



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 10:58 AM EST

PDB ID : 7LVZ  
Title : Crystal structure of ADO  
Authors : Bingman, C.A.; Fernandez, R.L.; Smith, R.W.; Fox, B.G.; Brunold, T.C.  
Deposited on : 2021-02-26  
Resolution : 1.89 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  
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

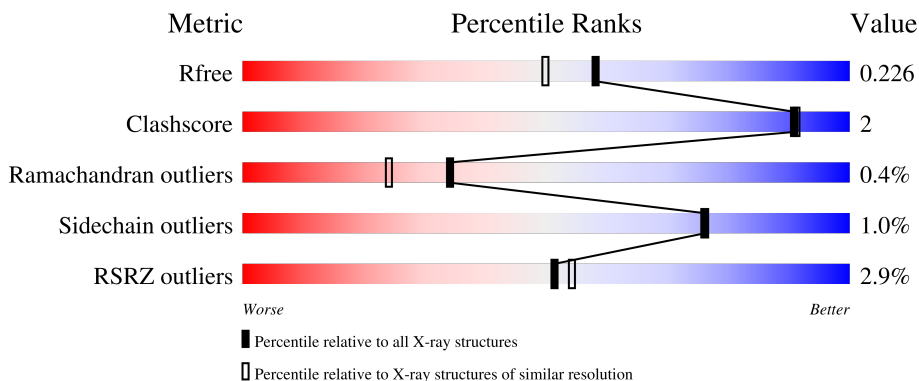
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	256	
1	B	256	
1	C	256	
1	D	256	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15672 atoms, of which 7504 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 2-aminoethanethiol dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	236	3709	1188	1844	328	338	11	0	1	0
1	B	245	3845	1227	1910	343	352	13	0	2	0
1	C	238	3736	1195	1857	331	341	12	0	3	0
1	D	246	3811	1217	1893	338	352	11	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0

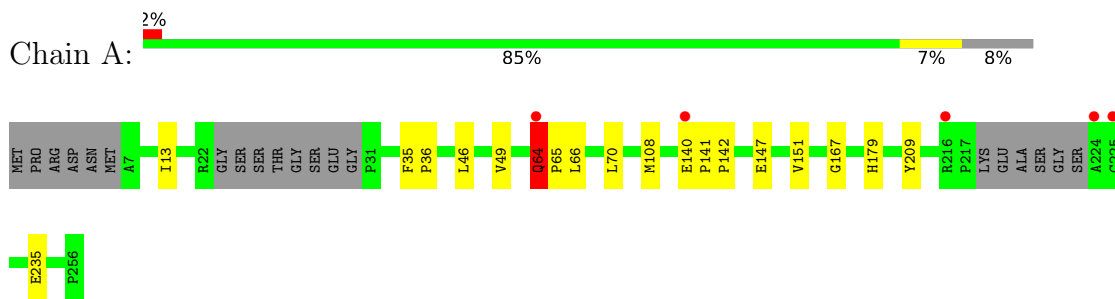
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total 153	O 153	0	3
5	B	196	Total 198	O 198	0	2
5	C	102	Total 103	O 103	0	1
5	D	106	Total 107	O 107	0	1

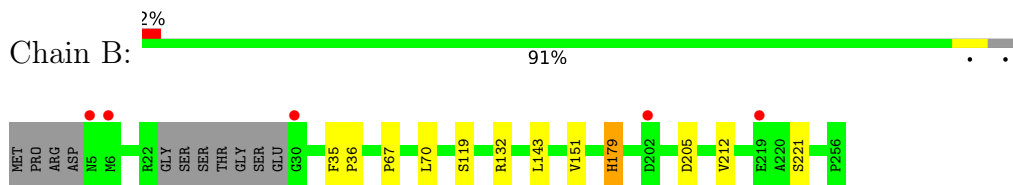
### 3 Residue-property plots [i](#)

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.

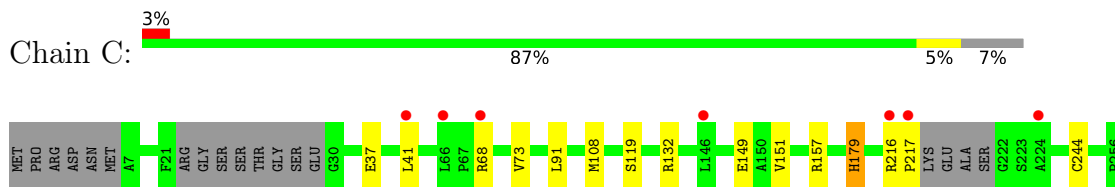
- Molecule 1: 2-aminoethanethiol dioxygenase



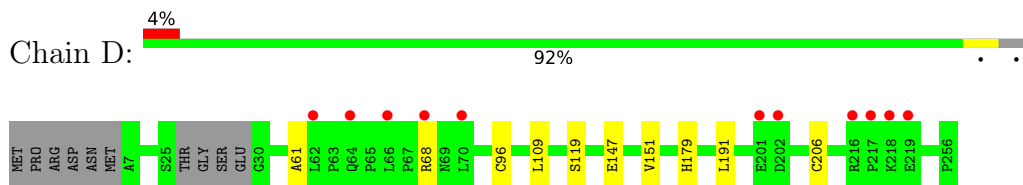
- Molecule 1: 2-aminoethanethiol dioxygenase



- Molecule 1: 2-aminoethanethiol dioxygenase



- Molecule 1: 2-aminoethanethiol dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.30Å 139.53Å 142.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.17 – 1.89 99.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.17-1.89) 83.1 (99.52-1.85)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.86Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.191 , 0.228 0.190 , 0.226	Depositor DCC
$R_{free}$ test set	2519 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: FE2, MG, CL

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	0.46	0/1921	0.61	0/2622
1	B	0.51	0/1992	0.63	0/2717
1	C	0.46	0/1942	0.60	0/2652
1	D	0.42	1/1975 (0.1%)	0.57	0/2695
All	All	0.46	1/7830 (0.0%)	0.60	0/10686

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	CYS	CB-SG	-5.17	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLU	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	1865	1844	1843	9	0
1	B	1935	1910	1910	6	0
1	C	1879	1857	1845	9	0
1	D	1918	1893	1892	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	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	1	0	0	0	0
4	B	1	0	0	0	0
5	A	153	0	0	0	0
5	B	198	0	0	0	0
5	C	103	0	0	1	0
5	D	107	0	0	0	0
All	All	8168	7504	7490	26	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 2.

All (26) 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:A:46:LEU:HD22	1:A:108:MET:HG2	1.75	0.66
1:A:147:GLU:O	1:A:151:VAL:HG23	2.11	0.50
1:A:66:LEU:HD22	1:A:70:LEU:HD22	1.93	0.49
1:B:67:PRO:HD2	1:B:70:LEU:HD12	1.95	0.48
1:C:157:ARG:NH2	5:C:403:HOH:O	2.47	0.48
1:A:64:GLN:N	1:A:65:PRO:CD	2.78	0.47
1:C:216:ARG:HB3	1:C:217:PRO:HD2	1.97	0.46
1:C:132[B]:ARG:NH2	1:C:149:GLU:OE2	2.48	0.46
1:A:46:LEU:HD22	1:A:108:MET:CG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:N	1:B:221:SER:OG	2.49	0.44
1:B:35:PHE:N	1:B:36:PRO:HD2	2.33	0.44
1:C:37:GLU:O	1:C:41:LEU:HD13	2.18	0.44
1:A:209:TYR:CE2	1:A:235:GLU:HG3	2.53	0.44
1:D:147:GLU:O	1:D:151:VAL:HG23	2.19	0.43
1:C:132[A]:ARG:NH1	1:C:151:VAL:O	2.50	0.43
1:D:109:LEU:HA	1:D:191:LEU:O	2.18	0.43
1:A:13:ILE:HD11	1:A:49:VAL:CG2	2.49	0.43
1:C:119:SER:O	1:C:179:HIS:HA	2.19	0.42
1:D:119:SER:O	1:D:179:HIS:HA	2.19	0.42
1:B:143:LEU:HD21	1:B:212:VAL:HG11	2.02	0.42
1:A:35:PHE:N	1:A:36:PRO:HD2	2.34	0.42
1:B:119:SER:O	1:B:179:HIS:HA	2.20	0.42
1:C:91:LEU:HD12	1:C:91:LEU:N	2.35	0.42
1:B:132:ARG:NH1	1:B:151:VAL:O	2.47	0.41
1:C:73:VAL:O	1:C:244:CYS:HA	2.20	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	231/256 (90%)	225 (97%)	3 (1%)	3 (1%)	12	4
1	B	243/256 (95%)	240 (99%)	3 (1%)	0	100	100
1	C	235/256 (92%)	229 (97%)	6 (3%)	0	100	100
1	D	242/256 (94%)	239 (99%)	2 (1%)	1 (0%)	34	24
All	All	951/1024 (93%)	933 (98%)	14 (2%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	PRO
1	D	61	ALA
1	A	64	GLN
1	A	142	PRO

### 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	205/219 (94%)	203 (99%)	2 (1%)	76	76
1	B	212/219 (97%)	210 (99%)	2 (1%)	78	79
1	C	207/219 (94%)	205 (99%)	2 (1%)	76	76
1	D	210/219 (96%)	208 (99%)	2 (1%)	76	76
All	All	834/876 (95%)	826 (99%)	8 (1%)	76	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	179	HIS
1	B	179	HIS
1	B	205	ASP
1	C	68	ARG
1	C	179	HIS
1	D	68	ARG
1	D	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN

### 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 10 ligands modelled in this entry, 10 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

### 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	236/256 (92%)	0.16	5 (2%) 63 66	26, 39, 84, 130	0
1	B	245/256 (95%)	0.13	5 (2%) 65 68	24, 36, 62, 101	0
1	C	238/256 (92%)	0.18	7 (2%) 51 54	28, 43, 74, 113	0
1	D	246/256 (96%)	0.35	11 (4%) 33 36	29, 52, 90, 118	0
All	All	965/1024 (94%)	0.21	28 (2%) 51 54	24, 42, 79, 130	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	LYS	4.6
1	A	224	ALA	4.2
1	D	66	LEU	4.2
1	D	217	PRO	3.3
1	D	62	LEU	3.2
1	C	146	LEU	3.1
1	D	219	GLU	3.1
1	D	70	LEU	2.9
1	D	201	GLU	2.9
1	B	30	GLY	2.7
1	A	216	ARG	2.7
1	B	5	ASN	2.7
1	B	202	ASP	2.6
1	C	216	ARG	2.6
1	C	224	ALA	2.5
1	C	66	LEU	2.5
1	D	64	GLN	2.4
1	B	6	MET	2.3
1	B	219	GLU	2.3
1	D	202	ASP	2.3
1	C	41	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	217	PRO	2.3
1	C	68	ARG	2.2
1	A	140	GLU	2.2
1	A	64	GLN	2.2
1	D	68	ARG	2.0
1	D	216	ARG	2.0
1	A	225	CYS	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](#)

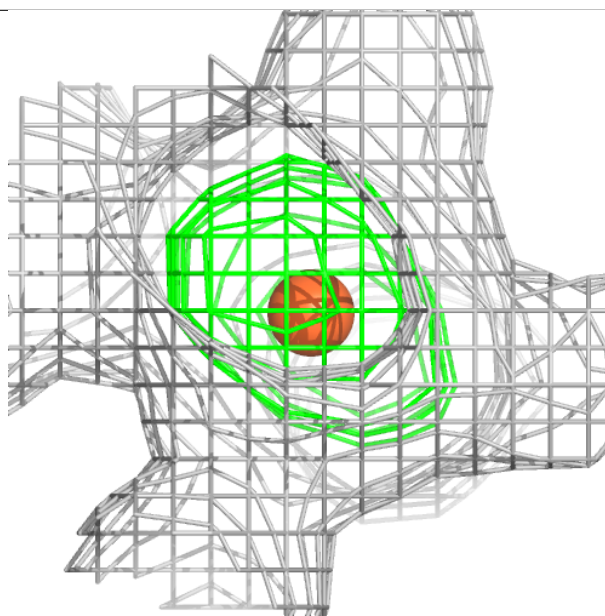
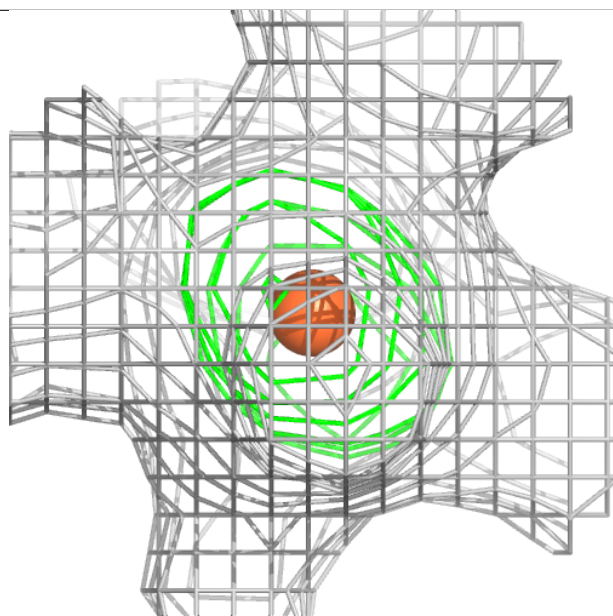
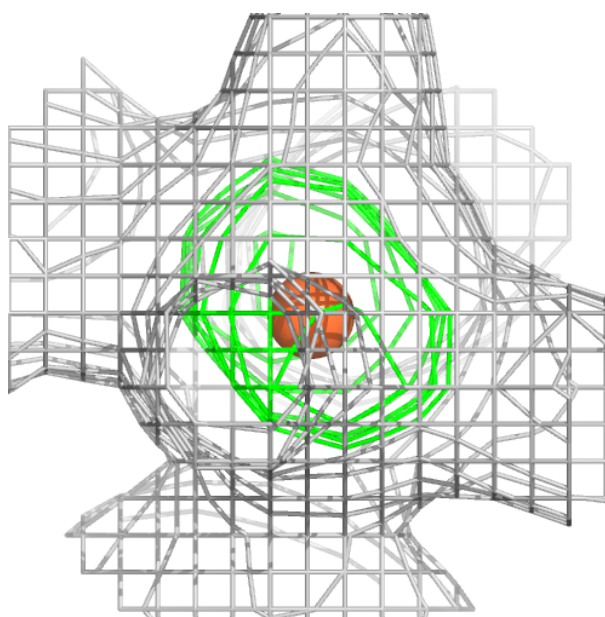
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CL	D	302	1/1	0.88	0.12	70,70,70,70	0
4	MG	B	303	1/1	0.93	0.05	58,58,58,58	0
3	CL	C	302	1/1	0.97	0.10	47,47,47,47	0
3	CL	A	302	1/1	0.98	0.08	42,42,42,42	0
2	FE2	D	301	1/1	0.99	0.23	42,42,42,42	0
2	FE2	C	301	1/1	0.99	0.17	31,31,31,31	0
4	MG	A	303	1/1	0.99	0.05	42,42,42,42	0
3	CL	B	302	1/1	0.99	0.10	35,35,35,35	0
2	FE2	A	301	1/1	1.00	0.17	30,30,30,30	0
2	FE2	B	301	1/1	1.00	0.16	26,26,26,26	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.

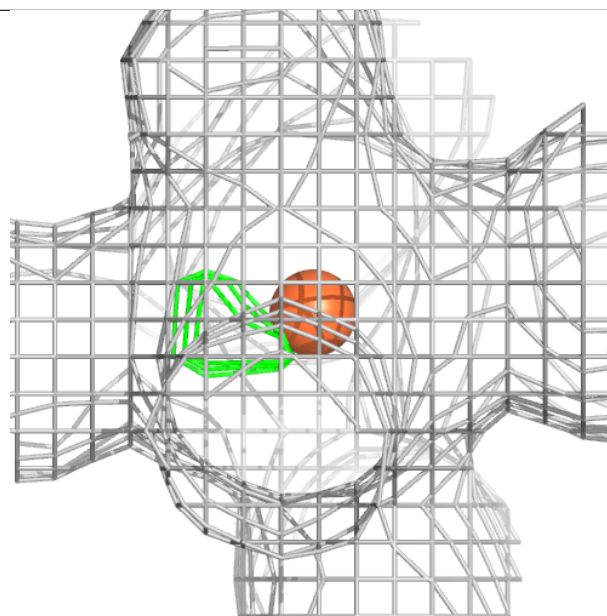
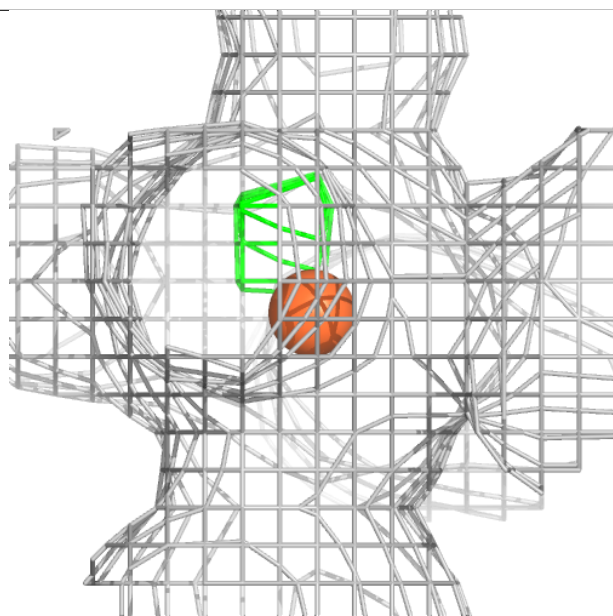
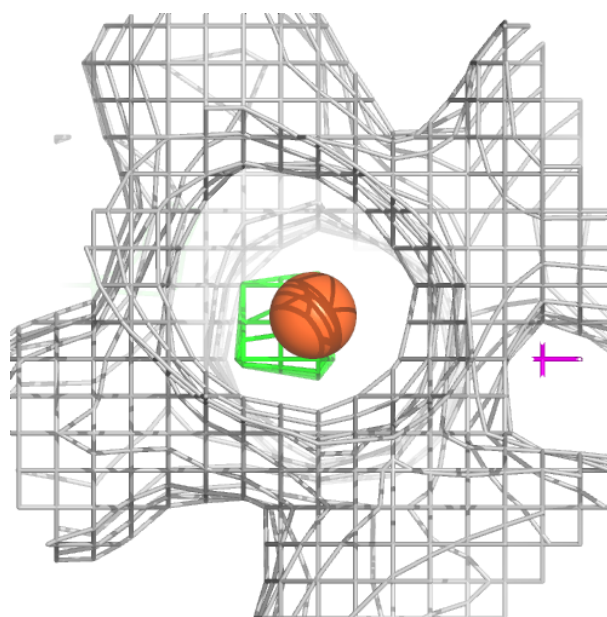
**Electron density around FE2 D 301:**

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



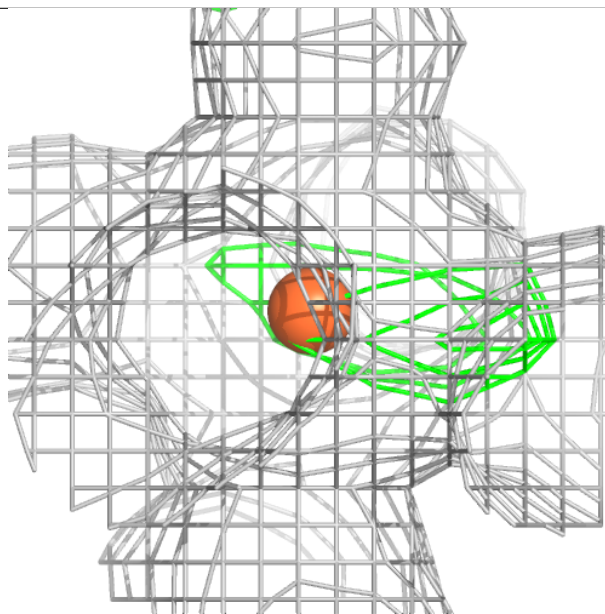
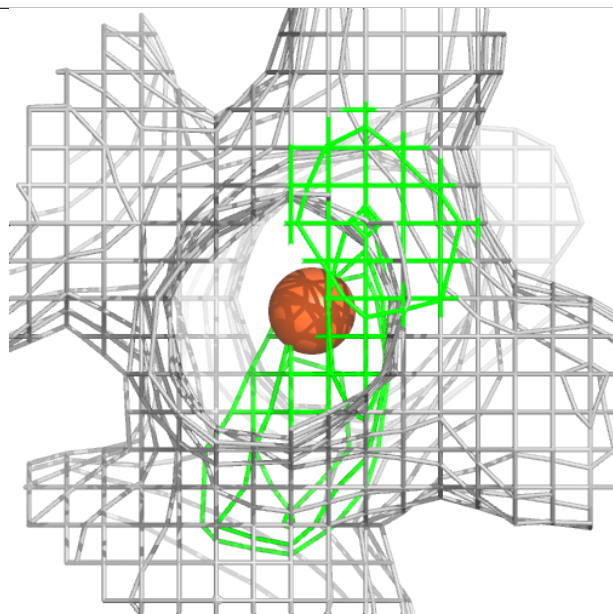
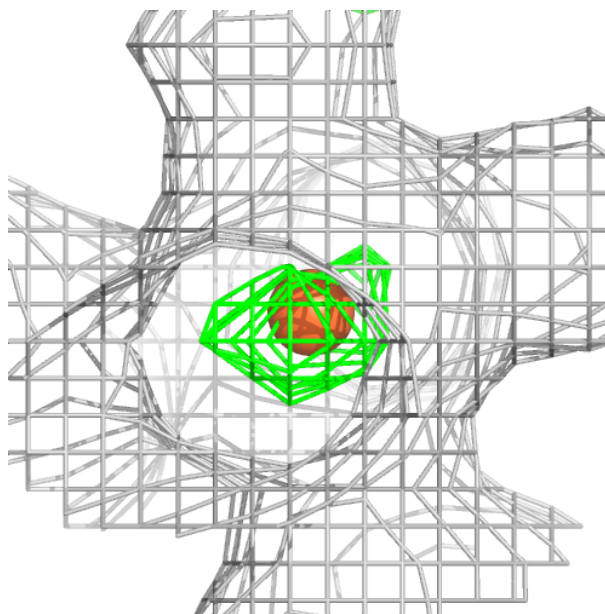
**Electron density around FE2 C 301:**

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

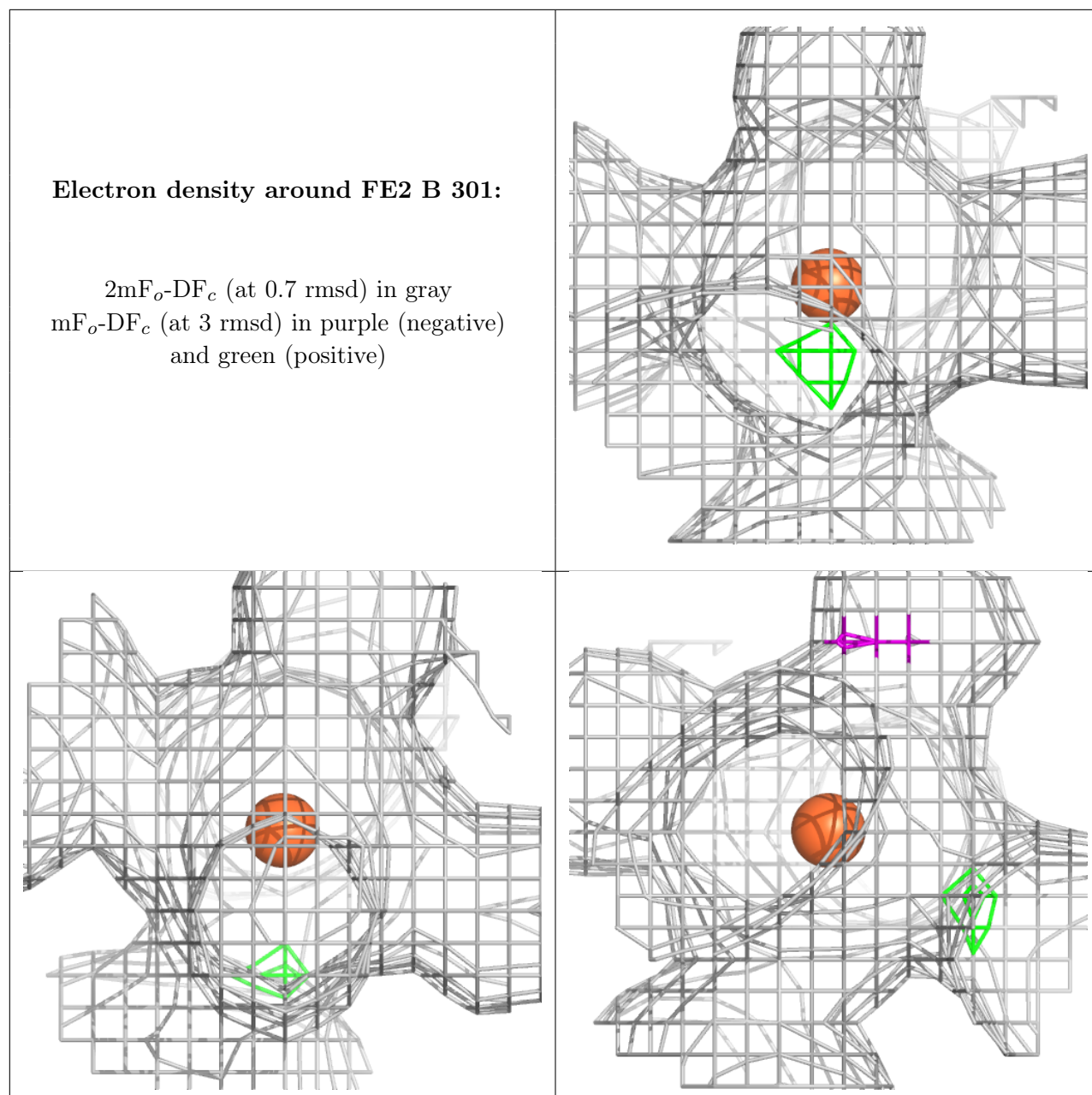


**Electron density around FE2 A 301:**

$2mF_o-DF_c$  (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.