

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

### Apr 12, 2023 – 02:37 pm BST

PDB ID : 8AVM

Title : Mutant of Superoxide Dismutase sodfm2 from Bacteroides fragilis

Authors : Basle, A.; Barwinska-Sendra, A.; Sendra, K.M.; Waldron, K.

Deposited on : 2022-08-26

Resolution : 2.00 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$ 

EDS : 2.32.2buster-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)

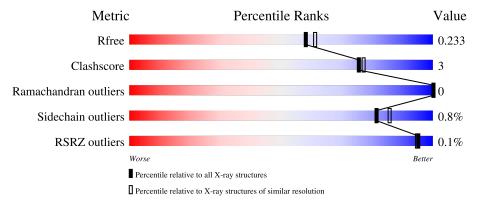
Validation Pipeline (wwPDB-VP) : 2.32.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	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 >=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	192	94%	6%
1	В	192	92%	7% •
1	С	192	91%	9%
1	D	192	95%	5%
1	Е	192	95%	5%

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Mol	Chain	Length	Quality of chain		
1	F	192	90%	10% •	



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18176 atoms, of which 8442 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 Superoxide dismutase [Fe].

Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace	
1	Λ	192	Total	С	Н	N	О	S	0	0	0	
1	A	192	2943	988	1407	260	285	3	0	U		
1	В	192	Total	С	Н	N	О	S	0	0	0	
1	Ъ	192	2943	988	1407	260	285	3	0	U		
1	С	102	192	Total	С	Н	N	О	S	0	0	0
1		192	2943	988	1407	260	285	3	0			
1	D	192	Total	С	Н	N	О	S	0	0	0	
1	D	192	2943	988	1407	260	285	3	0			
1	Е	192	Total	С	Н	N	О	S	0	0	0	
1	l Li	192	2943	988	1407	260	285	3	0			
1	F	192	Total	С	Н	N	О	S	0	0	0	
	I.	132	2943	988	1407	260	285	3	U	U	U	

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P53638
A	156	THR	GLY	engineered mutation	UNP P53638
A	157	CYS	PHE	engineered mutation	UNP P53638
В	1	MET	-	initiating methionine	UNP P53638
В	156	THR	GLY	engineered mutation	UNP P53638
В	157	CYS	PHE	engineered mutation	UNP P53638
С	1	MET	-	initiating methionine	UNP P53638
С	156	THR	GLY	engineered mutation	UNP P53638
С	157	CYS	PHE	engineered mutation	UNP P53638
D	1	MET	-	initiating methionine	UNP P53638
D	156	THR	GLY	engineered mutation	UNP P53638
D	157	CYS	PHE	engineered mutation	UNP P53638
Е	1	MET	-	initiating methionine	UNP P53638
Е	156	THR	GLY	engineered mutation	UNP P53638
Е	157	CYS	PHE	engineered mutation	UNP P53638
F	1	MET	-	initiating methionine	UNP P53638
F	156	THR	GLY	engineered mutation	UNP P53638

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Chain	Residue	Modelled	Actual	Comment	Reference
F	157	CYS	PHE	engineered mutation	UNP P53638

• 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 1 1	0	0
2	В	1	Total Fe 1 1	0	0
2	С	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	В	95	Total O 95 95	0	0
3	С	113	Total O 113 113	0	0
3	D	87	Total O 87 87	0	0
3	Е	70	Total O 70 70	0	0
3	F	38	Total O 38 38	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: Superoxide dismutase [Fe]







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	79.43Å 117.11Å 139.33Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	69.00 - 2.00	Depositor
resolution (A)	69.00 - 2.00	EDS
% Data completeness	100.0 (69.00-2.00)	Depositor
(in resolution range)	100.0 (69.00-2.00)	EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
P.P.	0.193 , $0.229$	Depositor
$R, R_{free}$	0.201 , $0.233$	DCC
$R_{free}$ test set	4329  reflections  (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 28.8	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18176	wwPDB-VP
Average B, all atoms $(Å^2)$	42.0	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 23.39 % 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 4.7062e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: 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	Boı	nd lengths	Bond angles		
IVIOI	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.57	1/1580 (0.1%)	0.78	1/2147 (0.0%)	
1	В	0.53	1/1580 (0.1%)	0.78	1/2147 (0.0%)	
1	С	0.59	0/1580	0.85	2/2147 (0.1%)	
1	D	0.55	0/1580	0.75	0/2147	
1	Е	0.54	0/1580	0.77	0/2147	
1	F	0.49	0/1580	0.77	4/2147 (0.2%)	
All	All	0.54	2/9480 (0.0%)	0.78	8/12882 (0.1%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
1	В	111	GLU	CD-OE2	-6.19	1.18	1.25
1	A	181	GLU	CD-OE1	-5.63	1.19	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	148	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	F	171	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	148	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	В	172	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	191	ARG	NE-CZ-NH2	-5.28	117.66	120.30

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	1536	1407	1491	8	0
1	В	1536	1407	1491	7	0
1	С	1536	1407	1491	17	0
1	D	1536	1407	1491	6	0
1	Ε	1536	1407	1491	6	0
1	F	1536	1407	1491	13	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Ε	1	0	0	0	0
2	F	1	0	0	0	0
3	A	109	0	0	3	0
3	В	95	0	0	0	0
3	С	113	0	0	4	0
3	D	87	0	0	2	0
3	Е	70	0	0	2	0
3	F	38	0	0	7	0
All	All	9734	8442	8946	57	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 3.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ ( ext{Å}) \end{aligned}$	
1:C:152:LYS:HD3	3:C:360:HOH:O	1.43	1.19	
1:A:171:ARG:NH1	3:A:301:HOH:O	1.75	1.11	
1:F:46:GLU:OE1	3:F:301:HOH:O	1.73	1.04	
1:A:100:ARG:HH12	1:A:134:LYS:HD3	1.25	1.01	
1:E:171:ARG:NH1	3:E:301:HOH:O	2.03	0.91	

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	Perce	ntiles
1	A	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
1	В	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
1	$\mathbf{C}$	190/192 (99%)	185 (97%)	5 (3%)	0	100	100
1	D	190/192 (99%)	185 (97%)	5 (3%)	0	100	100
1	E	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
1	F	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
All	All	1140/1152 (99%)	1106 (97%)	34 (3%)	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	Rotameric Outliers	
1	A	161/161 (100%)	161 (100%)	0	100 100
1	В	161/161 (100%)	158 (98%)	3 (2%)	57 61
1	С	161/161 (100%)	160 (99%)	1 (1%)	86 90
1	D	161/161 (100%)	160 (99%)	1 (1%)	86 90
1	E	161/161 (100%)	161 (100%)	0	100 100
1	F	161/161 (100%)	158 (98%)	3 (2%)	57 61
All	All	966/966 (100%)	958 (99%)	8 (1%)	81 86

5 of 8 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	F	99	LYS
1	F	87	LYS
1	D	40	SER
1	С	46	GLU
1	F	1	MET

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 6 ligands modelled in this entry, 6 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>	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	$192/192\ (100\%)$	-0.50	0 100 100	28, 36, 55, 65	0
1	В	$192/192\ (100\%)$	-0.43	0 100 100	26, 38, 62, 81	0
1	С	192/192 (100%)	-0.55	0 100 100	29, 35, 47, 59	0
1	D	192/192 (100%)	-0.55	0 100 100	30, 39, 57, 67	0
1	E	192/192 (100%)	-0.46	0 100 100	33, 40, 59, 79	0
1	F	$192/192\ (100\%)$	-0.22	1 (0%) 91 90	34, 48, 74, 95	0
All	All	1152/1152 (100%)	-0.45	1 (0%) 95 95	26, 39, 61, 95	0

### All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	VAL	2.9

## 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.

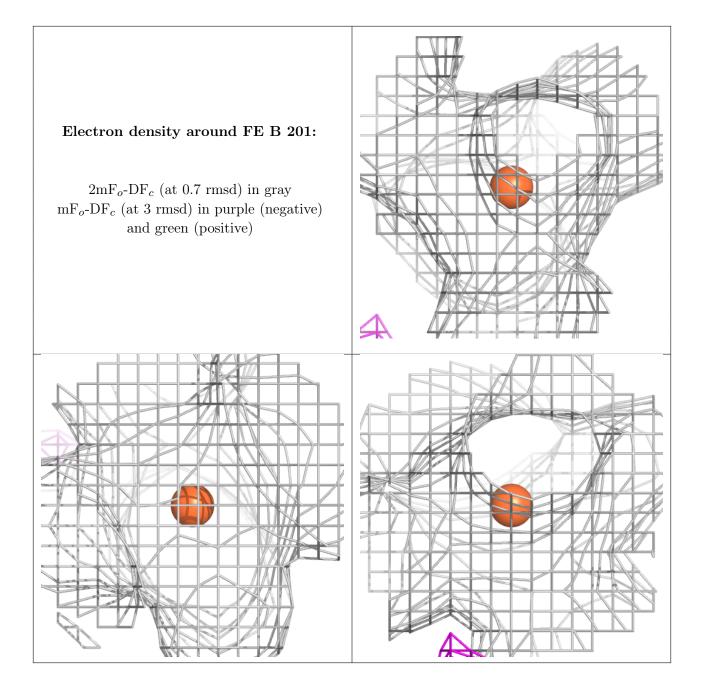


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	FE	A	201	1/1	1.00	0.13	29,29,29,29	0
2	FE	В	201	1/1	1.00	0.13	30,30,30,30	0
2	FE	С	201	1/1	1.00	0.14	30,30,30,30	0
2	FE	D	201	1/1	1.00	0.12	31,31,31,31	0
2	FE	E	201	1/1	1.00	0.13	33,33,33,33	0
2	FE	F	201	1/1	1.00	0.13	36,36,36,36	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 201: $2mF_o$ -DF<sub>c</sub> (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

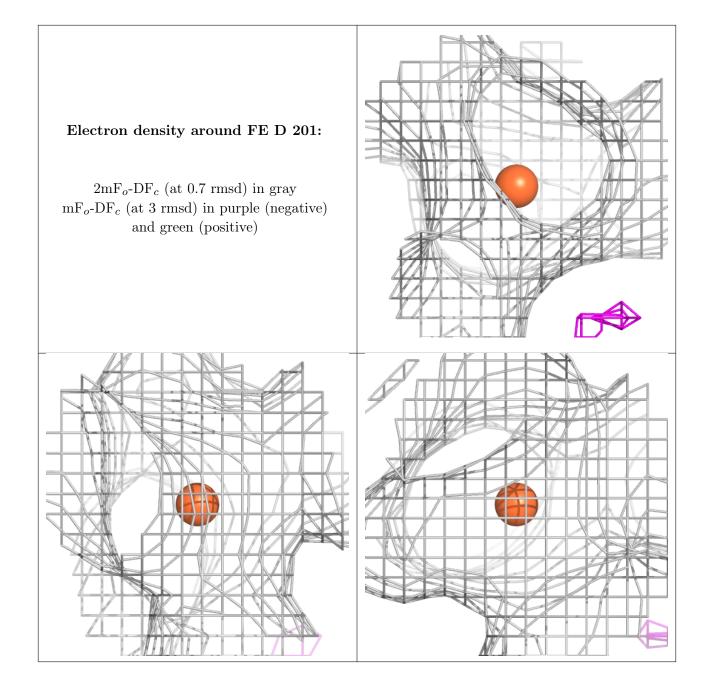






# Electron density around FE C 201: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

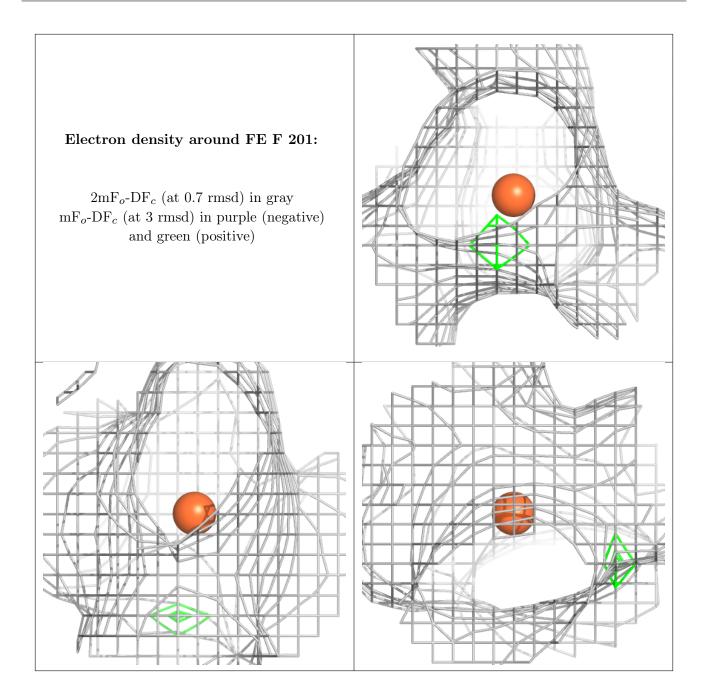






# Electron density around FE E 201: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

