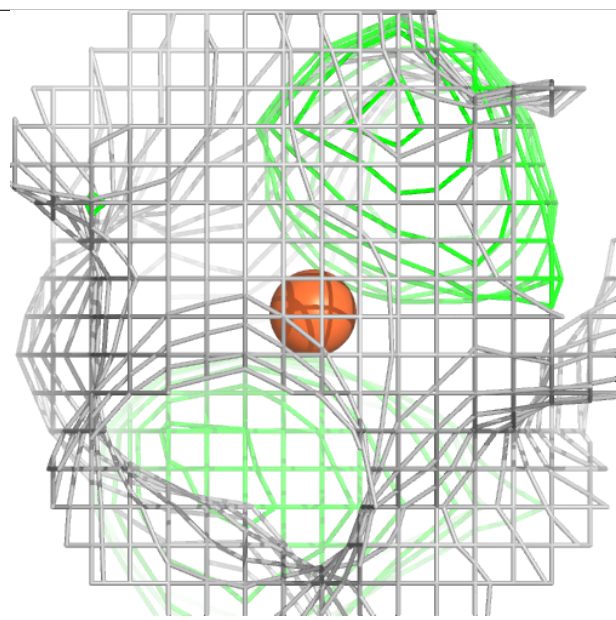
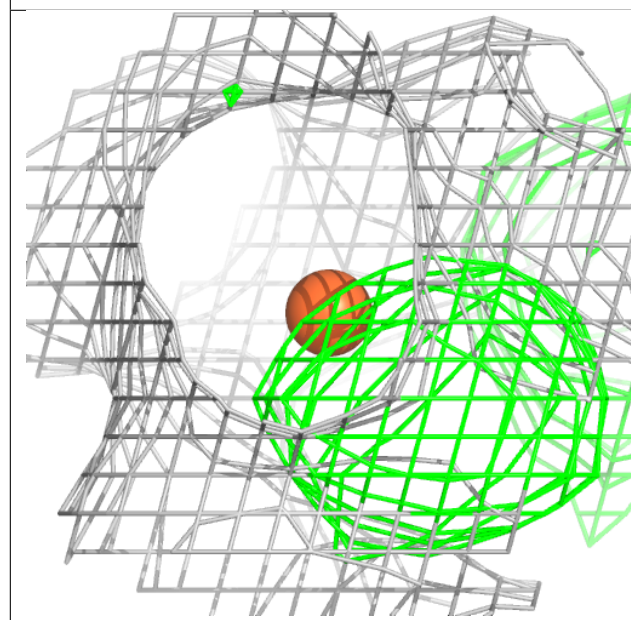
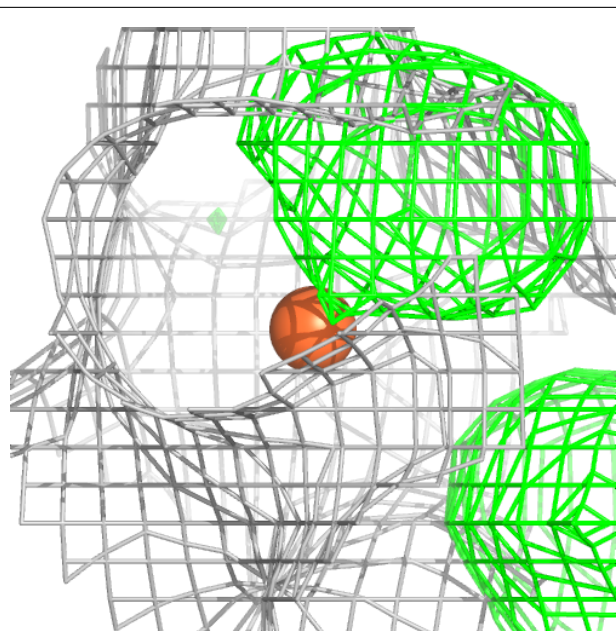
**Electron density around FE B 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



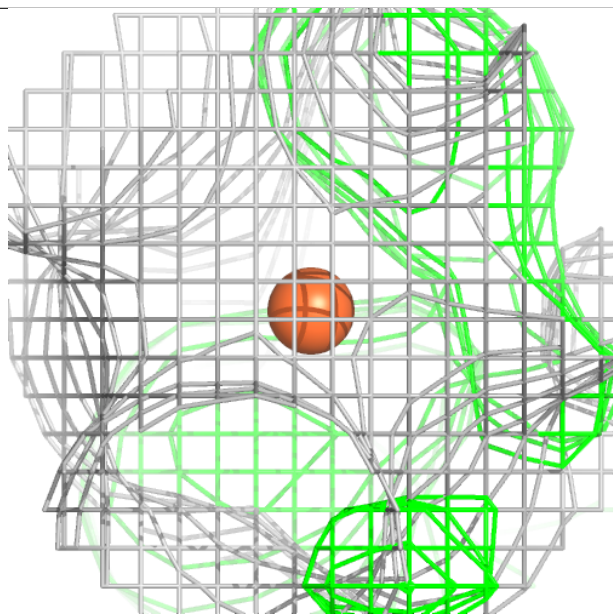
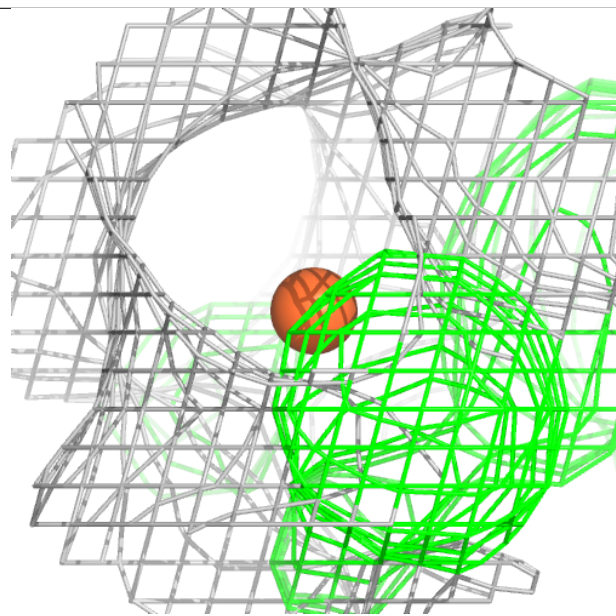
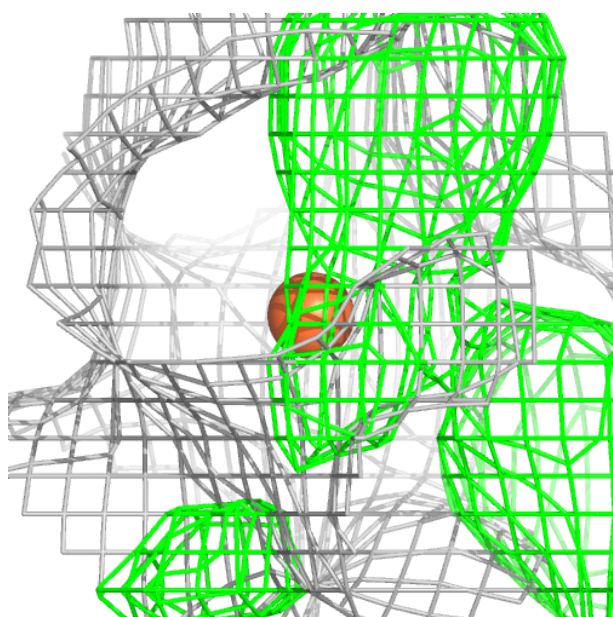
**Electron density around FE C 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

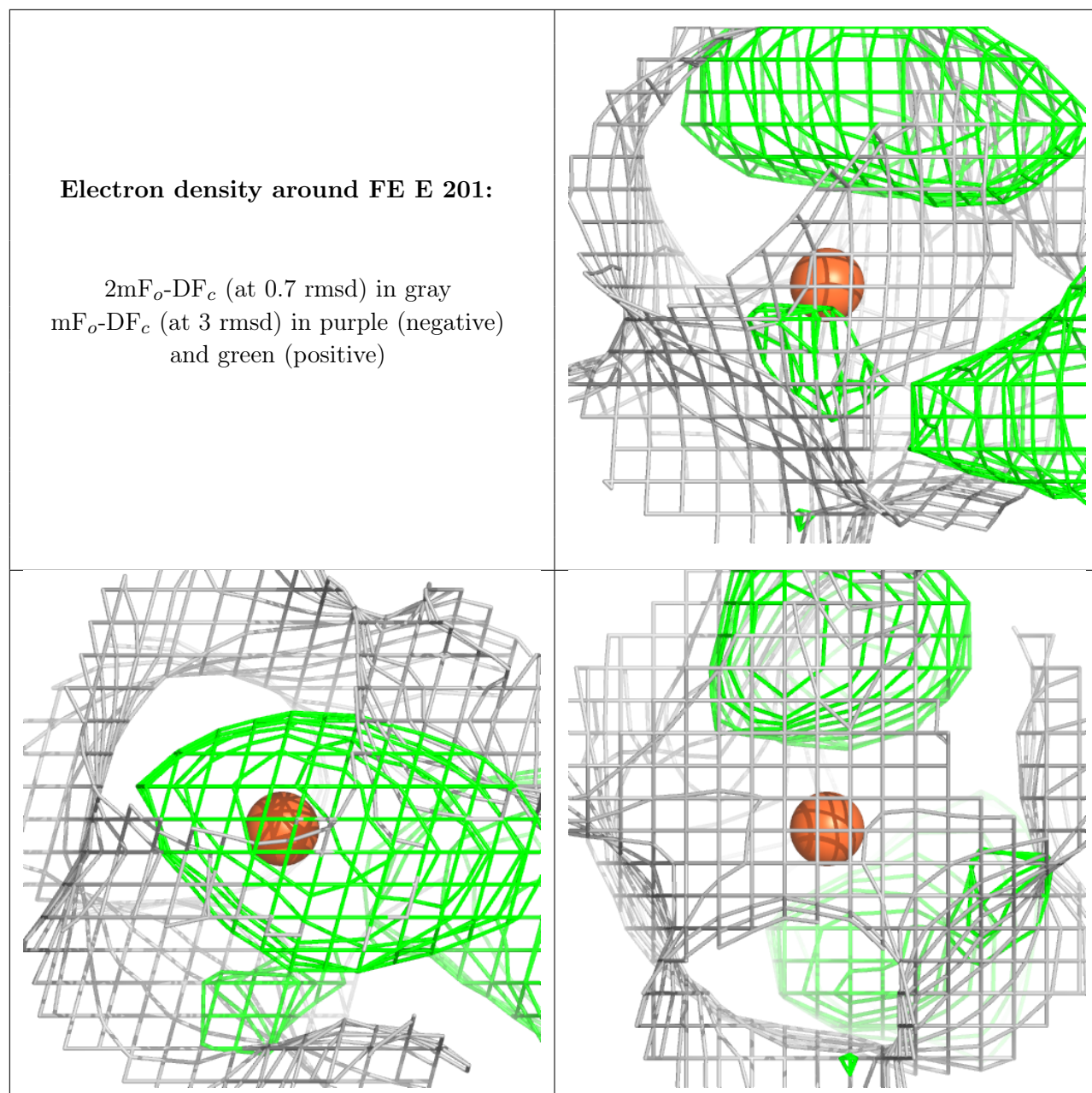


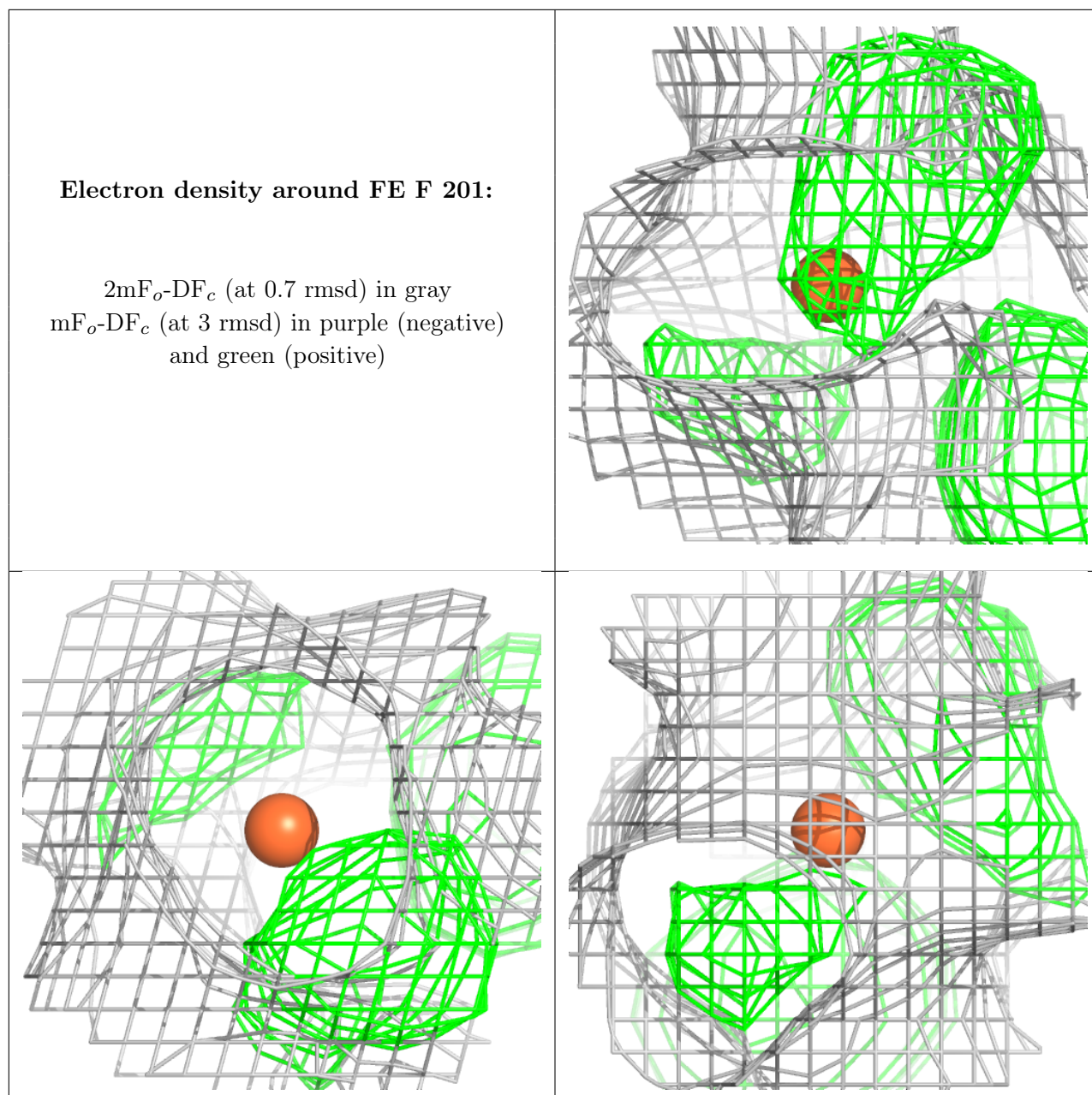
**Electron density around FE D 201:**

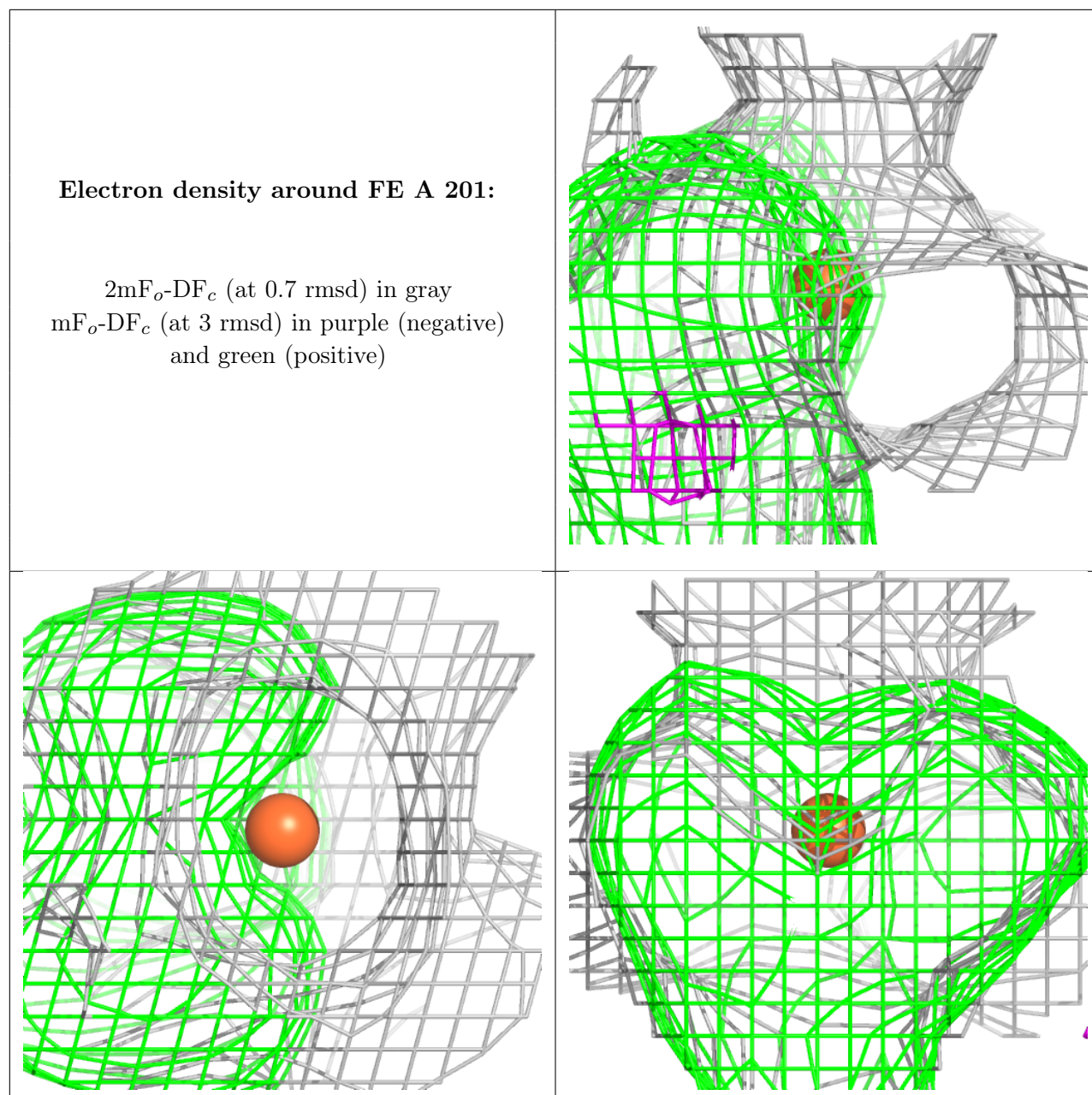
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)











## 6.5 Other polymers [i](#)

There are no such residues in this entry.