

wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 08:02 pm GMT

PDB ID : 6ZMA

Title: Structure of the tRNA-Monooxygenase enzyme MiaE frozen under 140 bar of

krypton using the soak and freeze methodology

Authors : Carpentier, P.; Atta, M.

Deposited on : 2020-07-02

Resolution : 2.15 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:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

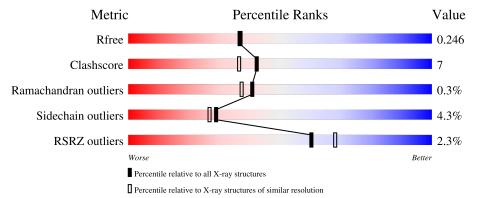
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	В	205	85%	9%	•	-	
1	С	205	84%	11%	•	-	

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
8	KR	В	311	-	-	X	-
8	KR	С	308	-	-	X	-
8	KR	С	309	-	-	-	X



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 3483 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 tRNA hydroxylase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	В	199	Total 1589	C 1007	N 286	O 289	S 7	15	3	0
1	С	199	Total 1579	C 1003	N 284	O 284	S 8	7	2	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Fe 2 2	0	0
2	С	2	Total Fe 2 2	0	0

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

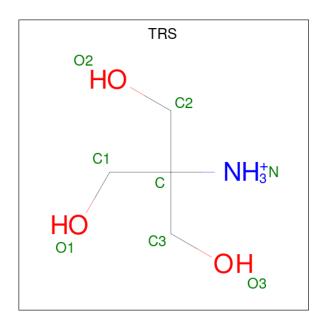
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Cl 1 1	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	2	Total Ca 2 2	0	0

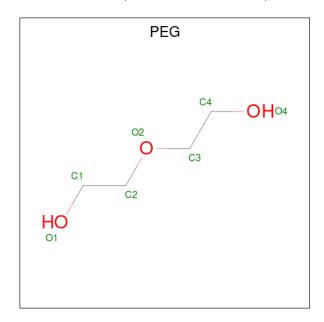
• Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
5	В	1	Total 8		N 1		0	0
5	С	1	Total 8	C 4	N 1	O 3	0	0

 $\bullet \ \ Molecule \ 6 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 7 4 3	0	0
6	В	1	Total C O 7 4 3	0	0

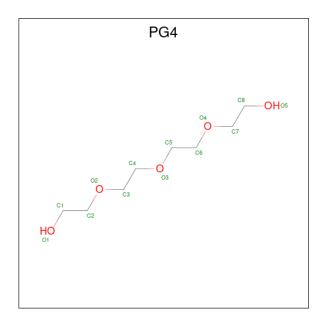
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 7 4 3	0	0
6	С	1	Total C O 7 4 3	0	0
6	С	1	Total C O 7 4 3	0	0
6	С	1	Total C O 7 4 3	0	0
6	С	1	Total C O 7 4 3	0	0

• Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



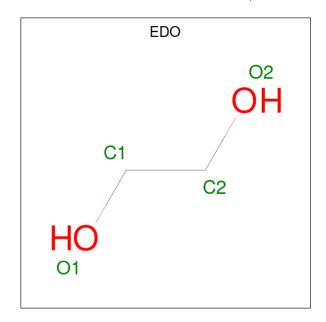
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total C O 13 8 5	0	0

• Molecule 8 is KRYPTON (three-letter code: KR) (formula: Kr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	2	Total Kr 2 2	0	0
8	С	4	Total Kr 4 4	0	0



 \bullet Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total C O 4 2 2	0	0
9	С	1	Total C O 4 2 2	0	0
9	С	1	Total C O 4 2 2	0	0

• Molecule 10 is water.

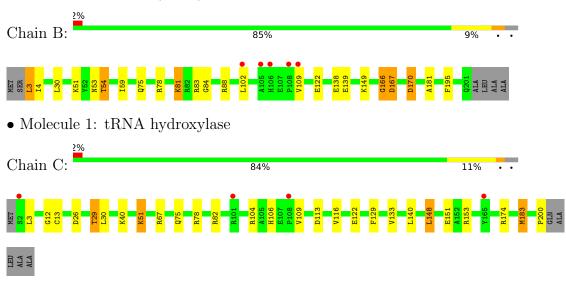
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	97	Total O 97 97	0	0
10	С	115	Total O 115 115	0	0



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: tRNA hydroxylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	117.62Å 52.30Å 79.41Å	Depositor
a, b, c, α , β , γ	90.00° 90.74° 90.00°	Depositor
Resolution (Å)	79.40 - 2.15	Depositor
resolution (A)	47.79 - 2.15	EDS
% Data completeness	94.6 (79.40-2.15)	Depositor
(in resolution range)	94.6 (47.79-2.15)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.09 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
Ρ. Р.	0.180 , 0.244	Depositor
R, R_{free}	0.189 , 0.246	DCC
R_{free} test set	1290 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 60.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3483	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: PEG, FE, PG4, KR, CA, TRS, EDO, 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		Bo	nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	В	1.83	$13/1621 \ (0.8\%)$	1.97	11/2195 (0.5%)
1	С	1.47	5/1611 (0.3%)	2.50	6/2178 (0.3%)
All	All	1.66	$18/3232 \ (0.6\%)$	2.25	17/4373 (0.4%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(A)
1	В	149	LYS	CE-NZ	-50.79	0.22	1.49
1	С	82	ARG	CZ-NH2	-44.08	0.75	1.33
1	В	78	ARG	CD-NE	-27.67	0.99	1.46
1	С	51	LYS	CE-NZ	-26.27	0.83	1.49
1	В	149	LYS	CD-CE	-24.31	0.90	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	82	ARG	NE-CZ-NH2	-73.55	83.53	120.30
1	С	82	ARG	NE-CZ-NH1	-73.27	83.66	120.30
1	В	170	ASP	CB-CG-OD1	-60.12	64.20	118.30
1	В	170	ASP	CB-CG-OD2	51.48	164.63	118.30
1	С	82	ARG	NH1-CZ-NH2	32.43	155.07	119.40



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	166	GLY	Peptide

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	В	1589	0	1582	15	0
1	С	1579	0	1577	20	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	В	1	0	0	0	0
4	В	2	0	0	1	0
5	В	8	0	11	2	0
5	С	8	0	11	5	0
6	В	21	0	30	0	0
6	С	28	0	40	3	0
7	В	13	0	18	0	0
8	В	2	0	0	5	0
8	С	4	0	0	6	0
9	В	4	0	6	1	0
9	С	8	0	12	1	0
10	В	97	0	0	5	0
10	С	115	0	0	9	1
All	All	3483	0	3287	45	1

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 7.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:200:PRO:HG3	10:C:441:HOH:O	1.52	1.05
6:C:305:PEG:O2	10:C:402:HOH:O	1.78	1.01
1:B:84:GLY:O	10:B:403:HOH:O	1.83	0.96

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Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
4:B:305:CA:CA	10:B:403:HOH:O	1.45	0.92
1:C:40:LYS:NZ	10:C:403:HOH:O	2.12	0.82

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
10:C:425:HOH:O	10:C:446:HOH:O[4_546]	1.56	0.64

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	entiles
1	В	200/205~(98%)	196 (98%)	3 (2%)	1 (0%)	29	22
1	C	199/205~(97%)	195 (98%)	4 (2%)	0	100	100
All	All	399/410 (97%)	391 (98%)	7 (2%)	1 (0%)	41	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	167	ASP

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	В	164/169 (97%)	155 (94%)	9 (6%)	21 17		
1	С	163/169 (96%)	156 (96%)	7 (4%)	29 27		
All	All	327/338 (97%)	311 (95%)	16 (5%)	29 21		

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	183[A]	MET
1	С	148	LEU
1	В	170	ASP
1	С	140	LEU
1	В	139	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	53	ASN
1	С	75	GLN
1	С	156	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 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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	Trno	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	С	304	-	6,6,6	0.43	0	5,5,5	0.46	0
6	PEG	В	308	-	6,6,6	0.49	0	5,5,5	0.49	0
6	PEG	В	307	-	6,6,6	0.53	0	5,5,5	0.56	0
5	TRS	С	303	2	7,7,7	0.47	0	9,9,9	0.71	0
6	PEG	С	306	-	6,6,6	0.50	0	5,5,5	0.45	0
9	EDO	С	312	-	3,3,3	0.47	0	2,2,2	0.36	0
5	TRS	В	306	2	7,7,7	0.38	0	9,9,9	0.65	0
6	PEG	С	305	-	6,6,6	0.55	0	5,5,5	0.65	0
9	EDO	С	313	-	3,3,3	0.62	0	2,2,2	0.50	0
6	PEG	В	309	-	6,6,6	0.49	0	5,5,5	0.73	0
9	EDO	В	313	-	3,3,3	0.42	0	2,2,2	0.32	0
7	PG4	В	310	-	12,12,12	0.50	0	11,11,11	0.66	0
6	PEG	С	307	-	6,6,6	0.58	0	5,5,5	0.73	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	PEG	С	304	-	-	2/4/4/4	-
6	PEG	В	308	-	-	1/4/4/4	-
6	PEG	В	307	-	-	3/4/4/4	-
5	TRS	С	303	2	-	3/9/9/9	-
6	PEG	С	306	-	-	1/4/4/4	-
9	EDO	С	312	-	-	1/1/1/1	-
5	TRS	В	306	2	-	5/9/9/9	-
6	PEG	С	305	-	-	3/4/4/4	-
9	EDO	С	313	-	-	1/1/1/1	-
6	PEG	В	309	-	-	2/4/4/4	-
9	EDO	В	313	-	-	1/1/1/1	
7	PG4	В	310	-	-	7/10/10/10	-
6	PEG	С	307	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	306	TRS	C1-C-C2-O2
5	В	306	TRS	C3-C-C2-O2
5	В	306	TRS	N-C-C2-O2
7	В	310	PG4	O2-C3-C4-O3
6	В	309	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	303	TRS	5	0
5	В	306	TRS	2	0
6	С	305	PEG	3	0
9	С	313	EDO	1	0
9	В	313	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (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>	>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	В	199/205 (97%)	0.03	5 (2%) 57	65	31, 46, 75, 92	5 (2%)
1	С	199/205~(97%)	0.06	4 (2%) 65	72	31, 43, 71, 100	4 (2%)
All	All	398/410 (97%)	0.05	9 (2%) 60	68	31, 45, 72, 100	9 (2%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	109	VAL	3.7
1	В	106	HIS	3.4
1	С	2	SER	2.9
1	В	105	ALA	2.6
1	В	108	PRO	2.6

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)

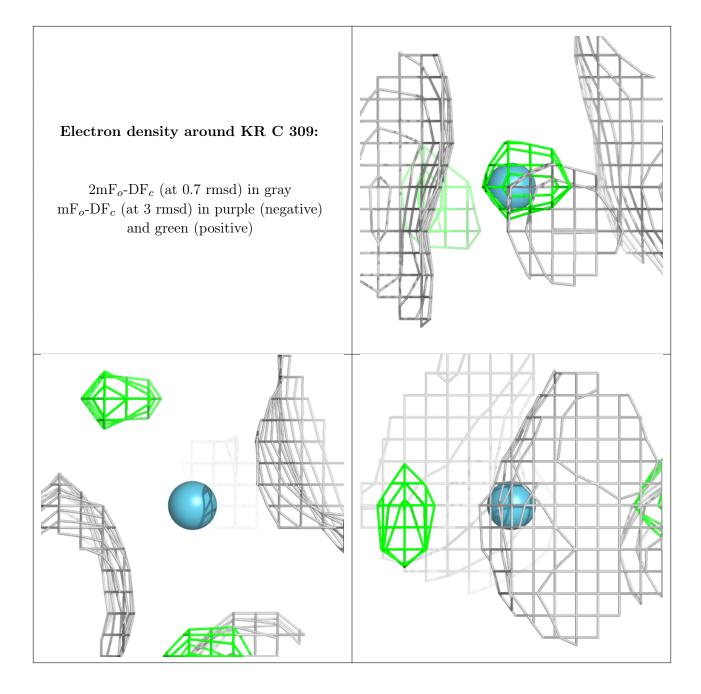
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



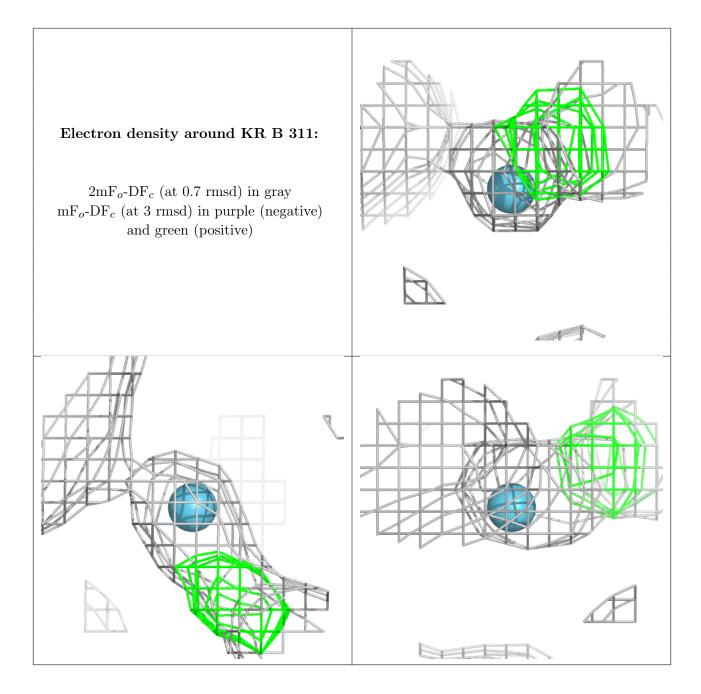
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
8	KR	С	309	1/1	0.24	0.83	43,43,43,43	1
9	EDO	В	313	4/4	0.49	0.20	87,89,89,90	0
6	PEG	В	307	7/7	0.56	0.25	70,77,83,84	0
6	PEG	С	307	7/7	0.67	0.16	64,68,74,74	0
6	PEG	В	308	7/7	0.68	0.23	62,66,70,70	0
6	PEG	С	306	7/7	0.71	0.20	63,67,70,72	0
4	CA	В	305	1/1	0.73	0.21	118,118,118,118	1
8	KR	В	311	1/1	0.77	0.17	50,50,50,50	1
6	PEG	В	309	7/7	0.79	0.16	68,69,74,75	0
5	TRS	В	306	8/8	0.79	0.20	48,58,60,64	0
6	PEG	С	305	7/7	0.80	0.17	72,81,83,83	0
7	PG4	В	310	13/13	0.83	0.17	55,59,67,68	0
9	EDO	С	312	4/4	0.83	0.21	76,76,77,77	0
8	KR	С	308	1/1	0.87	0.19	48,48,48,48	1
9	EDO	С	313	4/4	0.88	0.14	62,65,65,67	0
6	PEG	С	304	7/7	0.89	0.14	63,67,68,70	0
5	TRS	С	303	8/8	0.90	0.21	39,58,61,71	0
8	KR	С	311	1/1	0.93	0.18	49,49,49,49	1
8	KR	В	312	1/1	0.94	0.16	35,35,35,35	1
2	FE	В	302	1/1	0.96	0.06	53,53,53,53	0
2	FE	В	301	1/1	0.97	0.09	47,47,47,47	0
8	KR	С	310	1/1	0.97	0.27	49,49,49,49	1
3	CL	В	303	1/1	0.98	0.10	45,45,45,45	0
2	FE	С	302	1/1	0.99	0.05	49,49,49,49	0
2	FE	С	301	1/1	0.99	0.11	40,40,40,40	0
4	CA	В	304	1/1	1.00	0.14	42,42,42,42	0

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

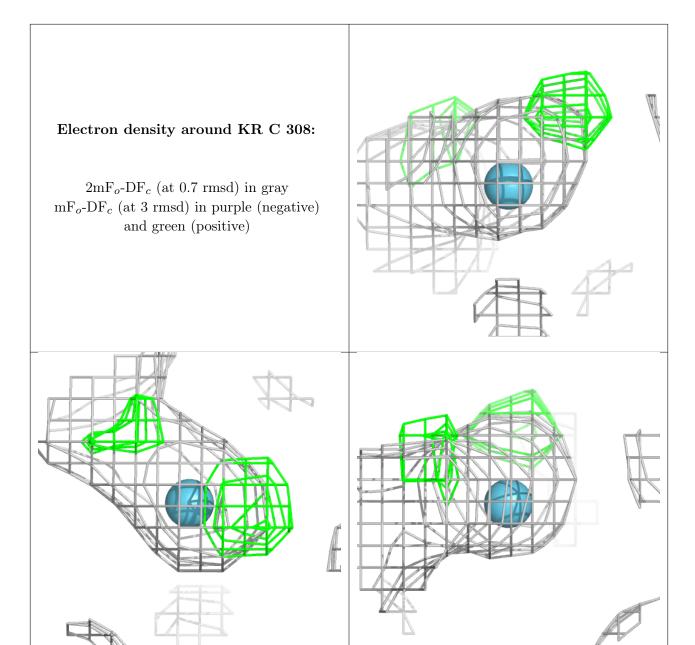




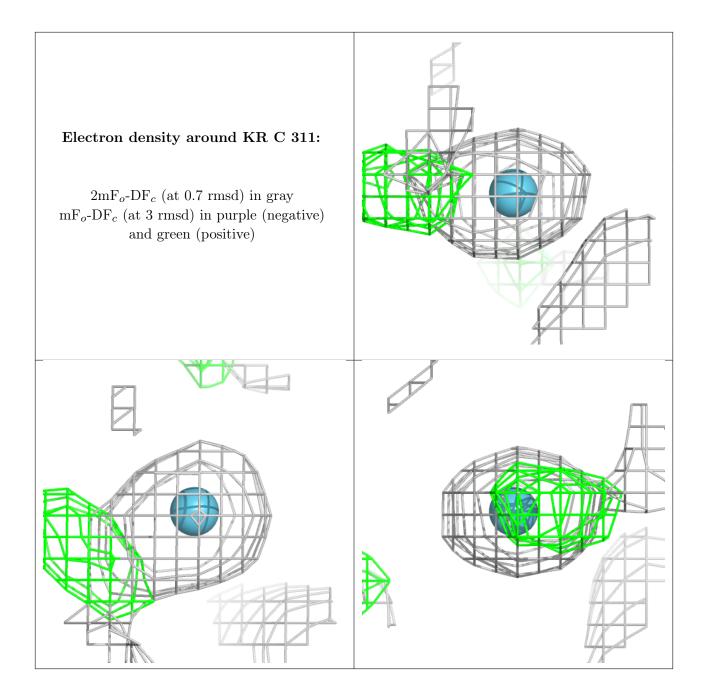




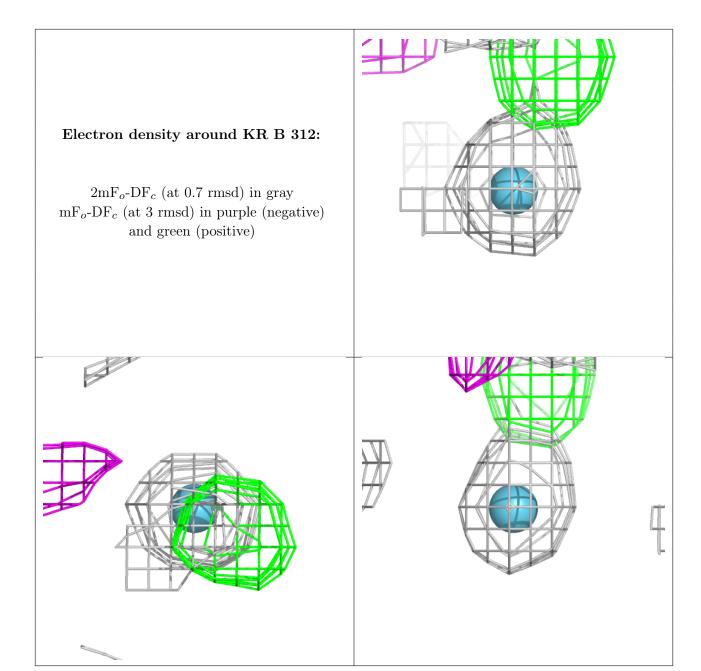




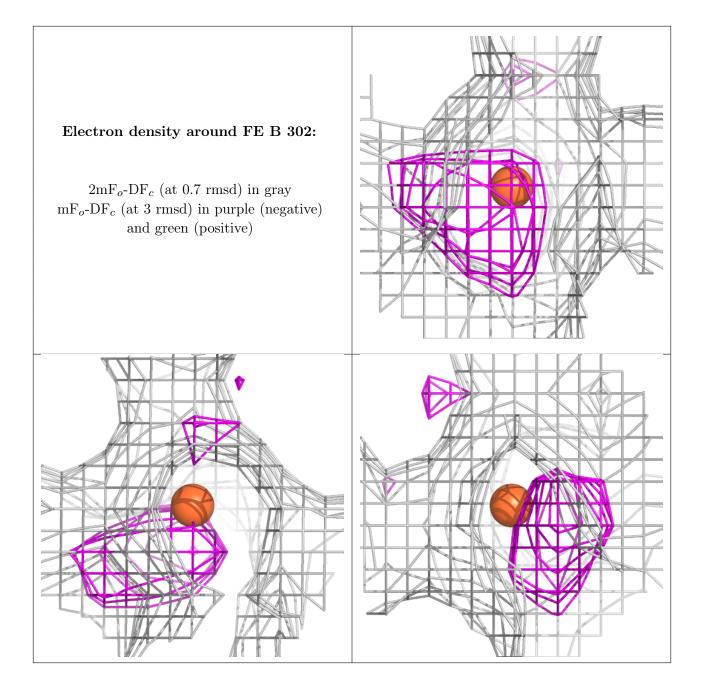












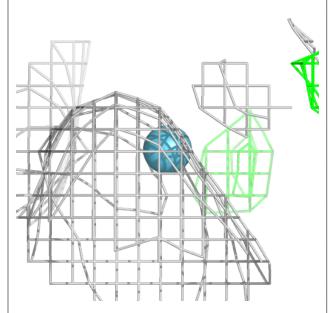


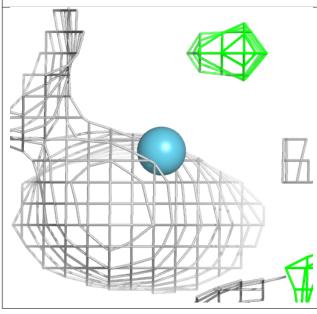
Electron density around FE B 301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)

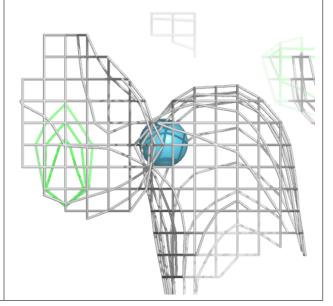


Electron density around KR C 310:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



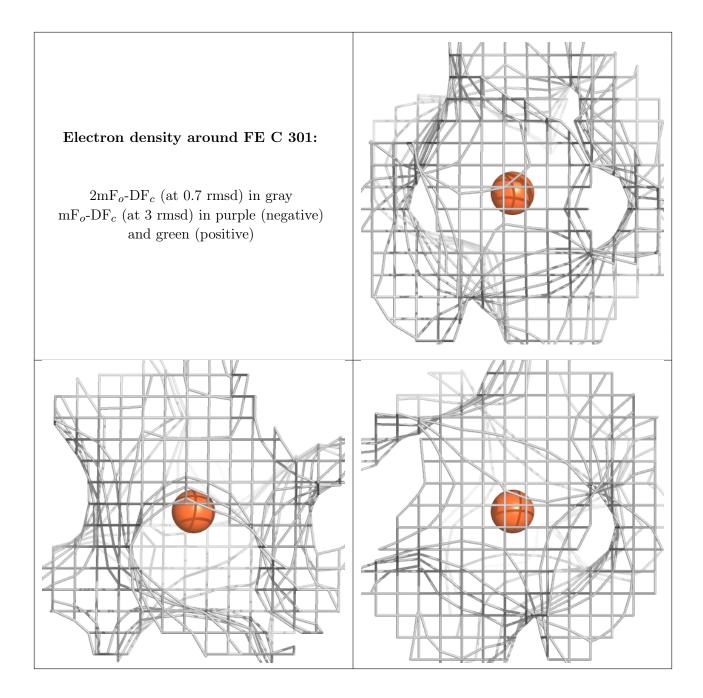






Electron density around FE C 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

