



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:52 PM UTC

PDB ID : 9M2A / pdb\_00009m2a  
Title : The crystal structure of the trypanosome alternative oxidase complexed with a trypanocidal phosphonium derivative (compound1)  
Authors : Ebiloma, G.U.; Balogun, E.O.; Dardonville, C.; De Koning, H.P.; Shiba, T.  
Deposited on : 2025-02-27  
Resolution : 3.01 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](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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

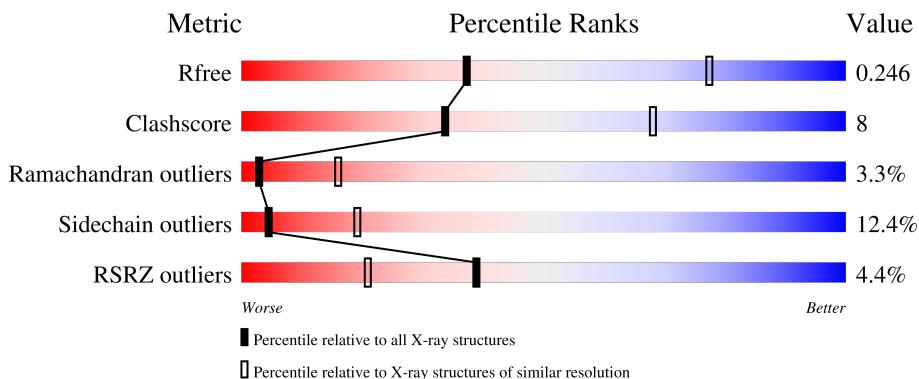
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
$R_{free}$	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	A	272	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>..</div> </div> </div>
1	B	272	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	272	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>.</div> </div> </div>
1	D	272	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8805 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 Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2175	1393	387	385	10			
1	B	268	Total	C	N	O	S	0	0	0
			2175	1393	387	385	10			
1	C	271	Total	C	N	O	S	0	0	0
			2198	1406	390	392	10			
1	D	271	Total	C	N	O	S	0	0	0
			2201	1408	390	392	11			

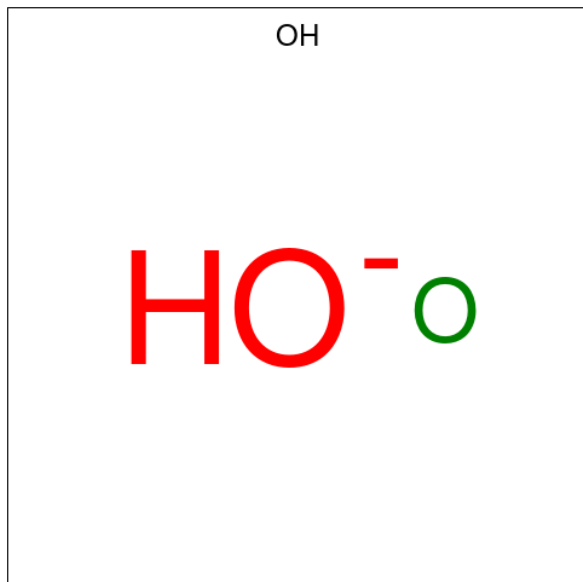
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	expression tag	UNP Q26710
A	31	ALA	-	expression tag	UNP Q26710
B	30	ALA	-	expression tag	UNP Q26710
B	31	ALA	-	expression tag	UNP Q26710
C	30	ALA	-	expression tag	UNP Q26710
C	31	ALA	-	expression tag	UNP Q26710
D	30	ALA	-	expression tag	UNP Q26710
D	31	ALA	-	expression tag	UNP Q26710

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

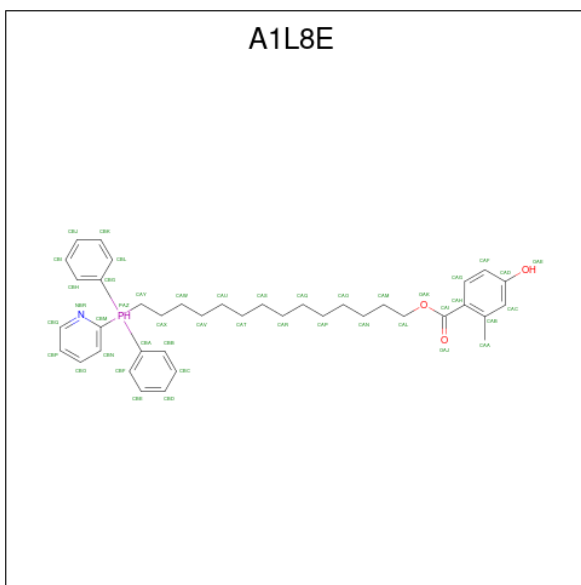
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



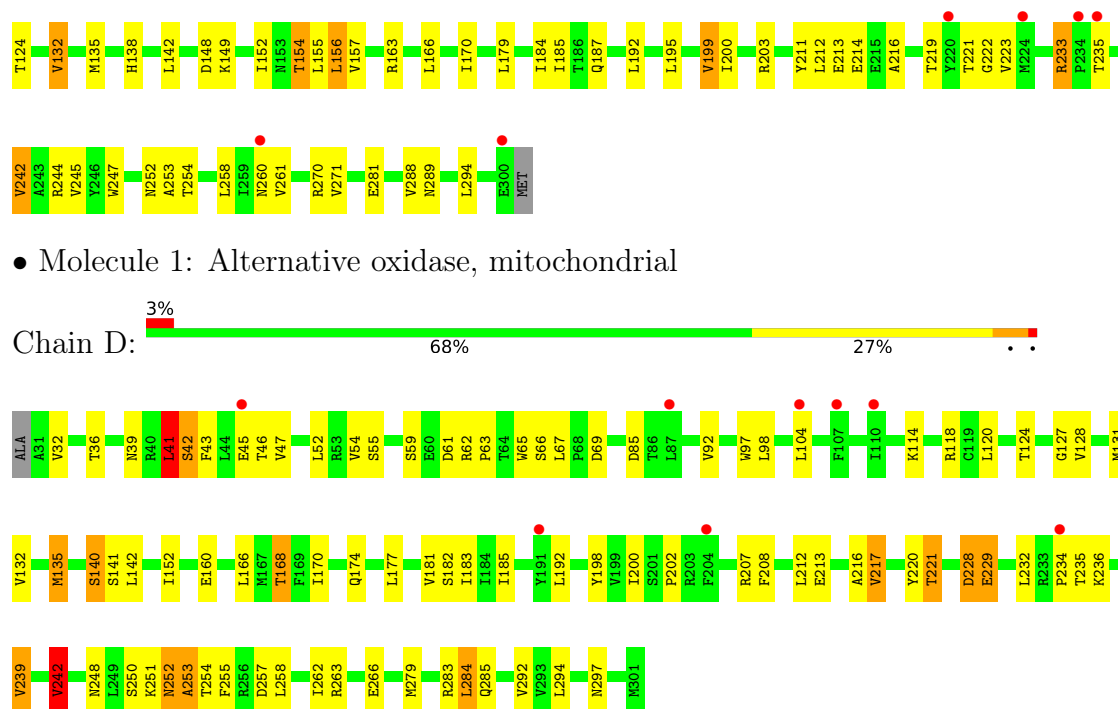
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

- Molecule 4 is 14-[diphenyl(pyridin-2-yl)- $\lambda^5$ -phosphanyl]tetradecyl 2-methyl-4-oxidan-yl-benzoate (CCD ID: A1L8E) (formula: C<sub>39</sub>H<sub>50</sub>NO<sub>3</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	39	1	3	1		





● Molecule 1: Alternative oxidase, mitochondrial

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.37Å 221.73Å 62.85Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	44.96 – 3.01 44.96 – 3.01	Depositor EDS
% Data completeness (in resolution range)	81.8 (44.96-3.01) 81.8 (44.96-3.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.195 , 0.254 0.193 , 0.246	Depositor DCC
$R_{free}$ test set	1495 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.166 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: OH, FE, A1L8E

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	0.74	0/2225	1.06	2/3023 (0.1%)
1	B	0.75	0/2225	1.09	4/3023 (0.1%)
1	C	0.71	0/2248	1.05	2/3054 (0.1%)
1	D	0.70	0/2251	1.08	4/3057 (0.1%)
All	All	0.72	0/8949	1.07	12/12157 (0.1%)

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	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ASN	N-CA-C	7.14	118.71	111.07
1	D	228	ASP	N-CA-C	-6.26	101.41	110.24
1	D	217	VAL	N-CA-C	-6.15	104.34	110.30
1	D	41	LEU	N-CA-C	-5.91	103.62	111.24
1	C	132	VAL	N-CA-CB	5.62	117.77	110.57

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ASN	Peptide
1	B	40	ARG	Peptide
1	D	235	THR	Peptide

## 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	2175	0	2206	47	0
1	B	2175	0	2206	31	0
1	C	2198	0	2223	37	0
1	D	2201	0	2227	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	0	0	0
All	All	8805	0	8862	136	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 8.

The worst 5 of 136 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:221:THR:HG22	1:B:263:ARG:HE	1.36	0.88
1:A:135:MET:HE2	1:B:135:MET:HE2	1.61	0.82
1:A:183:ILE:HD13	1:B:145:MET:HE1	1.72	0.71
1:B:217:VAL:O	1:B:221:THR:HG23	1.94	0.67
1:B:161:ASN:ND2	1:B:246:TYR:OH	2.25	0.64

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	A	266/272 (98%)	217 (82%)	40 (15%)	9 (3%)	3	15
1	B	266/272 (98%)	234 (88%)	24 (9%)	8 (3%)	3	18
1	C	269/272 (99%)	223 (83%)	39 (14%)	7 (3%)	4	21
1	D	269/272 (99%)	225 (84%)	33 (12%)	11 (4%)	2	12
All	All	1070/1088 (98%)	899 (84%)	136 (13%)	35 (3%)	3	16

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
1	A	242	VAL
1	B	104	LEU
1	B	229	GLU
1	C	60	GLU

### 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	A	242/245 (99%)	214 (88%)	28 (12%)	5	22
1	B	242/245 (99%)	212 (88%)	30 (12%)	4	19
1	C	244/245 (100%)	214 (88%)	30 (12%)	4	19
1	D	245/245 (100%)	212 (86%)	33 (14%)	4	16
All	All	973/980 (99%)	852 (88%)	121 (12%)	4	19

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	292	VAL
1	D	221	THR
1	C	156	LEU
1	D	192	LEU
1	D	292	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	297	ASN
1	C	289	ASN
1	C	260	ASN
1	D	72	ASN
1	A	297	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - 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
4	A1L8E	A	504	-	46,47,47	1.80	7 (15%)	57,60,60	1.98	9 (15%)

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
4	A1L8E	A	504	-	-	14/41/41/41	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	A1L8E	CAA-CAB	-6.25	1.39	1.51
4	A	504	A1L8E	PAZ-CBA	5.46	1.89	1.79
4	A	504	A1L8E	CAH-CAI	-4.65	1.40	1.50
4	A	504	A1L8E	PAZ-CAY	3.66	1.90	1.80
4	A	504	A1L8E	PAZ-CBG	3.34	1.85	1.79

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	A1L8E	CAY-PAZ-CBA	-7.42	94.09	109.60
4	A	504	A1L8E	CAY-PAZ-CBG	-6.71	95.57	109.60
4	A	504	A1L8E	CBM-PAZ-CBG	5.09	122.99	107.96
4	A	504	A1L8E	CBG-PAZ-CBA	3.81	116.48	109.28
4	A	504	A1L8E	CBM-PAZ-CBA	3.77	119.10	107.96

There are no chirality outliers.

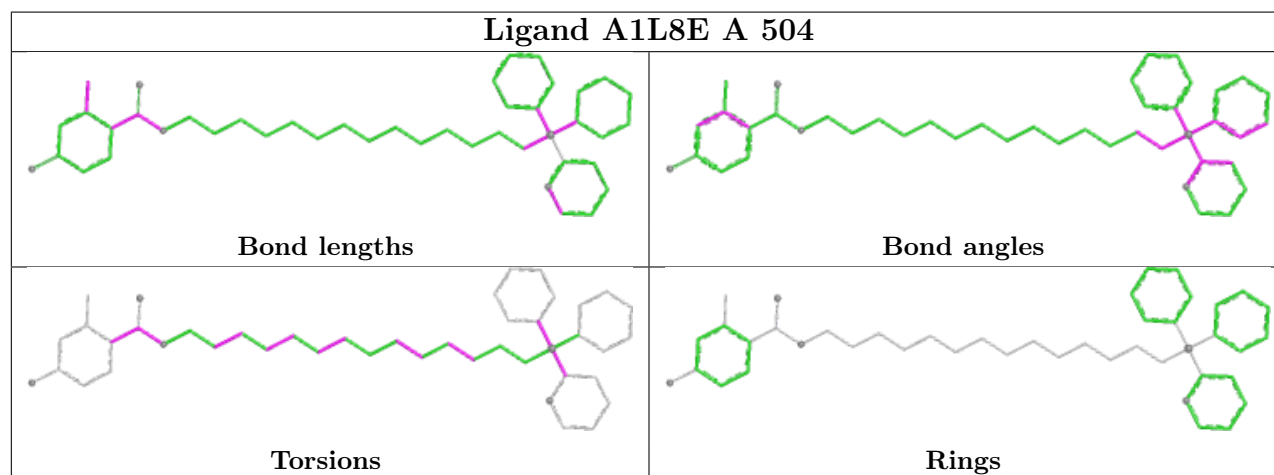
5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	A1L8E	NBR-CBM-PAZ-CBG
4	A	504	A1L8E	CBN-CBM-PAZ-CAY
4	A	504	A1L8E	CAH-CAI-OAK-CAL
4	A	504	A1L8E	OAJ-CAI-OAK-CAL
4	A	504	A1L8E	CAN-CAO-CAP-CAQ

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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<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	268/272 (98%)	0.24	6 (2%) 62 39	34, 56, 86, 128	0
1	B	268/272 (98%)	0.41	13 (4%) 35 18	38, 58, 87, 112	0
1	C	271/272 (99%)	0.55	20 (7%) 20 10	46, 70, 121, 141	0
1	D	271/272 (99%)	0.38	8 (2%) 52 30	47, 72, 117, 166	0
All	All	1078/1088 (99%)	0.39	47 (4%) 39 21	34, 64, 108, 166	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	GLU	5.2
1	C	260	ASN	4.6
1	D	110	ILE	4.2
1	C	99	PHE	4.2
1	C	104	LEU	4.0

### 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](#)

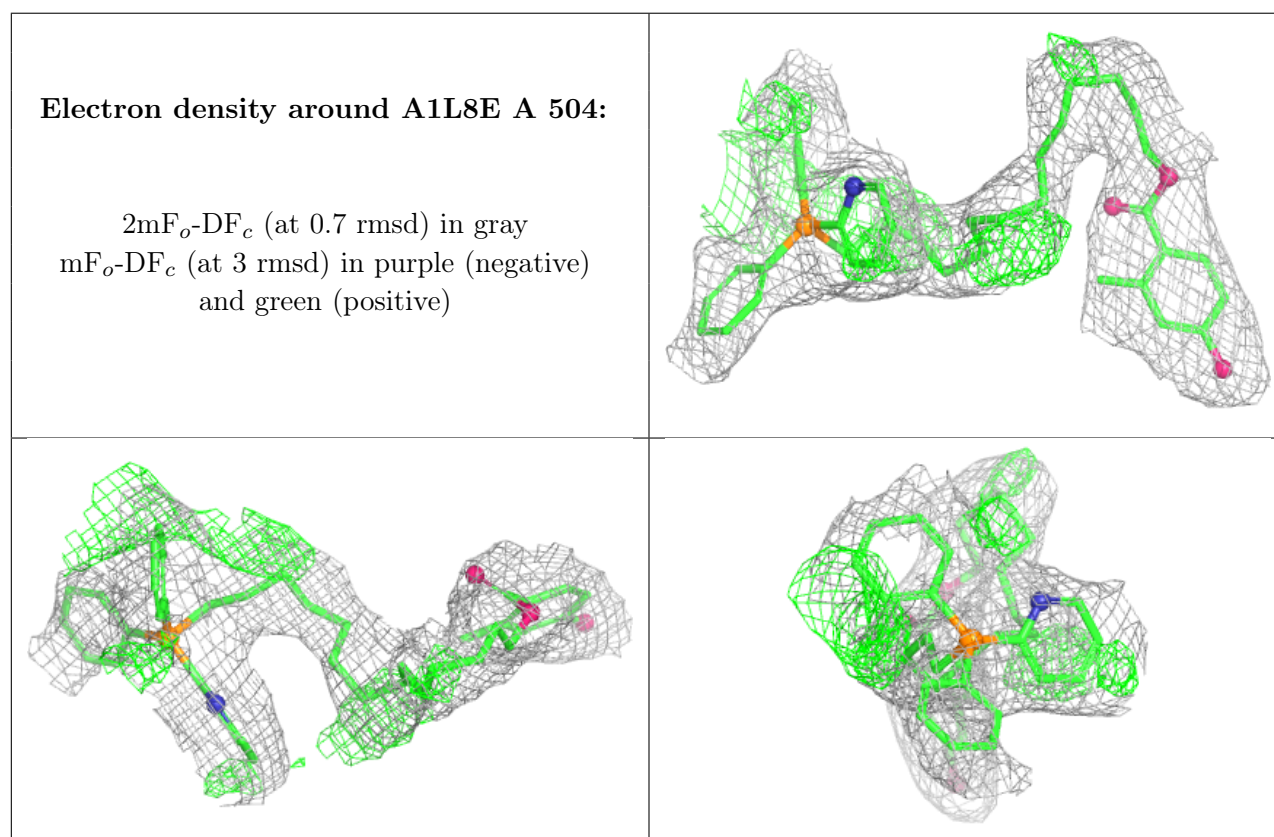
There are no oligosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
4	A1L8E	A	504	44/44	0.83	0.20	63,74,90,93	0
3	OH	C	503	1/1	0.95	0.06	25,25,25,25	0
3	OH	A	503	1/1	0.97	0.05	11,11,11,11	0
2	FE	C	502	1/1	0.98	0.06	49,49,49,49	0
3	OH	B	503	1/1	0.98	0.12	28,28,28,28	0
2	FE	A	502	1/1	0.99	0.03	43,43,43,43	0
2	FE	D	502	1/1	0.99	0.02	39,39,39,39	0
3	OH	D	503	1/1	0.99	0.03	20,20,20,20	0
2	FE	B	502	1/1	0.99	0.05	60,60,60,60	0
2	FE	B	501	1/1	1.00	0.03	45,45,45,45	0
2	FE	D	501	1/1	1.00	0.01	47,47,47,47	0
2	FE	A	501	1/1	1.00	0.01	45,45,45,45	0
2	FE	C	501	1/1	1.00	0.02	51,51,51,51	0

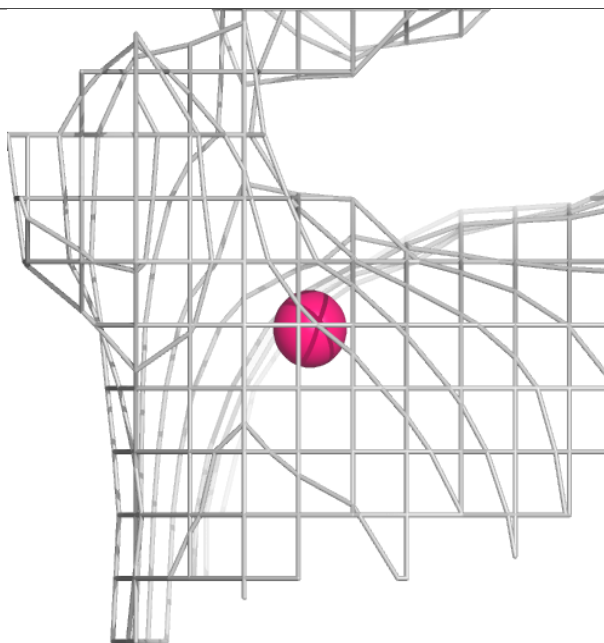
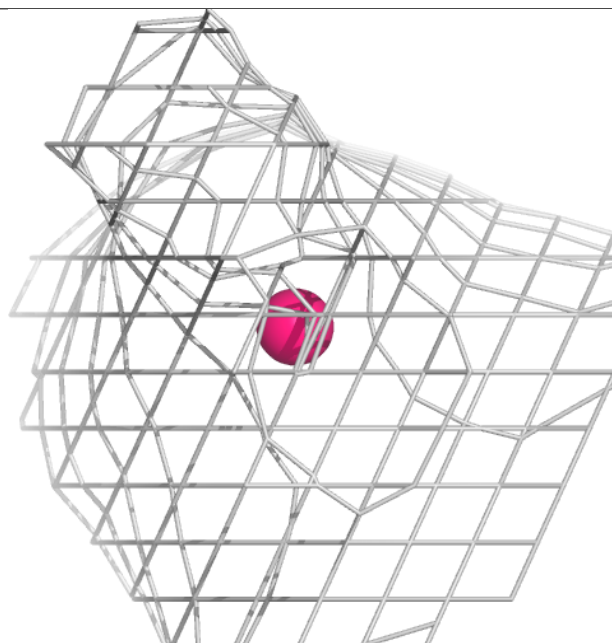
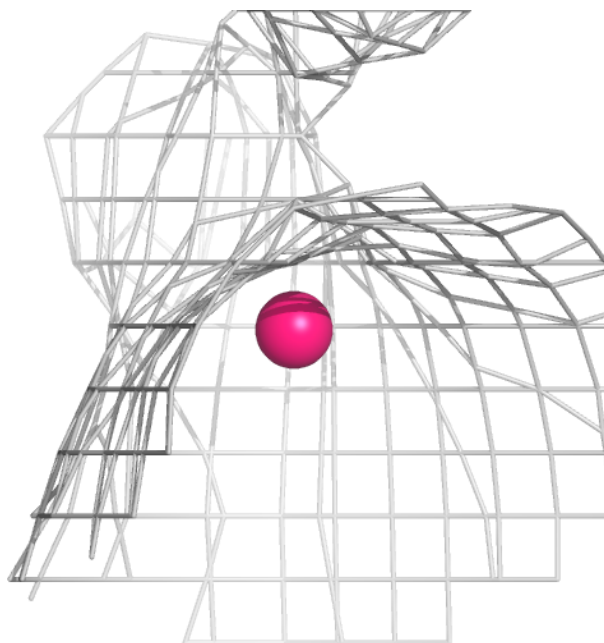
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





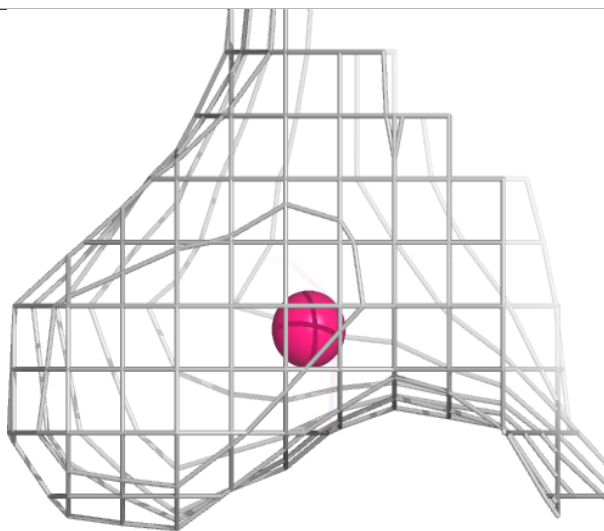
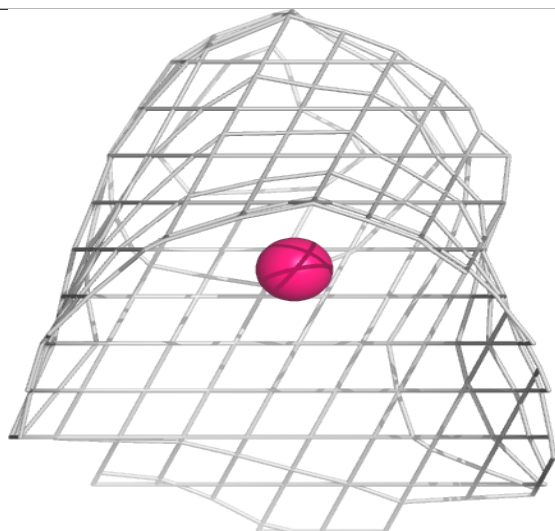
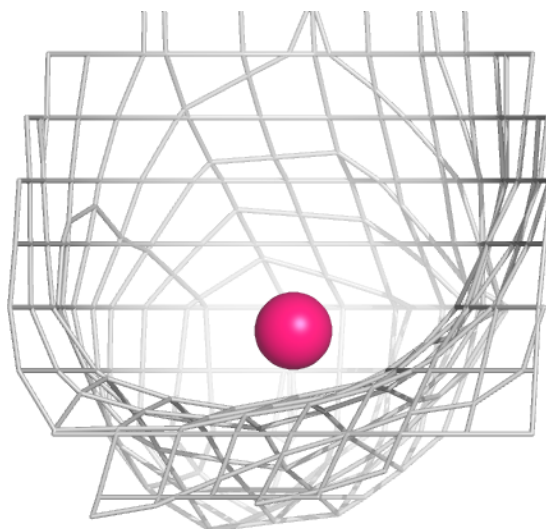
**Electron density around OH C 503:**

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



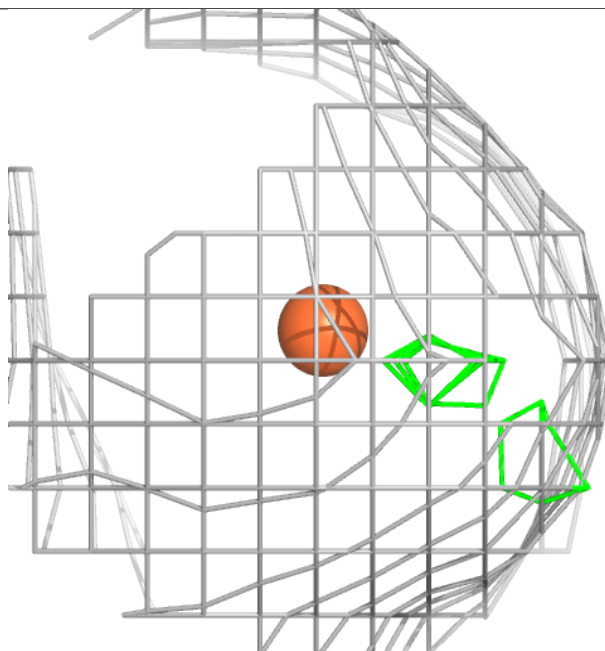
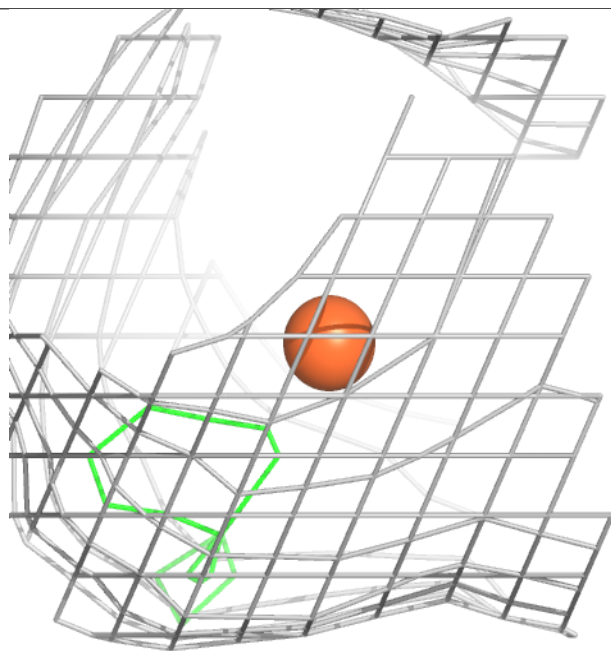
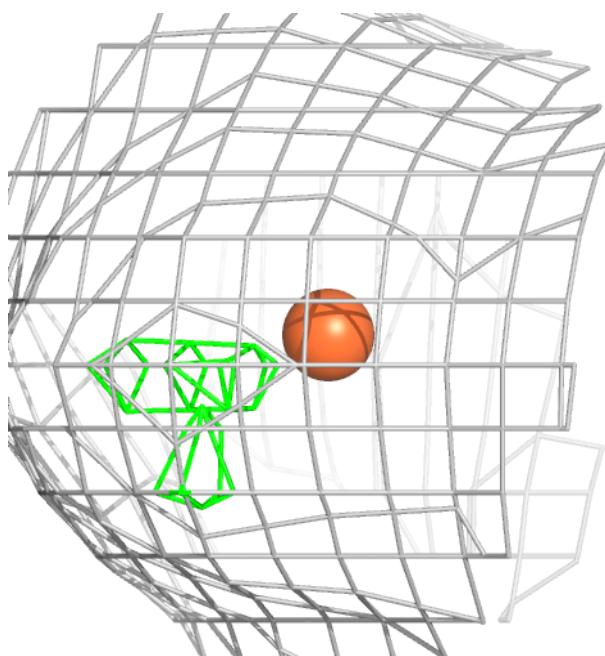
**Electron density around OH A 503:**

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



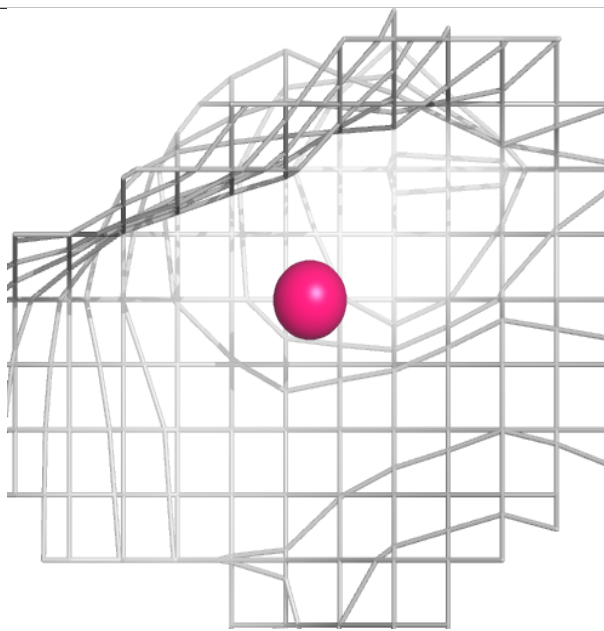
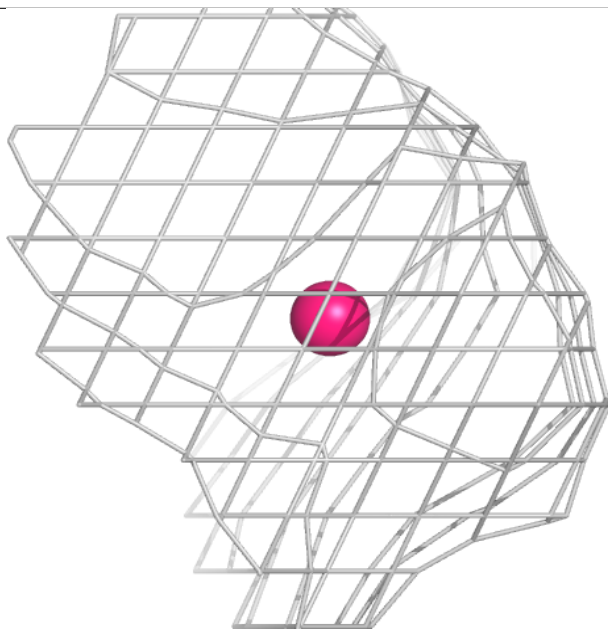
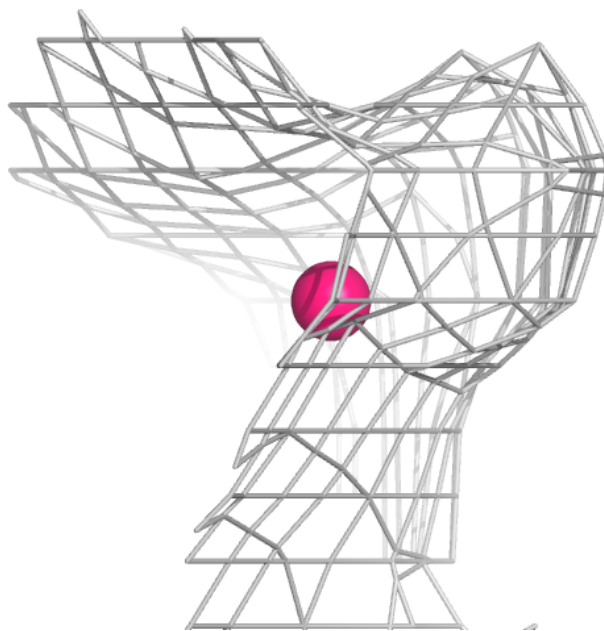
**Electron density around FE C 502:**

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



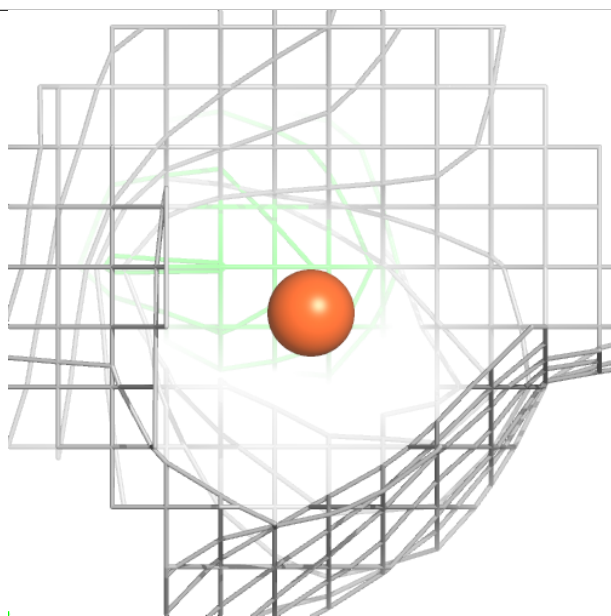
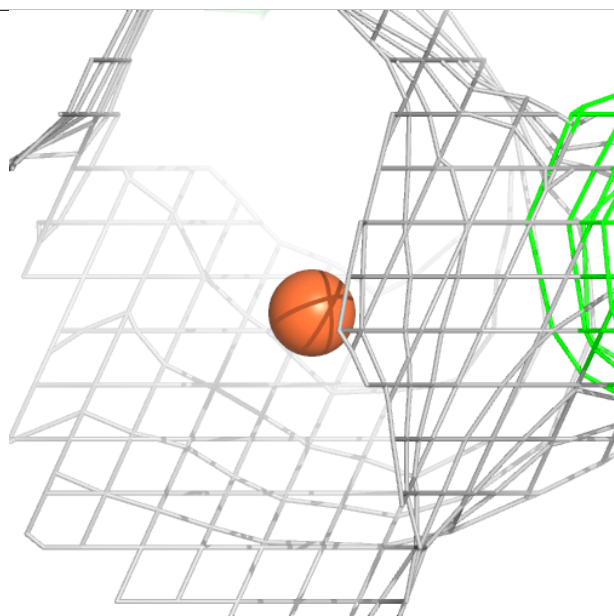
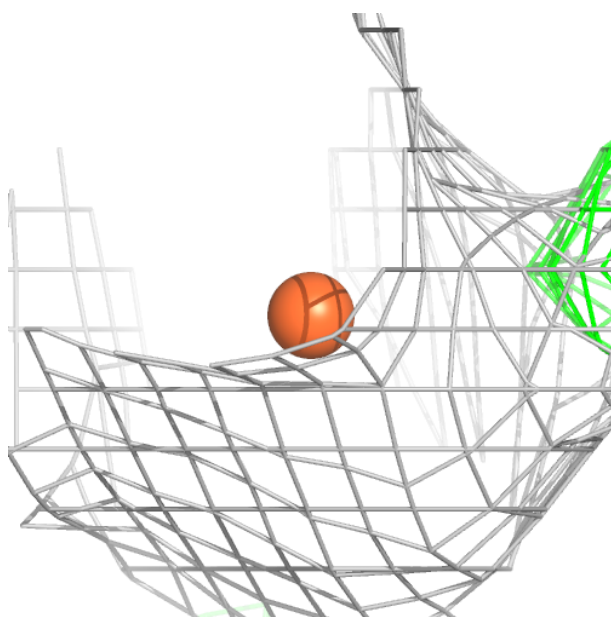
**Electron density around OH B 503:**

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



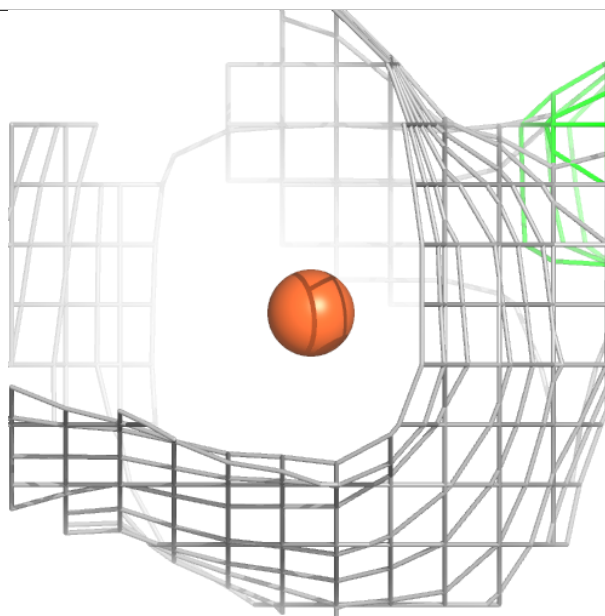
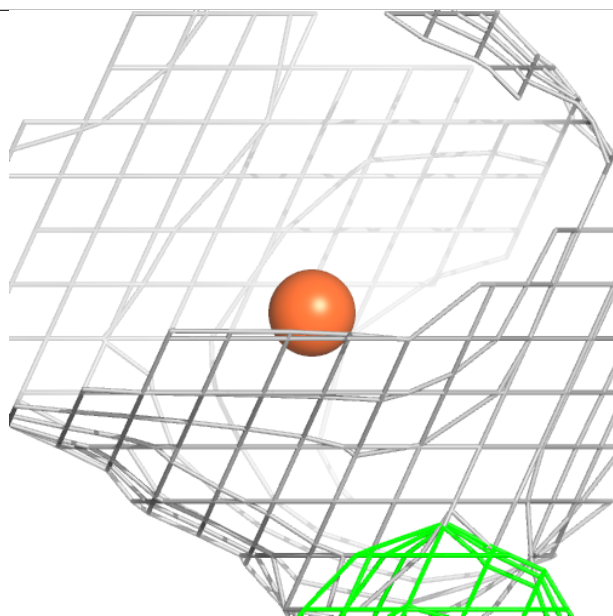
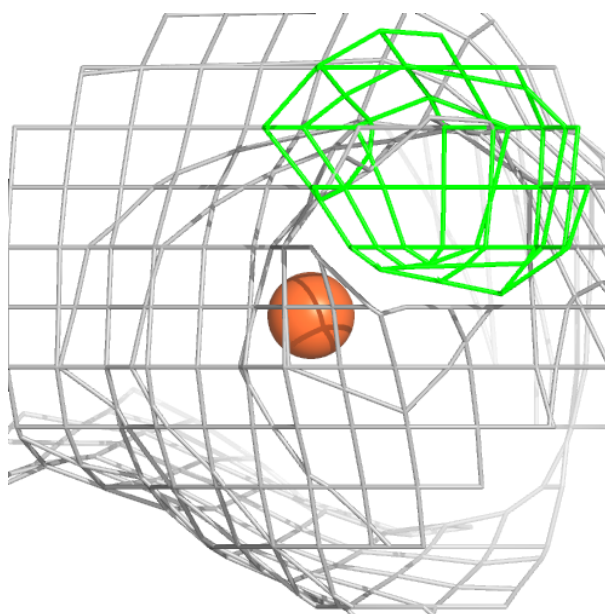
**Electron density around FE A 502:**

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



**Electron density around FE D 502:**

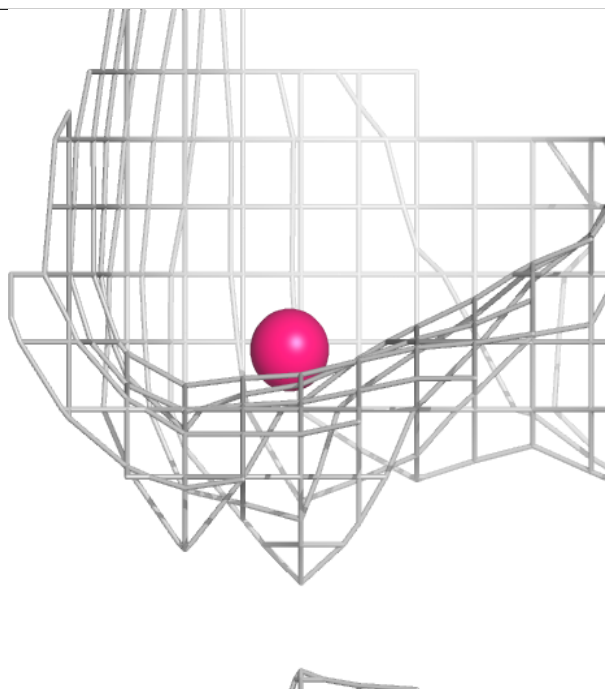
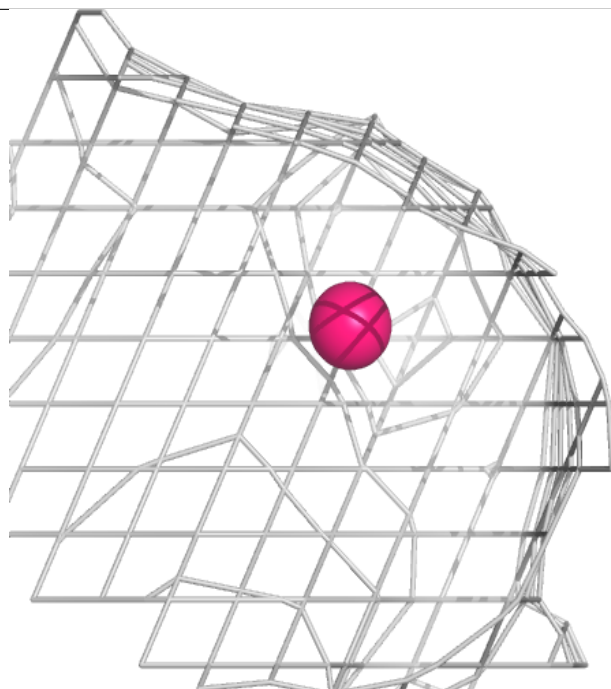
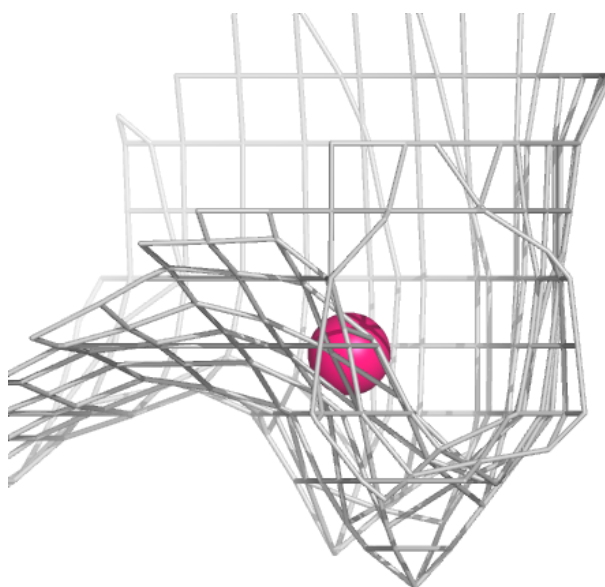
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





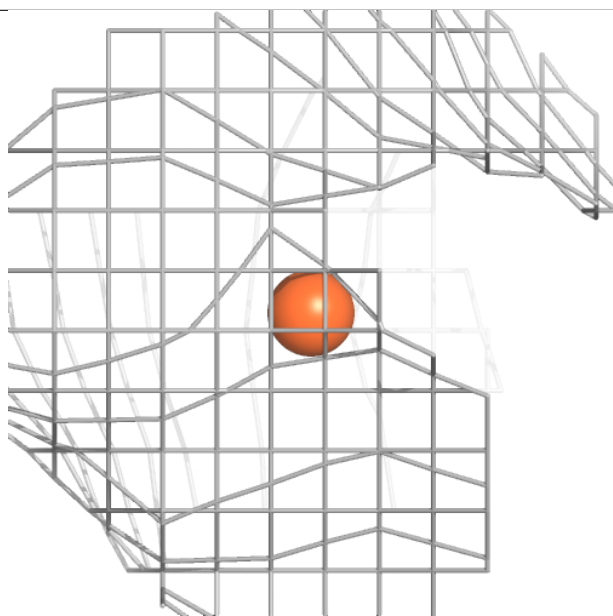
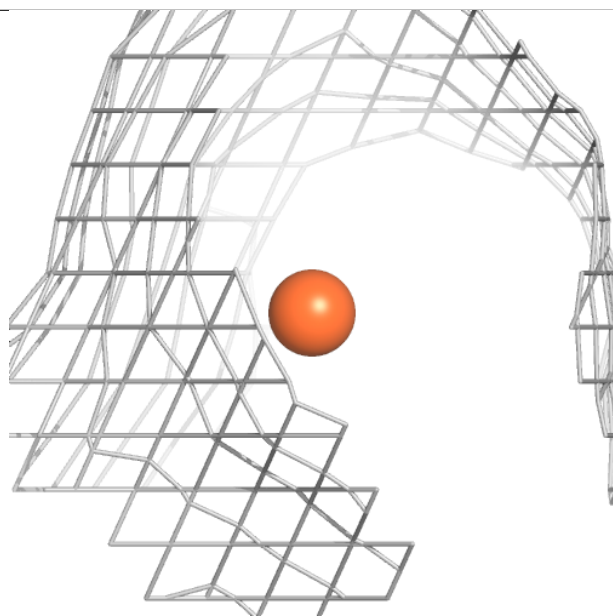
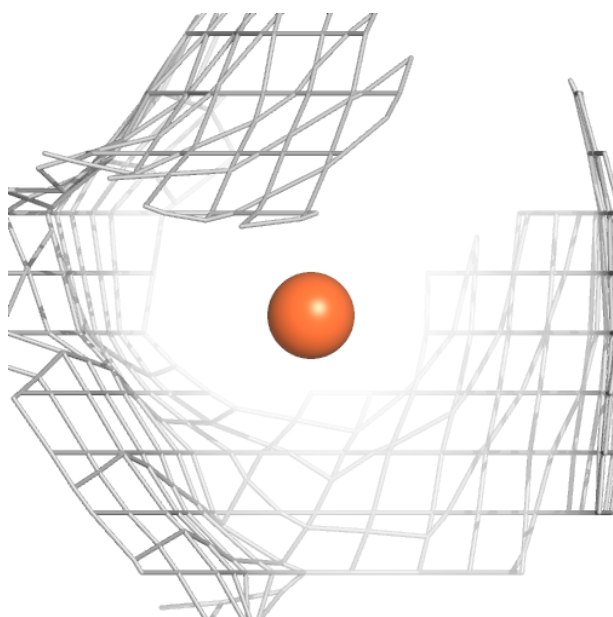
**Electron density around OH D 503:**

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



**Electron density around FE B 502:**

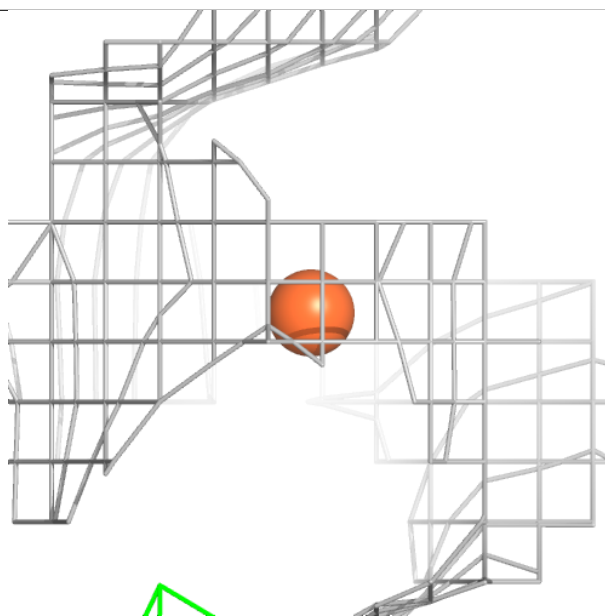
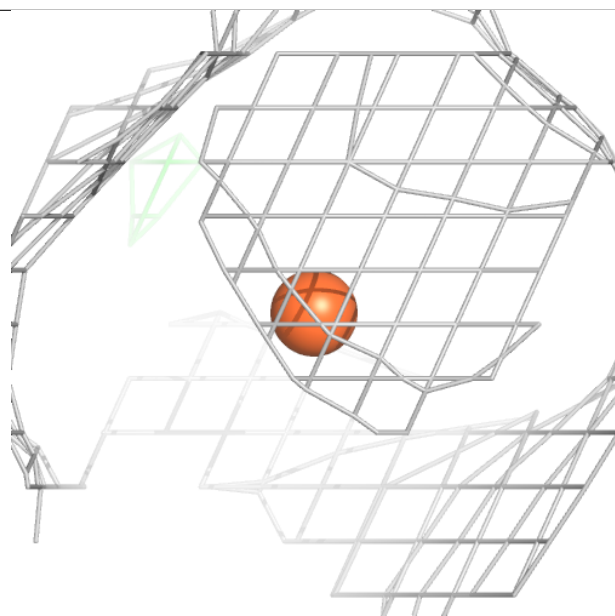
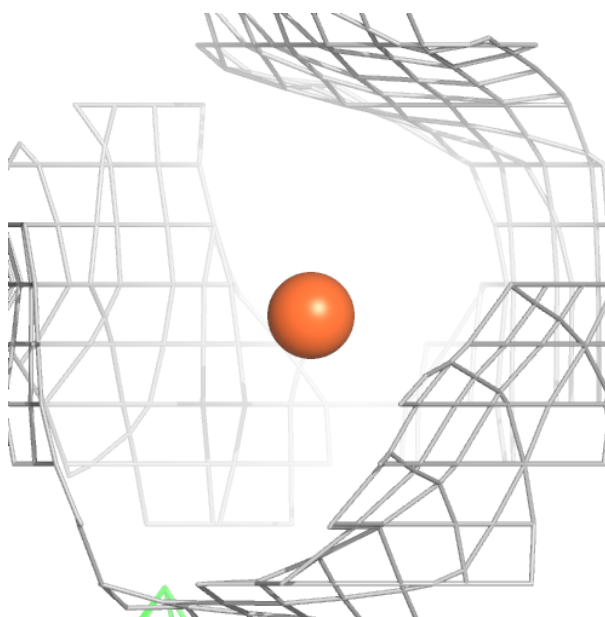
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





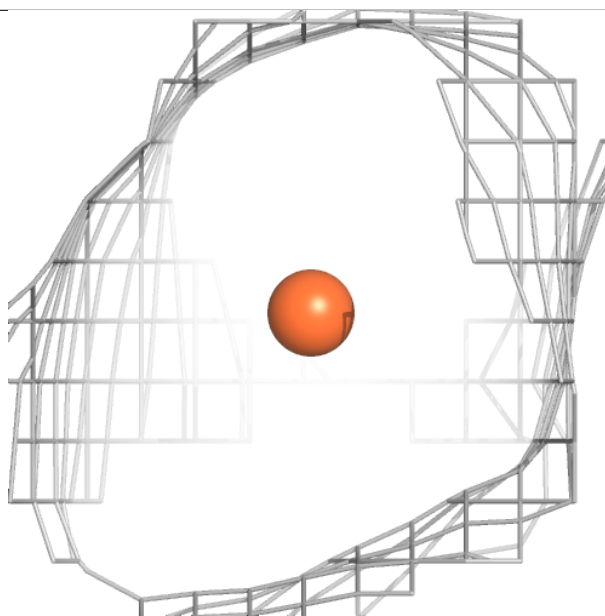
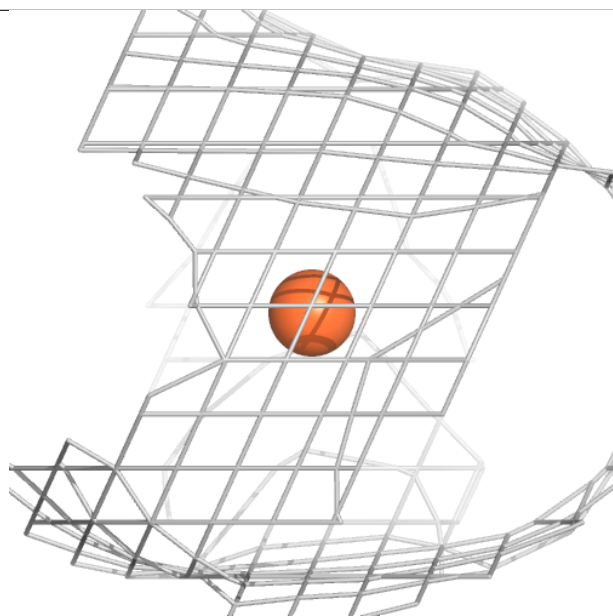
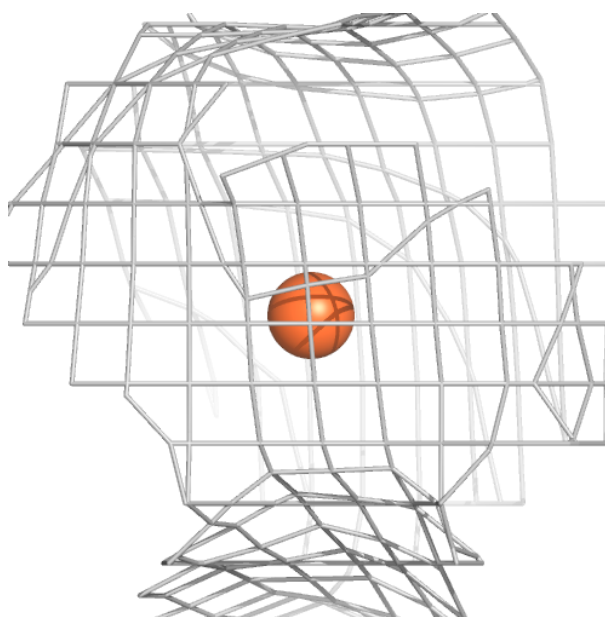
**Electron density around FE B 501:**

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



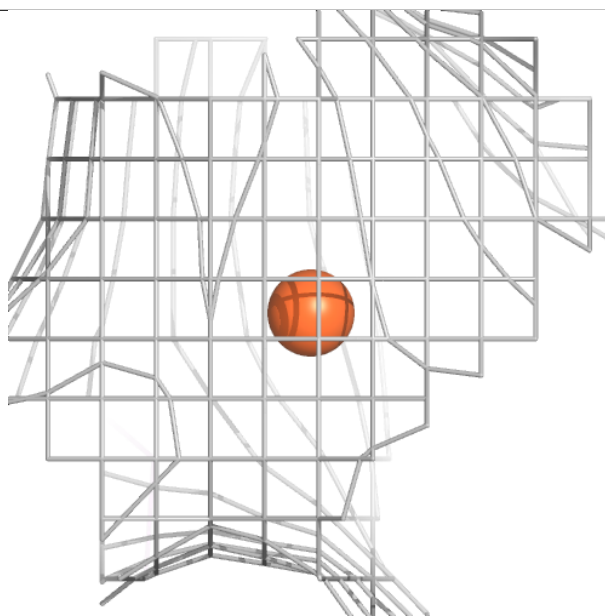
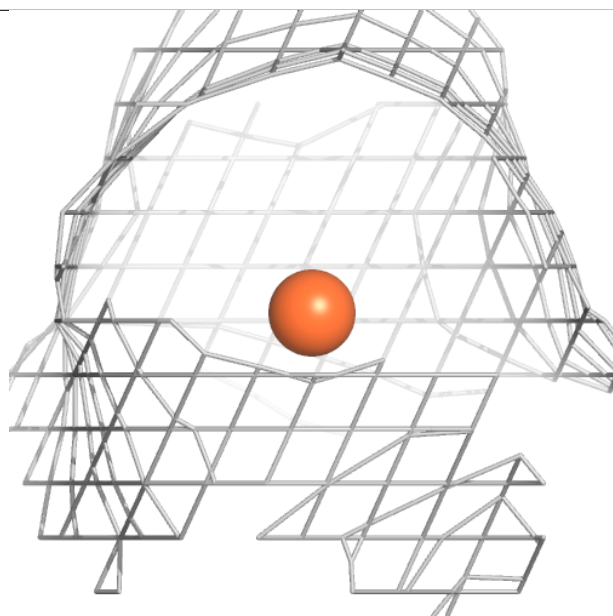
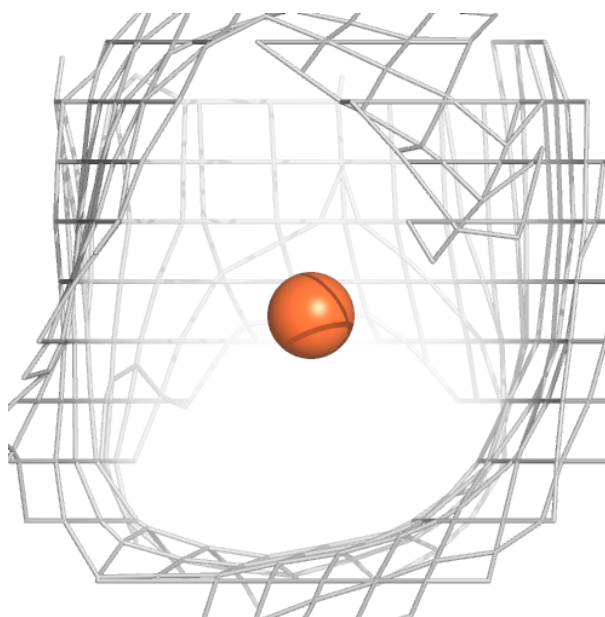
**Electron density around FE D 501:**

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



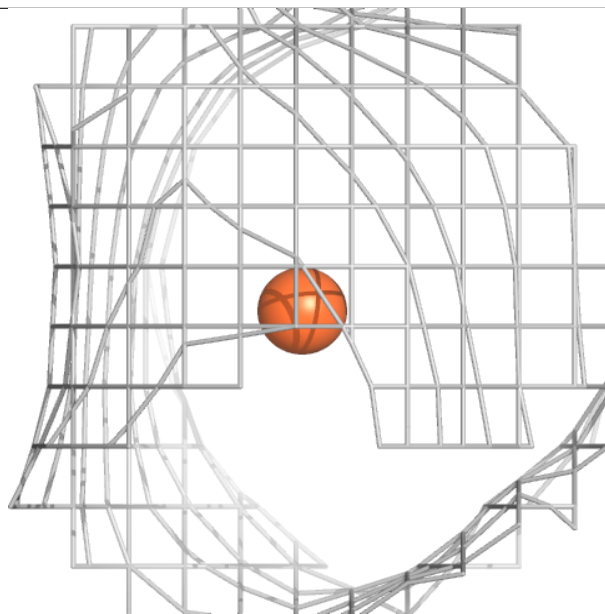
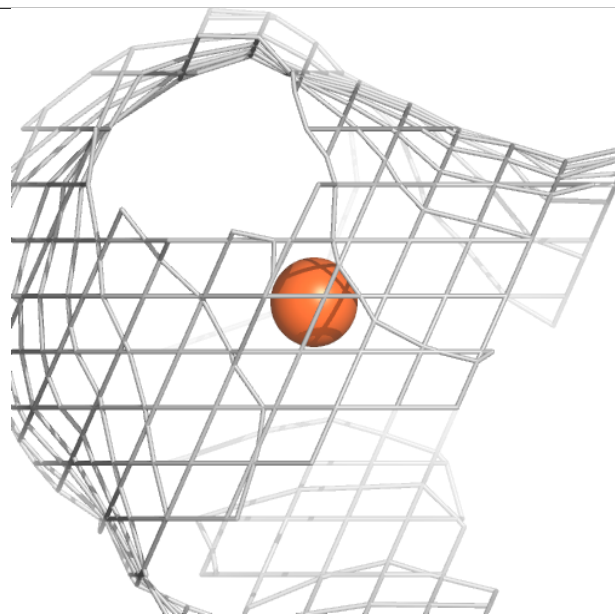
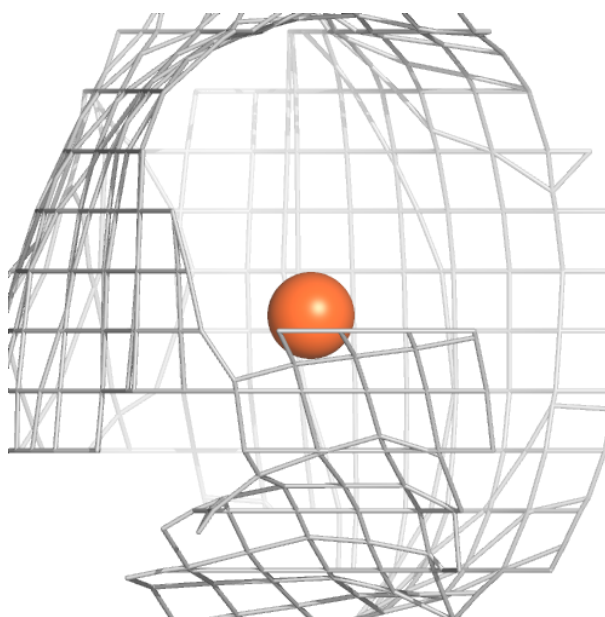
**Electron density around FE A 501:**

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



**Electron density around FE C 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.