



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 04:13 PM EDT

PDB ID : 9YPM / pdb\_00009ypm  
Title : MboA with Leu-Ala-Arg peptide substrate and two Fe(II) ions bound  
Authors : Badding, E.D.; Kissman, E.N.; Chang, M.C.Y.  
Deposited on : 2025-10-14  
Resolution : 2.45 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>.

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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
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

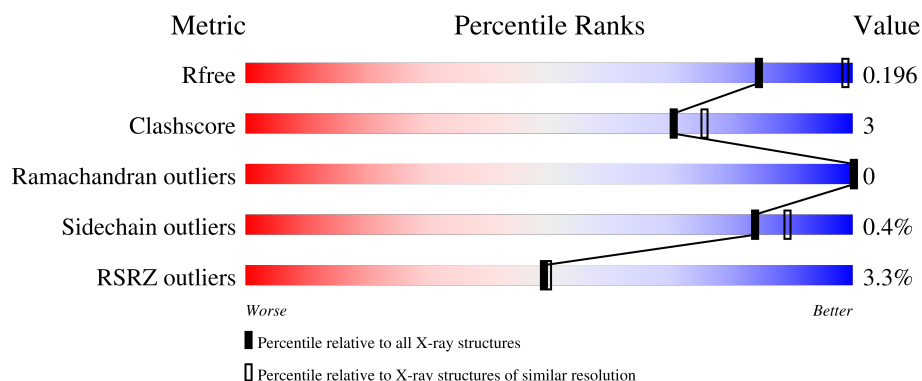
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.




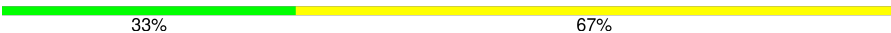

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	250	 4% 88% 7% 5%
1	B	250	 % 84% 6% 9%
1	C	250	 4% 83% 7% 10%
1	D	250	 4% 88% 7% 5%
2	J	3	 67% 33%

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Mol	Chain	Length	Quality of chain
2	K	3	 <div>33% 67%</div>
2	L	3	 <div>33% 67%</div>
2	M	3	 <div>67% 33%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	311	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8119 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 Mangotoxin biosynthesis protein MboA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	3	0
			1906	1221	307	364	14			
1	B	227	Total	C	N	O	S	0	2	0
			1812	1162	287	348	15			
1	C	226	Total	C	N	O	S	0	2	0
			1803	1156	287	345	15			
1	D	238	Total	C	N	O	S	0	3	0
			1905	1221	304	366	14			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A244EXR3
A	-23	GLY	-	expression tag	UNP A0A244EXR3
A	-22	HIS	-	expression tag	UNP A0A244EXR3
A	-21	HIS	-	expression tag	UNP A0A244EXR3
A	-20	HIS	-	expression tag	UNP A0A244EXR3
A	-19	HIS	-	expression tag	UNP A0A244EXR3
A	-18	HIS	-	expression tag	UNP A0A244EXR3
A	-17	HIS	-	expression tag	UNP A0A244EXR3
A	-16	HIS	-	expression tag	UNP A0A244EXR3
A	-15	HIS	-	expression tag	UNP A0A244EXR3
A	-14	HIS	-	expression tag	UNP A0A244EXR3
A	-13	HIS	-	expression tag	UNP A0A244EXR3
A	-12	SER	-	expression tag	UNP A0A244EXR3
A	-11	SER	-	expression tag	UNP A0A244EXR3
A	-10	GLY	-	expression tag	UNP A0A244EXR3
A	-9	HIS	-	expression tag	UNP A0A244EXR3
A	-8	LEU	-	expression tag	UNP A0A244EXR3
A	-7	GLU	-	expression tag	UNP A0A244EXR3
A	-6	VAL	-	expression tag	UNP A0A244EXR3
A	-5	LEU	-	expression tag	UNP A0A244EXR3
A	-4	PHE	-	expression tag	UNP A0A244EXR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	expression tag	UNP A0A244EXR3
A	-2	GLY	-	expression tag	UNP A0A244EXR3
A	-1	PRO	-	expression tag	UNP A0A244EXR3
A	0	HIS	-	expression tag	UNP A0A244EXR3
B	-24	MET	-	initiating methionine	UNP A0A244EXR3
B	-23	GLY	-	expression tag	UNP A0A244EXR3
B	-22	HIS	-	expression tag	UNP A0A244EXR3
B	-21	HIS	-	expression tag	UNP A0A244EXR3
B	-20	HIS	-	expression tag	UNP A0A244EXR3
B	-19	HIS	-	expression tag	UNP A0A244EXR3
B	-18	HIS	-	expression tag	UNP A0A244EXR3
B	-17	HIS	-	expression tag	UNP A0A244EXR3
B	-16	HIS	-	expression tag	UNP A0A244EXR3
B	-15	HIS	-	expression tag	UNP A0A244EXR3
B	-14	HIS	-	expression tag	UNP A0A244EXR3
B	-13	HIS	-	expression tag	UNP A0A244EXR3
B	-12	SER	-	expression tag	UNP A0A244EXR3
B	-11	SER	-	expression tag	UNP A0A244EXR3
B	-10	GLY	-	expression tag	UNP A0A244EXR3
B	-9	HIS	-	expression tag	UNP A0A244EXR3
B	-8	LEU	-	expression tag	UNP A0A244EXR3
B	-7	GLU	-	expression tag	UNP A0A244EXR3
B	-6	VAL	-	expression tag	UNP A0A244EXR3
B	-5	LEU	-	expression tag	UNP A0A244EXR3
B	-4	PHE	-	expression tag	UNP A0A244EXR3
B	-3	GLN	-	expression tag	UNP A0A244EXR3
B	-2	GLY	-	expression tag	UNP A0A244EXR3
B	-1	PRO	-	expression tag	UNP A0A244EXR3
B	0	HIS	-	expression tag	UNP A0A244EXR3
C	-24	MET	-	initiating methionine	UNP A0A244EXR3
C	-23	GLY	-	expression tag	UNP A0A244EXR3
C	-22	HIS	-	expression tag	UNP A0A244EXR3
C	-21	HIS	-	expression tag	UNP A0A244EXR3
C	-20	HIS	-	expression tag	UNP A0A244EXR3
C	-19	HIS	-	expression tag	UNP A0A244EXR3
C	-18	HIS	-	expression tag	UNP A0A244EXR3
C	-17	HIS	-	expression tag	UNP A0A244EXR3
C	-16	HIS	-	expression tag	UNP A0A244EXR3
C	-15	HIS	-	expression tag	UNP A0A244EXR3
C	-14	HIS	-	expression tag	UNP A0A244EXR3
C	-13	HIS	-	expression tag	UNP A0A244EXR3
C	-12	SER	-	expression tag	UNP A0A244EXR3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP A0A244EXR3
C	-10	GLY	-	expression tag	UNP A0A244EXR3
C	-9	HIS	-	expression tag	UNP A0A244EXR3
C	-8	LEU	-	expression tag	UNP A0A244EXR3
C	-7	GLU	-	expression tag	UNP A0A244EXR3
C	-6	VAL	-	expression tag	UNP A0A244EXR3
C	-5	LEU	-	expression tag	UNP A0A244EXR3
C	-4	PHE	-	expression tag	UNP A0A244EXR3
C	-3	GLN	-	expression tag	UNP A0A244EXR3
C	-2	GLY	-	expression tag	UNP A0A244EXR3
C	-1	PRO	-	expression tag	UNP A0A244EXR3
C	0	HIS	-	expression tag	UNP A0A244EXR3
D	-24	MET	-	initiating methionine	UNP A0A244EXR3
D	-23	GLY	-	expression tag	UNP A0A244EXR3
D	-22	HIS	-	expression tag	UNP A0A244EXR3
D	-21	HIS	-	expression tag	UNP A0A244EXR3
D	-20	HIS	-	expression tag	UNP A0A244EXR3
D	-19	HIS	-	expression tag	UNP A0A244EXR3
D	-18	HIS	-	expression tag	UNP A0A244EXR3
D	-17	HIS	-	expression tag	UNP A0A244EXR3
D	-16	HIS	-	expression tag	UNP A0A244EXR3
D	-15	HIS	-	expression tag	UNP A0A244EXR3
D	-14	HIS	-	expression tag	UNP A0A244EXR3
D	-13	HIS	-	expression tag	UNP A0A244EXR3
D	-12	SER	-	expression tag	UNP A0A244EXR3
D	-11	SER	-	expression tag	UNP A0A244EXR3
D	-10	GLY	-	expression tag	UNP A0A244EXR3
D	-9	HIS	-	expression tag	UNP A0A244EXR3
D	-8	LEU	-	expression tag	UNP A0A244EXR3
D	-7	GLU	-	expression tag	UNP A0A244EXR3
D	-6	VAL	-	expression tag	UNP A0A244EXR3
D	-5	LEU	-	expression tag	UNP A0A244EXR3
D	-4	PHE	-	expression tag	UNP A0A244EXR3
D	-3	GLN	-	expression tag	UNP A0A244EXR3
D	-2	GLY	-	expression tag	UNP A0A244EXR3
D	-1	PRO	-	expression tag	UNP A0A244EXR3
D	0	HIS	-	expression tag	UNP A0A244EXR3

- Molecule 2 is a protein called LEU-ALA-ARG peptide substrate.

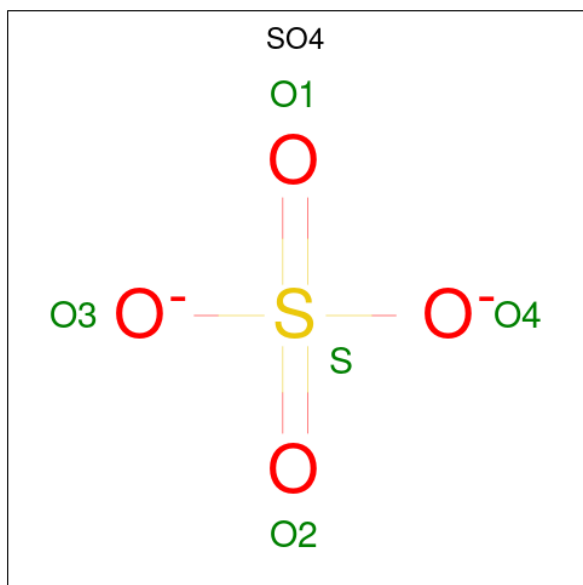
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	3	Total	C	N	O	0	0	0
			25	15	6	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			25	15	6	4			
2	L	3	Total	C	N	O	0	0	0
			25	15	6	4			
2	M	3	Total	C	N	O	0	0	0
			25	15	6	4			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Cl	0	0
			4	4		
4	B	4	Total	Cl	0	0
			4	4		
4	C	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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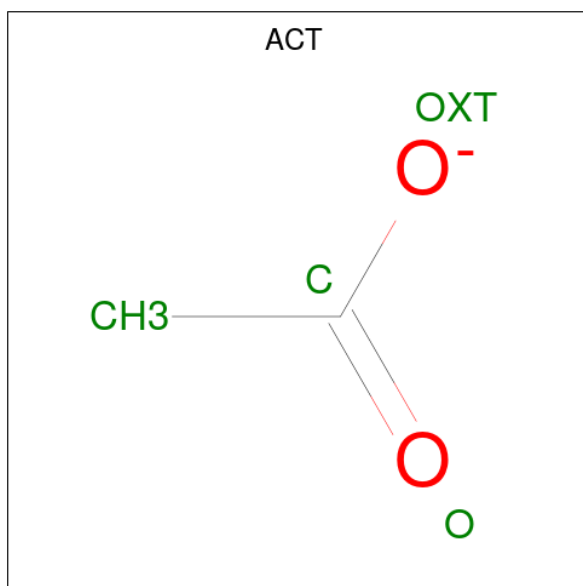
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	87	Total	O	0	0
			87	87		
8	B	62	Total	O	0	0
			62	62		
8	C	69	Total	O	0	0
			69	69		
8	D	47	Total	O	0	0
			47	47		
8	J	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	2	Total	O	0	0
			2	2		
8	M	1	Total	O	0	0
			1	1		



L300  
A301  
R302

- Molecule 2: LEU-ALA-ARG peptide substrate

Chain K:  33% 67%

L303  
A304  
R305

- Molecule 2: LEU-ALA-ARG peptide substrate

Chain L:  33% 67%

L306  
A307  
R308

- Molecule 2: LEU-ALA-ARG peptide substrate

Chain M:  67% 33%

L309  
A310  
R311

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.09Å 157.09Å 157.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.76 – 2.45 90.76 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.76-2.45) 100.0 (90.76-2.45)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.45Å)	Xtriage
Refinement program	PHENIX 2.0_5761	Depositor
R, $R_{free}$	0.163 , 0.195 0.163 , 0.196	Depositor DCC
$R_{free}$ test set	3592 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.005 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: GOL, CL, SO4, FE2, ACT

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	0.17	0/1955	0.35	0/2642
1	B	0.15	0/1857	0.31	0/2508
1	C	0.16	0/1848	0.33	0/2497
1	D	0.14	0/1953	0.29	0/2639
2	J	0.11	0/24	0.35	0/29
2	K	0.14	0/24	0.37	0/29
2	L	0.14	0/24	0.26	0/29
2	M	0.10	0/24	0.26	0/29
All	All	0.16	0/7709	0.32	0/10402

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	1906	0	1812	15	0
1	B	1812	0	1728	12	0
1	C	1803	0	1713	16	0
1	D	1905	0	1807	11	0
2	J	25	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	25	0	28	2	0
2	L	25	0	28	2	0
2	M	25	0	28	1	0
3	A	20	0	0	0	0
3	B	25	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	72	0	96	9	0
6	B	42	0	56	3	0
6	C	60	0	80	5	0
6	D	42	0	56	2	0
7	B	4	0	3	0	0
7	C	8	0	6	0	0
8	A	87	0	0	0	0
8	B	62	0	0	0	0
8	C	69	0	0	0	0
8	D	47	0	0	0	0
8	J	2	0	0	0	0
8	K	2	0	0	1	0
8	M	1	0	0	1	0
All	All	8119	0	7469	52	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 52 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:40:GLU:H	6:C:312:GOL:H2	1.52	0.73
1:C:50[B]:CYS:HG	2:L:306:LEU:N	1.87	0.72
1:B:50[B]:CYS:HG	2:K:303:LEU:N	1.85	0.72
1:A:92:MET:HE1	1:A:175:PHE:CD2	2.27	0.70
1:A:221:ARG:HE	6:A:315:GOL:H12	1.60	0.67

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	239/250 (96%)	237 (99%)	2 (1%)	0	100	100
1	B	227/250 (91%)	224 (99%)	3 (1%)	0	100	100
1	C	226/250 (90%)	223 (99%)	3 (1%)	0	100	100
1	D	239/250 (96%)	238 (100%)	1 (0%)	0	100	100
2	J	1/3 (33%)	1 (100%)	0	0	100	100
2	K	1/3 (33%)	1 (100%)	0	0	100	100
2	L	1/3 (33%)	1 (100%)	0	0	100	100
2	M	1/3 (33%)	1 (100%)	0	0	100	100
All	All	935/1012 (92%)	926 (99%)	9 (1%)	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	201/211 (95%)	199 (99%)	2 (1%)	68	77
1	B	191/211 (90%)	190 (100%)	1 (0%)	81	87
1	C	189/211 (90%)	189 (100%)	0	100	100
1	D	200/211 (95%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	2 (100%)	0	100	100
All	All	789/852 (93%)	786 (100%)	3 (0%)	84	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-12	SER
1	A	57	ASN
1	B	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	172	HIS
1	D	95	GLN
1	C	89	HIS
1	D	66	GLN
1	C	57	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 20 are monoatomic - leaving 54 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	SO4	A	301	-	4,4,4	0.68	0	6,6,6	0.14	0
6	GOL	B	315	-	5,5,5	0.34	0	5,5,5	0.37	0
6	GOL	D	311	-	5,5,5	0.34	0	5,5,5	0.38	0
6	GOL	C	312	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	A	320	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	C	309	-	5,5,5	0.32	0	5,5,5	0.39	0
7	ACT	C	318	-	3,3,3	1.15	0	3,3,3	1.21	0
3	SO4	A	304	-	4,4,4	0.66	0	6,6,6	0.12	0
3	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.11	0
3	SO4	B	303	-	4,4,4	0.67	0	6,6,6	0.12	0
6	GOL	D	308	-	5,5,5	0.32	0	5,5,5	0.40	0
6	GOL	C	310	-	5,5,5	0.31	0	5,5,5	0.33	0
6	GOL	A	321	-	5,5,5	0.33	0	5,5,5	0.43	0
6	GOL	A	312	-	5,5,5	0.32	0	5,5,5	0.42	0
3	SO4	B	305	-	4,4,4	0.69	0	6,6,6	0.07	0
6	GOL	D	313	-	5,5,5	0.33	0	5,5,5	0.40	0
3	SO4	C	302	-	4,4,4	0.67	0	6,6,6	0.11	0
6	GOL	C	308	-	5,5,5	0.31	0	5,5,5	0.48	0
3	SO4	D	303	-	4,4,4	0.67	0	6,6,6	0.11	0
6	GOL	C	316	-	5,5,5	0.32	0	5,5,5	0.34	0
6	GOL	A	317	-	5,5,5	0.32	0	5,5,5	0.24	0
6	GOL	A	319	-	5,5,5	0.33	0	5,5,5	0.44	0
6	GOL	B	312	-	5,5,5	0.32	0	5,5,5	0.41	0
6	GOL	A	315	-	5,5,5	0.33	0	5,5,5	0.39	0
3	SO4	A	302	-	4,4,4	0.66	0	6,6,6	0.09	0
6	GOL	C	311	-	5,5,5	0.33	0	5,5,5	0.36	0
6	GOL	C	317	-	5,5,5	0.33	0	5,5,5	0.46	0
6	GOL	D	309	-	5,5,5	0.33	0	5,5,5	0.38	0
6	GOL	D	310	-	5,5,5	0.35	0	5,5,5	0.44	0
6	GOL	A	316	-	5,5,5	0.28	0	5,5,5	0.52	0
6	GOL	A	314	-	5,5,5	0.33	0	5,5,5	0.29	0
6	GOL	A	322	-	5,5,5	0.34	0	5,5,5	0.29	0
6	GOL	B	318	-	5,5,5	0.31	0	5,5,5	0.41	0
6	GOL	B	313	-	5,5,5	0.34	0	5,5,5	0.30	0
3	SO4	A	303	-	4,4,4	0.68	0	6,6,6	0.16	0
6	GOL	C	315	-	5,5,5	0.34	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	D	312	-	5,5,5	0.32	0	5,5,5	0.43	0
6	GOL	A	311	-	5,5,5	0.34	0	5,5,5	0.42	0
6	GOL	A	313	-	5,5,5	0.35	0	5,5,5	0.44	0
3	SO4	B	304	-	4,4,4	0.68	0	6,6,6	0.08	0
6	GOL	B	314	-	5,5,5	0.33	0	5,5,5	0.38	0
6	GOL	C	314	-	5,5,5	0.34	0	5,5,5	0.28	0
7	ACT	B	319	-	3,3,3	1.14	0	3,3,3	1.26	0
6	GOL	B	316	-	5,5,5	0.31	0	5,5,5	0.30	0
3	SO4	B	302	-	4,4,4	0.68	0	6,6,6	0.13	0
3	SO4	C	303	-	4,4,4	0.72	0	6,6,6	0.09	0
6	GOL	A	318	-	5,5,5	0.33	0	5,5,5	0.40	0
6	GOL	C	313	-	5,5,5	0.34	0	5,5,5	0.29	0
3	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.09	0
6	GOL	D	314	-	5,5,5	0.31	0	5,5,5	0.43	0
7	ACT	C	319	-	3,3,3	1.18	0	3,3,3	1.14	0
3	SO4	D	302	-	4,4,4	0.68	0	6,6,6	0.16	0
3	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.06	0
6	GOL	B	317	-	5,5,5	0.34	0	5,5,5	0.43	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
6	GOL	B	315	-	-	0/4/4/4	-
6	GOL	D	311	-	-	0/4/4/4	-
6	GOL	C	312	-	-	2/4/4/4	-
6	GOL	A	320	-	-	2/4/4/4	-
6	GOL	C	309	-	-	0/4/4/4	-
6	GOL	D	308	-	-	0/4/4/4	-
6	GOL	C	310	-	-	2/4/4/4	-
6	GOL	A	321	-	-	1/4/4/4	-
6	GOL	A	312	-	-	1/4/4/4	-
6	GOL	D	313	-	-	2/4/4/4	-
6	GOL	C	308	-	-	1/4/4/4	-
6	GOL	C	316	-	-	0/4/4/4	-
6	GOL	A	317	-	-	2/4/4/4	-
6	GOL	A	319	-	-	2/4/4/4	-
6	GOL	B	312	-	-	0/4/4/4	-
6	GOL	A	315	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	311	-	-	2/4/4/4	-
6	GOL	C	317	-	-	0/4/4/4	-
6	GOL	D	309	-	-	2/4/4/4	-
6	GOL	D	310	-	-	2/4/4/4	-
6	GOL	A	316	-	-	1/4/4/4	-
6	GOL	A	314	-	-	1/4/4/4	-
6	GOL	A	322	-	-	1/4/4/4	-
6	GOL	B	318	-	-	0/4/4/4	-
6	GOL	B	313	-	-	2/4/4/4	-
6	GOL	C	315	-	-	2/4/4/4	-
6	GOL	D	312	-	-	0/4/4/4	-
6	GOL	A	311	-	-	2/4/4/4	-
6	GOL	B	314	-	-	2/4/4/4	-
6	GOL	A	313	-	-	2/4/4/4	-
6	GOL	C	314	-	-	1/4/4/4	-
6	GOL	B	316	-	-	0/4/4/4	-
6	GOL	A	318	-	-	2/4/4/4	-
6	GOL	C	313	-	-	0/4/4/4	-
6	GOL	D	314	-	-	2/4/4/4	-
6	GOL	B	317	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	311	GOL	C1-C2-C3-O3
6	A	311	GOL	O2-C2-C3-O3
6	C	310	GOL	O1-C1-C2-C3
6	C	312	GOL	C1-C2-C3-O3
6	D	310	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	315	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	312	GOL	2	0
6	D	308	GOL	1	0
6	C	310	GOL	1	0
6	D	313	GOL	1	0
6	C	308	GOL	1	0
6	A	317	GOL	1	0
6	A	315	GOL	2	0
6	A	316	GOL	2	0
6	A	311	GOL	4	0
6	C	314	GOL	1	0
6	B	317	GOL	2	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 [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	238/250 (95%)	-0.30	10 (4%) 40 40	30, 51, 79, 95	3 (1%)
1	B	227/250 (90%)	-0.38	2 (0%) 81 82	23, 51, 82, 126	2 (0%)
1	C	226/250 (90%)	-0.29	9 (3%) 42 41	23, 52, 84, 110	2 (0%)
1	D	238/250 (95%)	-0.08	10 (4%) 40 40	30, 61, 96, 130	3 (1%)
2	J	3/3 (100%)	-0.40	0 100 100	50, 50, 55, 56	0
2	K	3/3 (100%)	-0.27	0 100 100	55, 55, 58, 64	0
2	L	3/3 (100%)	0.16	0 100 100	57, 57, 61, 65	0
2	M	3/3 (100%)	0.43	0 100 100	61, 61, 66, 66	0
All	All	941/1012 (92%)	-0.26	31 (3%) 49 50	23, 54, 87, 130	10 (1%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	PRO	5.4
1	A	89[A]	HIS	4.0
1	C	175	PHE	3.7
1	D	89	HIS	3.5
1	C	0	HIS	3.4

### 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

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
4	CL	A	308	1/1	0.62	0.10	126,126,126,126	0
6	GOL	A	316	6/6	0.64	0.31	62,78,95,115	0
6	GOL	B	315	6/6	0.65	0.23	102,110,117,121	0
6	GOL	A	321	6/6	0.70	0.24	76,100,116,116	0
3	SO4	B	303	5/5	0.72	0.14	90,98,124,149	1
6	GOL	C	312	6/6	0.74	0.25	77,89,96,102	0
7	ACT	C	319	4/4	0.74	0.26	71,81,103,115	0
6	GOL	C	315	6/6	0.77	0.25	87,102,118,126	0
6	GOL	D	308	6/6	0.77	0.18	90,107,112,114	0
6	GOL	B	317	6/6	0.77	0.29	73,92,100,113	0
6	GOL	A	313	6/6	0.78	0.28	79,94,100,101	0
4	CL	C	305	1/1	0.79	0.25	119,119,119,119	0
6	GOL	C	311	6/6	0.79	0.24	82,105,114,123	0
6	GOL	B	314	6/6	0.80	0.27	84,98,117,127	0
6	GOL	A	315	6/6	0.80	0.19	84,96,98,117	0
6	GOL	A	314	6/6	0.81	0.30	75,84,108,108	0
6	GOL	D	313	6/6	0.83	0.16	67,83,86,92	0
6	GOL	D	314	6/6	0.83	0.22	80,83,111,113	0
7	ACT	B	319	4/4	0.83	0.25	86,93,97,99	0
7	ACT	C	318	4/4	0.83	0.22	77,85,87,95	0
6	GOL	B	312	6/6	0.83	0.23	68,86,106,108	0
3	SO4	D	301	5/5	0.84	0.08	87,103,116,125	5
3	SO4	B	302	5/5	0.84	0.14	79,80,104,108	5
3	SO4	A	304	5/5	0.84	0.15	89,92,104,126	5
6	GOL	D	311	6/6	0.85	0.26	89,97,109,121	0
6	GOL	C	309	6/6	0.85	0.15	84,85,91,96	0
6	GOL	A	317	6/6	0.85	0.23	79,92,109,115	0
3	SO4	C	303	5/5	0.85	0.20	77,95,113,172	0
6	GOL	B	316	6/6	0.85	0.18	69,75,94,99	0
3	SO4	D	303	5/5	0.85	0.12	74,77,92,98	5
3	SO4	C	302	5/5	0.86	0.12	70,76,95,109	5
4	CL	B	308	1/1	0.86	0.26	95,95,95,95	0
3	SO4	B	304	5/5	0.86	0.12	76,88,119,145	5
6	GOL	B	318	6/6	0.86	0.20	75,89,104,105	0
6	GOL	A	312	6/6	0.86	0.22	79,90,101,107	0
6	GOL	C	316	6/6	0.87	0.22	74,89,96,101	0
6	GOL	A	318	6/6	0.88	0.20	84,90,115,117	0

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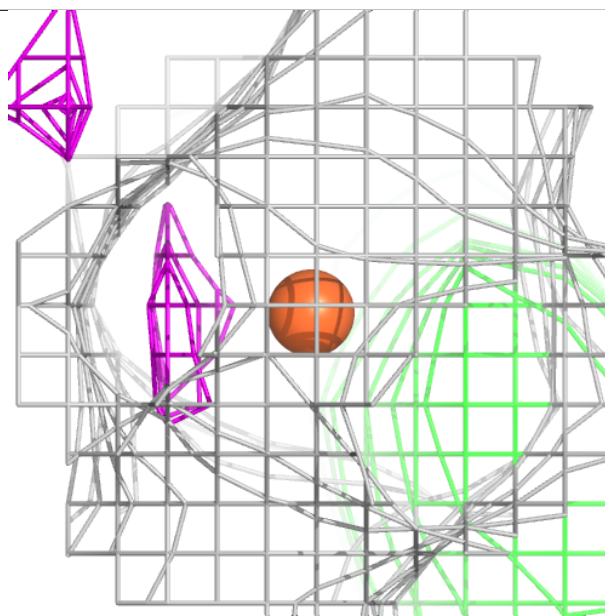
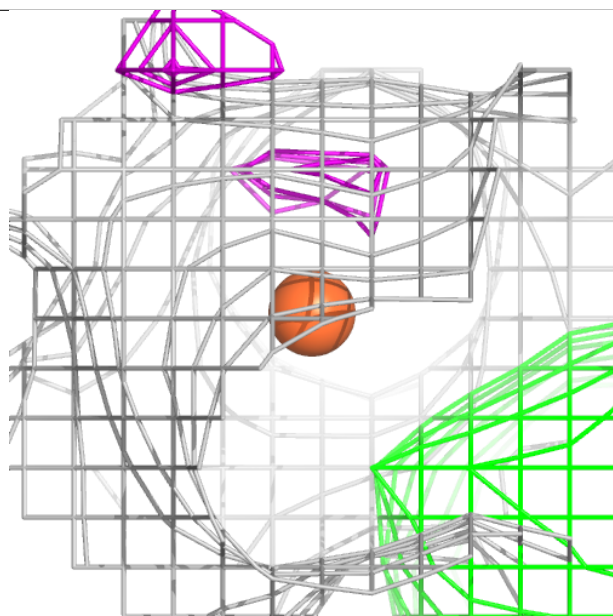
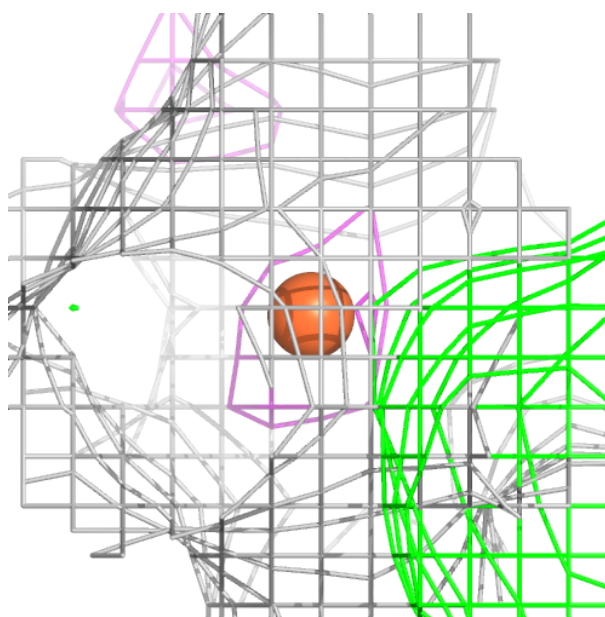
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	309	1/1	0.88	0.19	110,110,110,110	0
6	GOL	C	314	6/6	0.88	0.26	75,95,105,106	0
3	SO4	B	305	5/5	0.88	0.11	92,103,123,162	0
6	GOL	D	312	6/6	0.89	0.18	101,103,107,112	0
6	GOL	C	310	6/6	0.89	0.20	68,85,97,106	0
6	GOL	A	311	6/6	0.89	0.22	63,73,90,93	0
6	GOL	D	310	6/6	0.90	0.23	84,94,97,98	0
3	SO4	A	303	5/5	0.90	0.17	66,82,93,106	5
6	GOL	C	317	6/6	0.90	0.18	86,100,101,102	0
6	GOL	C	308	6/6	0.90	0.22	83,88,105,106	0
6	GOL	B	313	6/6	0.91	0.22	71,75,88,98	0
3	SO4	D	302	5/5	0.91	0.18	57,64,73,77	5
6	GOL	C	313	6/6	0.91	0.14	87,93,100,103	0
6	GOL	A	320	6/6	0.91	0.18	77,83,98,105	0
6	GOL	A	319	6/6	0.92	0.17	61,72,73,74	0
6	GOL	D	309	6/6	0.93	0.19	80,92,100,108	0
3	SO4	A	302	5/5	0.93	0.07	79,83,116,118	0
6	GOL	A	322	6/6	0.93	0.15	66,82,95,110	0
4	CL	D	304	1/1	0.94	0.12	104,104,104,104	0
4	CL	A	306	1/1	0.94	0.12	86,86,86,86	0
4	CL	B	306	1/1	0.94	0.12	83,83,83,83	0
4	CL	C	304	1/1	0.94	0.13	85,85,85,85	0
4	CL	B	307	1/1	0.94	0.12	79,79,79,79	0
3	SO4	B	301	5/5	0.95	0.08	61,76,79,92	5
3	SO4	C	301	5/5	0.95	0.07	72,78,94,102	5
5	FE2	A	309	1/1	0.95	0.06	67,67,67,67	0
3	SO4	A	301	5/5	0.96	0.08	68,68,71,75	0
4	CL	A	305	1/1	0.97	0.10	79,79,79,79	0
5	FE2	C	307	1/1	0.97	0.06	65,65,65,65	1
5	FE2	D	307	1/1	0.97	0.08	86,86,86,86	0
4	CL	A	307	1/1	0.98	0.07	51,51,51,51	0
5	FE2	D	306	1/1	0.98	0.05	70,70,70,70	0
5	FE2	A	310	1/1	0.98	0.07	60,60,60,60	0
5	FE2	B	311	1/1	0.99	0.04	70,70,70,70	0
5	FE2	C	306	1/1	0.99	0.02	81,81,81,81	0
4	CL	D	305	1/1	0.99	0.14	58,58,58,58	0
5	FE2	B	310	1/1	0.99	0.04	65,65,65,65	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.

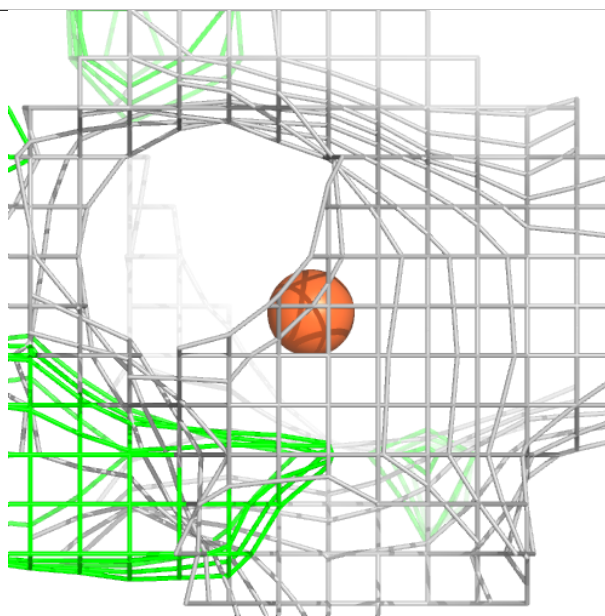
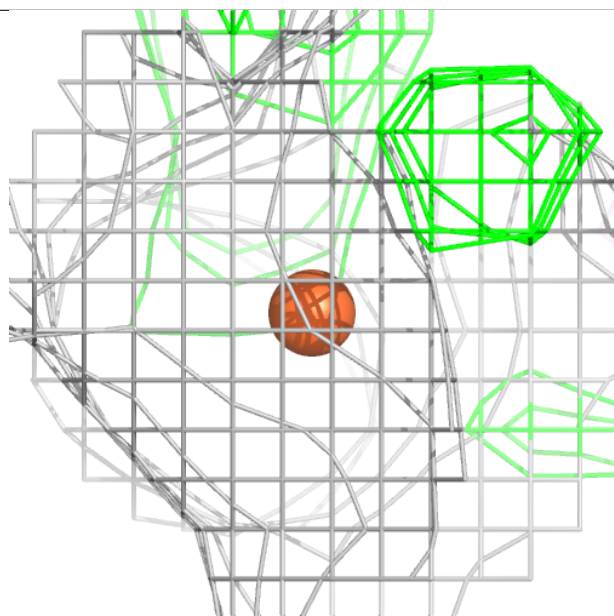
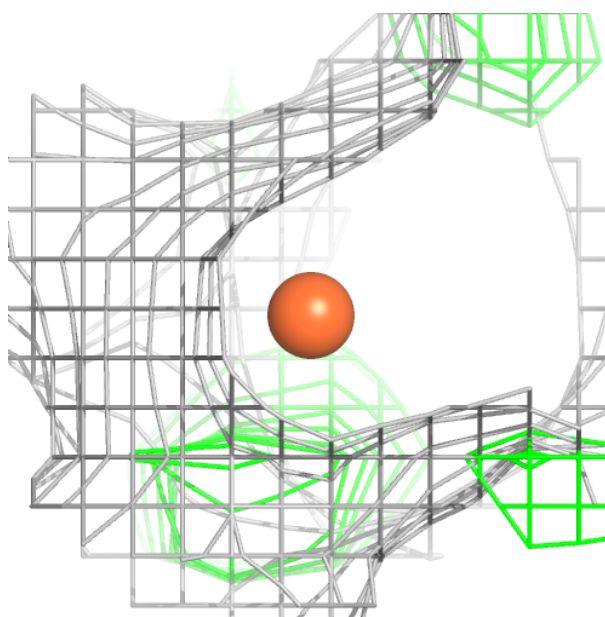
**Electron density around FE2 A 309:**

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



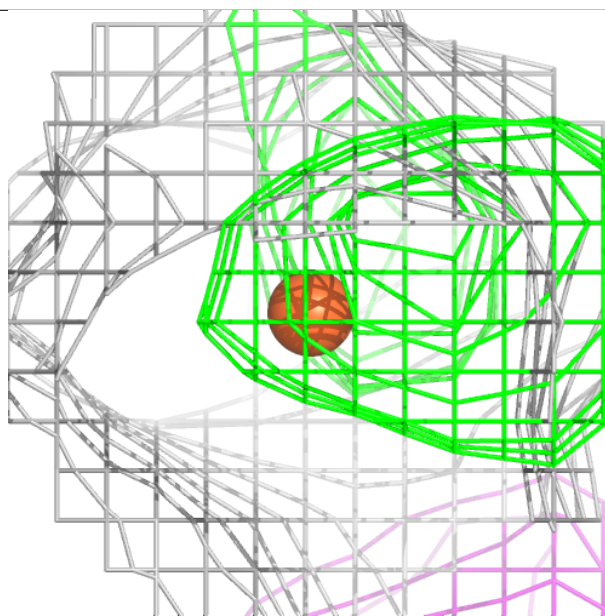
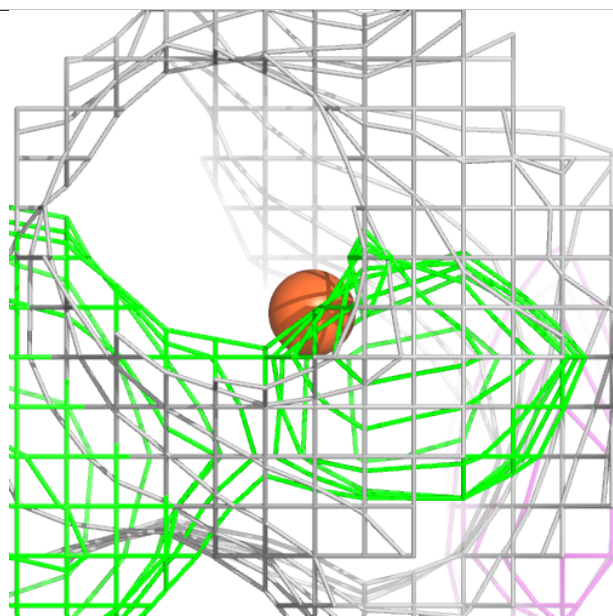
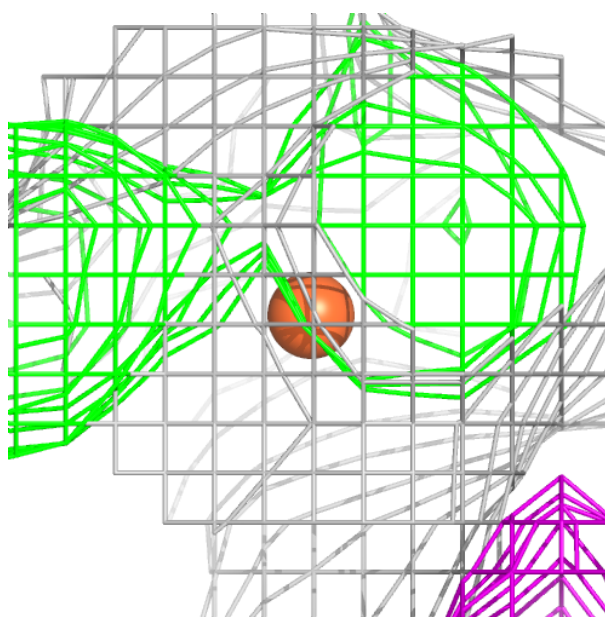
**Electron density around FE2 C 307:**

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



**Electron density around FE2 D 307:**

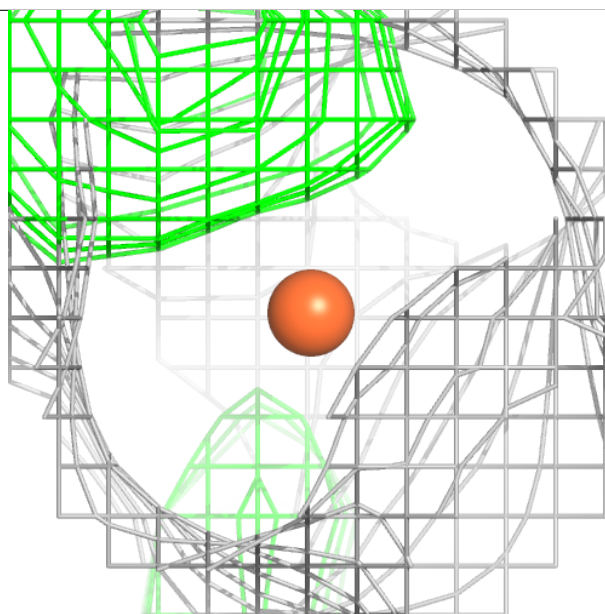
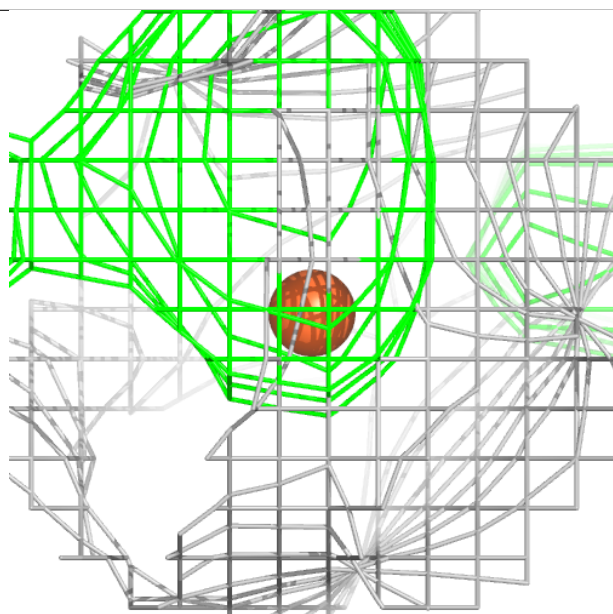
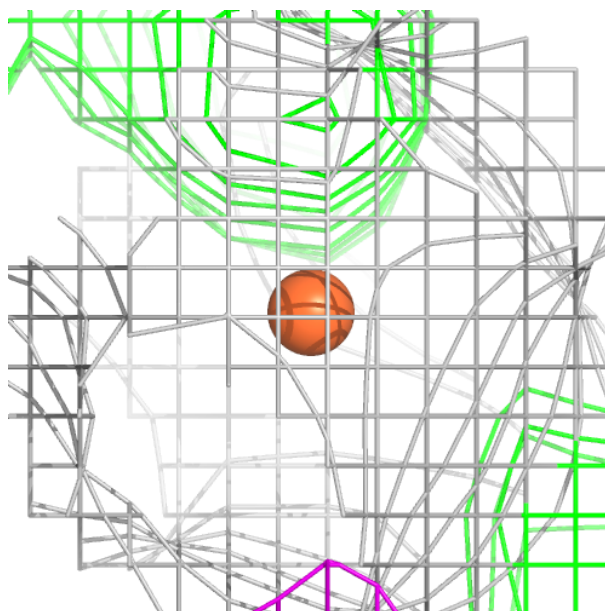
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





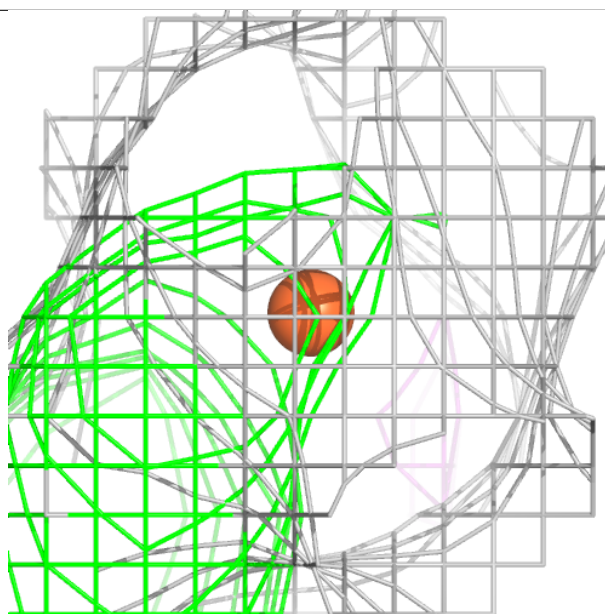
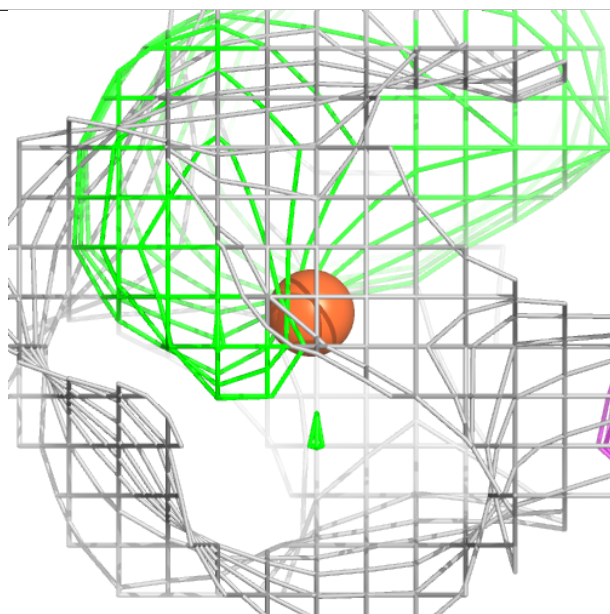
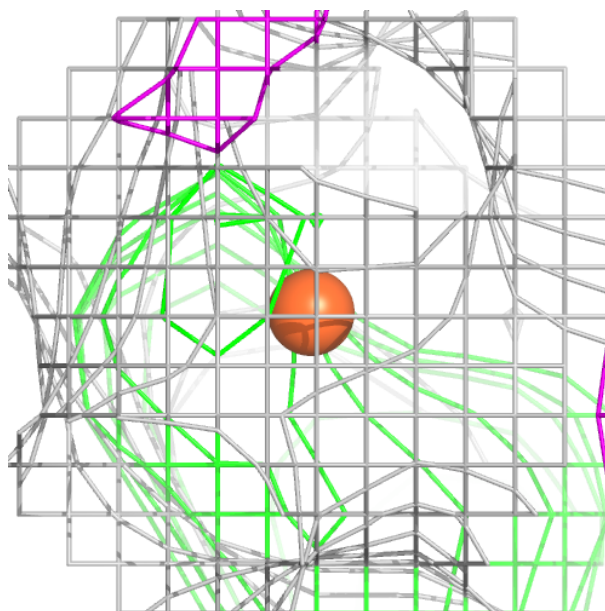
**Electron density around FE2 D 306:**

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



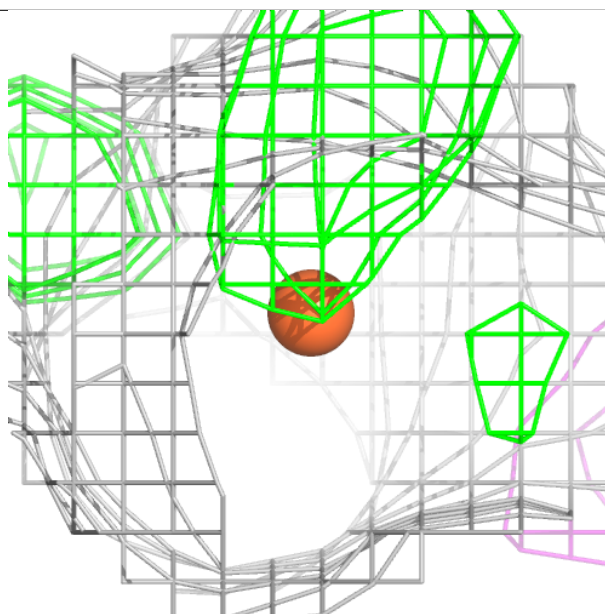
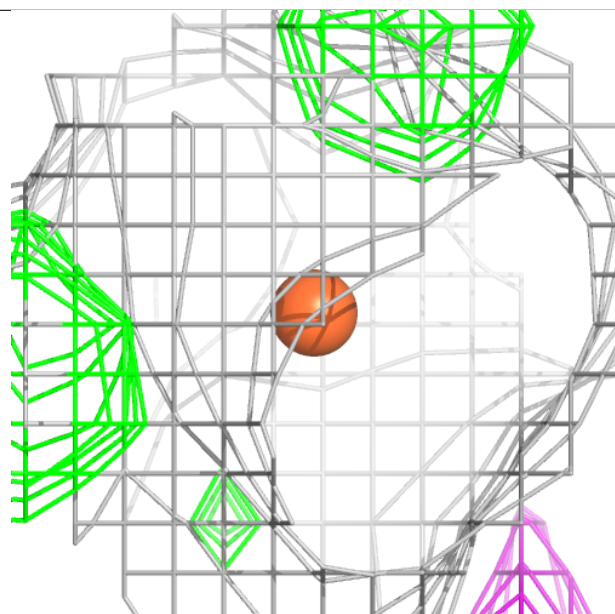
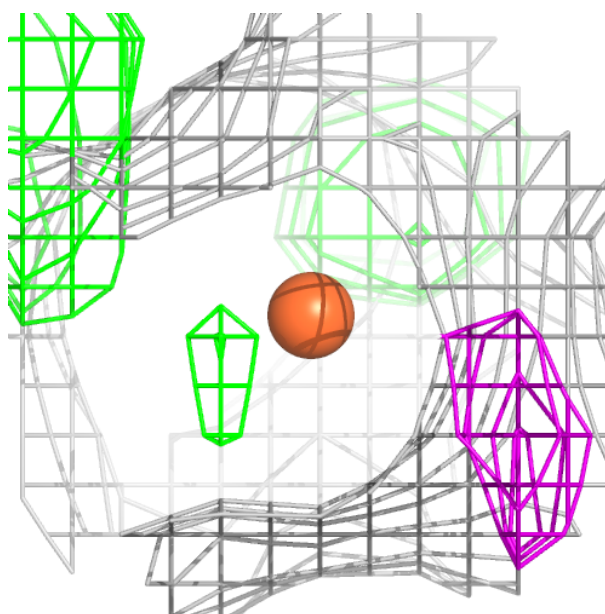
**Electron density around FE2 A 310:**

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



**Electron density around FE2 B 311:**

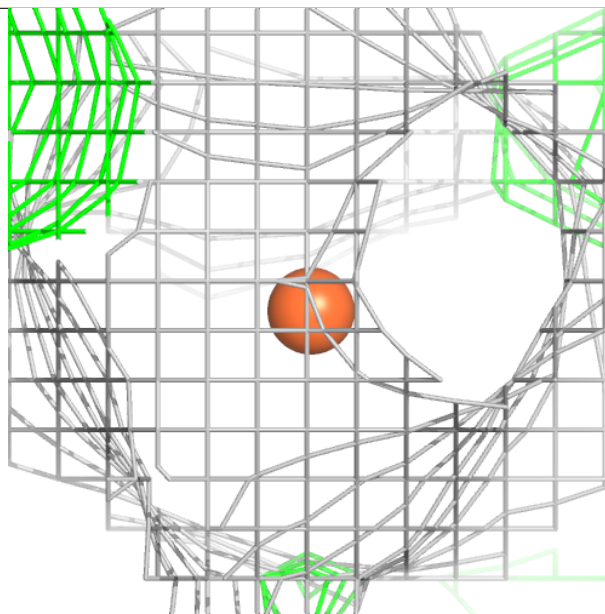
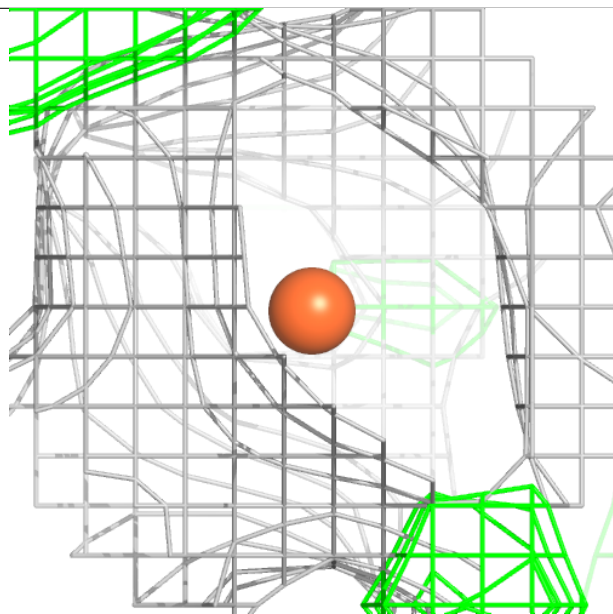
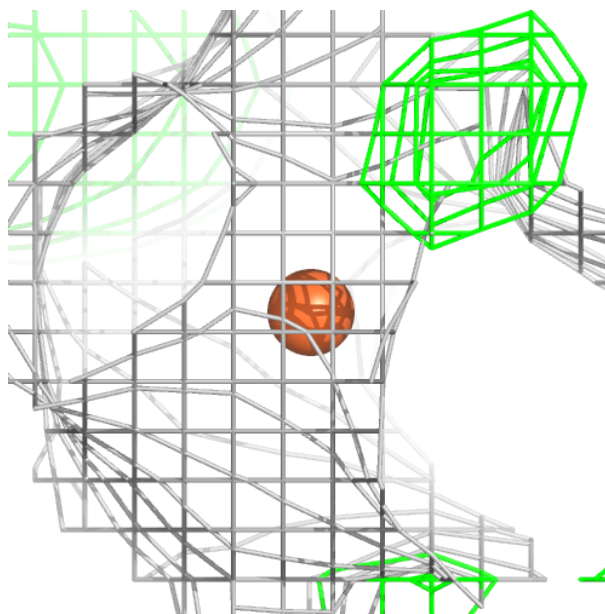
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





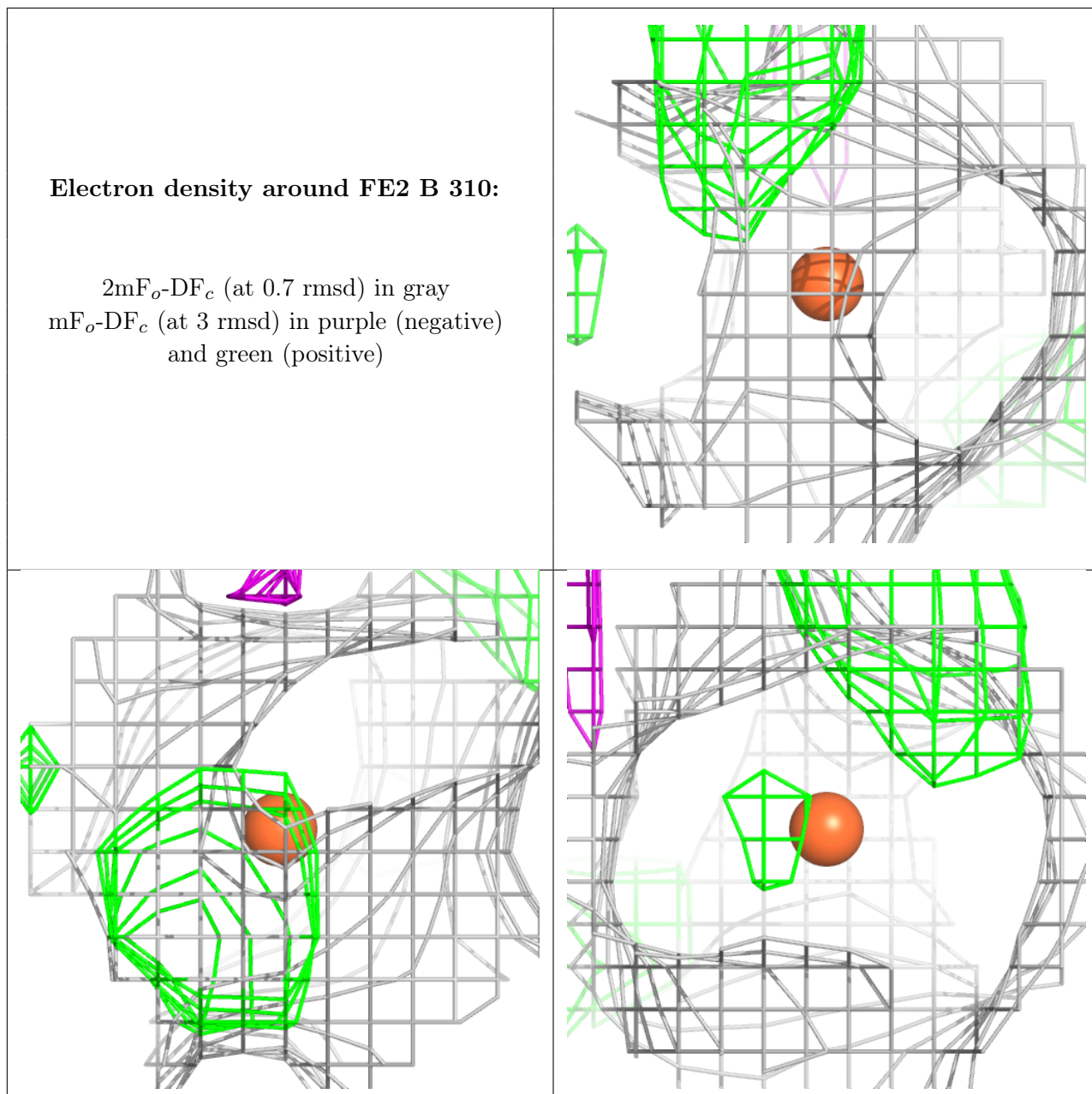
**Electron density around FE2 C 306:**

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



**Electron density around FE2 B 310:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.