



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 12:32 PM BST

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 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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

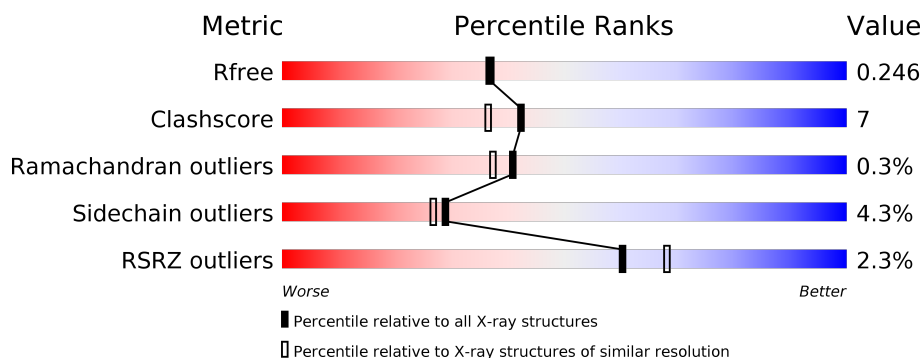
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 on 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	B	205	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	205	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </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
8	KR	B	311	-	-	X	-
8	KR	C	308	-	-	X	-
8	KR	C	309	-	-	-	X

## 2 Entry composition

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	B	199	Total	C	N	O	S	15	3	0
			1589	1007	286	289	7			
1	C	199	Total	C	N	O	S	7	2	0
			1579	1003	284	284	8			

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



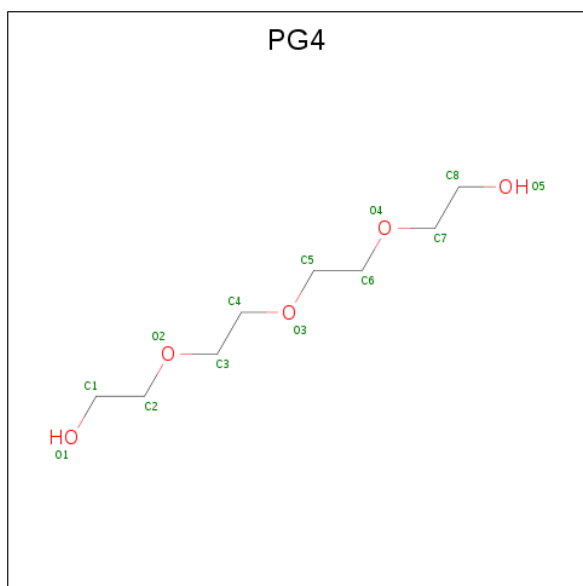
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Kr	0	0
			2	2		
8	C	4	Total	Kr	0	0
			4	4		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

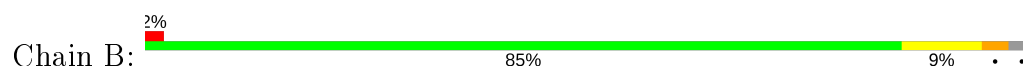
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	97	Total	O	0	0
			97	97		
10	C	115	Total	O	0	0
			115	115		

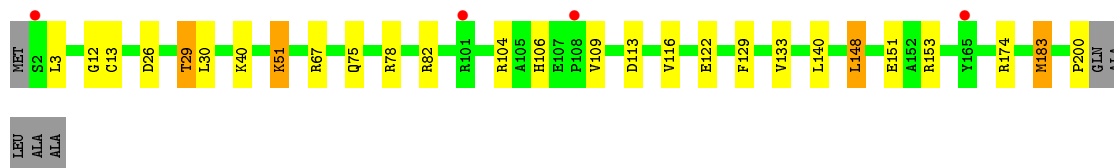
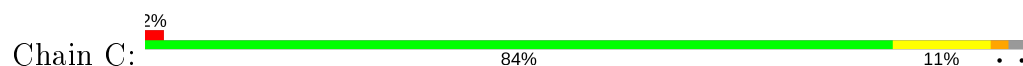
### 3 Residue-property plots [i](#)

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



- Molecule 1: tRNA hydroxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.62Å 52.30Å 79.41Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	79.40 – 2.15 47.79 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (79.40-2.15) 94.6 (47.79-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.180 , 0.244 0.189 , 0.246	Depositor DCC
$R_{free}$ test set	1290 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<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: CL, CA, EDO, KR, PG4, FE, TRS, PEG

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	B	1.83	13/1621 (0.8%)	1.97	11/2195 (0.5%)
1	C	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 mainchain group or atoms of a sidechain that are expected to be planar.

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	LYS	CE-NZ	-50.79	0.22	1.49
1	C	82	ARG	CZ-NH2	-44.08	0.75	1.33
1	B	78	ARG	CD-NE	-27.67	0.99	1.46
1	C	51	LYS	CE-NZ	-26.27	0.83	1.49
1	B	149	LYS	CD-CE	-24.31	0.90	1.51
1	B	81	LYS	CG-CD	-18.34	0.90	1.52
1	C	51	LYS	CD-CE	-12.42	1.20	1.51
1	B	78	ARG	NE-CZ	-11.16	1.18	1.33
1	B	78	ARG	CZ-NH1	-10.75	1.19	1.33
1	C	51	LYS	CG-CD	-10.56	1.16	1.52
1	B	78	ARG	CZ-NH2	-9.47	1.20	1.33
1	B	149	LYS	CB-CG	-8.65	1.29	1.52
1	B	170	ASP	CG-OD1	-8.14	1.06	1.25
1	B	81	LYS	CE-NZ	-7.52	1.30	1.49
1	B	170	ASP	CB-CG	-7.38	1.36	1.51
1	B	170	ASP	CG-OD2	-6.12	1.11	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	HIS	CG-CD2	-6.02	1.25	1.35
1	B	51	LYS	CG-CD	5.43	1.71	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ARG	NE-CZ-NH2	-73.55	83.53	120.30
1	C	82	ARG	NE-CZ-NH1	-73.27	83.66	120.30
1	B	170	ASP	CB-CG-OD1	-60.12	64.20	118.30
1	B	170	ASP	CB-CG-OD2	51.48	164.63	118.30
1	C	82	ARG	NH1-CZ-NH2	32.43	155.07	119.40
1	B	78	ARG	CD-NE-CZ	17.78	148.50	123.60
1	C	51	LYS	CG-CD-CE	16.01	159.93	111.90
1	C	51	LYS	CD-CE-NZ	14.04	144.00	111.70
1	B	78	ARG	CG-CD-NE	12.40	137.85	111.80
1	B	81	LYS	CG-CD-CE	11.22	145.55	111.90
1	B	81	LYS	CB-CG-CD	10.61	139.19	111.60
1	B	149	LYS	CB-CG-CD	9.64	136.65	111.60
1	B	170	ASP	CA-CB-CG	9.41	134.10	113.40
1	B	51	LYS	CB-CG-CD	-6.34	95.11	111.60
1	B	83	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	67	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	83	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	GLY	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	B	1589	0	1582	15	0
1	C	1579	0	1577	20	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
3	B	1	0	0	0	0
4	B	2	0	0	1	0
5	B	8	0	11	2	0
5	C	8	0	11	5	0
6	B	21	0	30	0	0
6	C	28	0	40	3	0
7	B	13	0	18	0	0
8	B	2	0	0	5	0
8	C	4	0	0	6	0
9	B	4	0	6	1	0
9	C	8	0	12	1	0
10	B	97	0	0	5	0
10	C	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.

All (45) 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: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
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
1:C:30:LEU:HD23	8:C:311:KR:KR	2.46	0.77
5:C:303:TRS:N	8:C:308:KR:KR	2.82	0.73
1:B:166:GLY:O	10:B:404:HOH:O	2.06	0.72
1:C:200:PRO:CG	10:C:441:HOH:O	2.25	0.68
1:C:104:ARG:NH1	10:C:406:HOH:O	2.28	0.67
5:C:303:TRS:HN3	8:C:308:KR:KR	2.39	0.66
1:B:195:PHE:CD2	8:B:311:KR:KR	3.11	0.65
1:C:122:GLU:OE1	1:C:151:GLU:OE2	2.14	0.65
1:B:54:THR:OG1	10:B:405:HOH:O	2.15	0.64
1:C:26:ASP:CG	1:C:29:THR:HG23	2.21	0.61
1:C:26:ASP:OD2	1:C:29:THR:HG23	2.01	0.61
6:C:305:PEG:C2	10:C:402:HOH:O	2.41	0.60
1:C:26:ASP:OD2	1:C:29:THR:CG2	2.51	0.58
5:C:303:TRS:H31	8:C:308:KR:KR	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	8:B:312:KR:KR	2.65	0.57
1:B:54:THR:HG22	10:B:465:HOH:O	2.06	0.55
1:C:3:LEU:O	1:C:3:LEU:HD12	2.06	0.54
1:C:12:GLY:O	1:C:183[A]:MET:CE	2.56	0.54
5:C:303:TRS:HN1	8:C:308:KR:KR	2.52	0.53
1:C:129:PHE:O	1:C:133:VAL:HG13	2.10	0.52
9:C:313:EDO:O1	10:C:404:HOH:O	2.18	0.52
5:C:303:TRS:C3	8:C:308:KR:KR	3.21	0.50
5:B:306:TRS:N	8:B:311:KR:KR	3.05	0.50
1:B:195:PHE:CE2	8:B:311:KR:KR	3.27	0.49
1:C:13:CYS:HB3	1:C:183[A]:MET:HE2	1.93	0.49
1:C:153:ARG:NH1	10:C:408:HOH:O	2.44	0.48
1:C:104:ARG:HG3	1:C:113:ASP:OD2	2.13	0.48
1:B:102:LEU:HD11	1:B:181:ALA:CB	2.44	0.48
1:B:102:LEU:HD11	1:B:181:ALA:HB3	1.96	0.48
1:C:148:LEU:C	1:C:148:LEU:HD12	2.36	0.46
1:C:104:ARG:HH21	1:C:109:VAL:HG21	1.81	0.46
1:B:3:LEU:HD22	1:B:4:ILE:H	1.80	0.46
1:B:166:GLY:CA	1:B:167:ASP:HB2	2.46	0.46
1:C:75:GLN:HE22	6:C:305:PEG:C2	2.28	0.45
1:C:200:PRO:CD	10:C:441:HOH:O	2.62	0.45
1:B:53:ASN:HA	1:B:59:ILE:HD11	2.00	0.44
1:B:75:GLN:HG2	9:B:313:EDO:H21	2.01	0.42
1:B:122:GLU:OE2	5:B:306:TRS:O2	2.37	0.42
1:B:195:PHE:CG	8:B:311:KR:KR	3.35	0.41
1:C:116:VAL:HG11	1:C:174:ARG:HG3	2.02	0.41

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	Interatomic distance (Å)	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	Percentiles	
1	B	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	B	167	ASP

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

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	LEU
1	B	54	THR
1	B	81	LYS
1	B	88[A]	ARG
1	B	88[B]	ARG
1	B	109	VAL
1	B	138	GLU
1	B	139	GLU
1	B	170	ASP
1	C	29	THR
1	C	51	LYS
1	C	78	ARG

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Mol	Chain	Res	Type
1	C	140	LEU
1	C	148	LEU
1	C	183[A]	MET
1	C	183[B]	MET

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

Mol	Chain	Res	Type
1	C	53	ASN
1	C	75	GLN
1	C	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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	EDO	B	313	-	3,3,3	0.42	0	2,2,2	0.32	0
6	PEG	C	304	-	6,6,6	0.43	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	C	313	-	3,3,3	0.62	0	2,2,2	0.50	0
6	PEG	B	308	-	6,6,6	0.49	0	5,5,5	0.49	0
6	PEG	C	306	-	6,6,6	0.50	0	5,5,5	0.45	0
6	PEG	C	307	-	6,6,6	0.58	0	5,5,5	0.73	0
5	TRS	C	303	2	7,7,7	0.47	0	9,9,9	0.71	0
6	PEG	B	307	-	6,6,6	0.53	0	5,5,5	0.56	0
9	EDO	C	312	-	3,3,3	0.47	0	2,2,2	0.36	0
6	PEG	B	309	-	6,6,6	0.49	0	5,5,5	0.73	0
6	PEG	C	305	-	6,6,6	0.55	0	5,5,5	0.65	0
7	PG4	B	310	-	12,12,12	0.50	0	11,11,11	0.66	0
5	TRS	B	306	2	7,7,7	0.38	0	9,9,9	0.65	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
9	EDO	B	313	-	-	1/1/1/1	-
6	PEG	C	304	-	-	2/4/4/4	-
9	EDO	C	313	-	-	1/1/1/1	-
6	PEG	B	308	-	-	1/4/4/4	-
6	PEG	C	306	-	-	1/4/4/4	-
6	PEG	C	307	-	-	2/4/4/4	-
5	TRS	C	303	2	-	3/9/9/9	-
6	PEG	B	307	-	-	3/4/4/4	-
9	EDO	C	312	-	-	1/1/1/1	-
6	PEG	B	309	-	-	2/4/4/4	-
6	PEG	C	305	-	-	3/4/4/4	-
7	PG4	B	310	-	-	7/10/10/10	-
5	TRS	B	306	2	-	5/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	306	TRS	C1-C-C2-O2

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms
5	B	306	TRS	C3-C-C2-O2
5	B	306	TRS	N-C-C2-O2
7	B	310	PG4	O2-C3-C4-O3
6	B	309	PEG	O1-C1-C2-O2
6	C	305	PEG	O2-C3-C4-O4
7	B	310	PG4	O4-C7-C8-O5
7	B	310	PG4	O3-C5-C6-O4
6	C	304	PEG	O1-C1-C2-O2
6	C	307	PEG	O1-C1-C2-O2
6	B	309	PEG	O2-C3-C4-O4
6	B	307	PEG	O2-C3-C4-O4
6	C	305	PEG	O1-C1-C2-O2
6	B	308	PEG	O1-C1-C2-O2
6	C	304	PEG	O2-C3-C4-O4
5	C	303	TRS	C1-C-C3-O3
6	C	306	PEG	O2-C3-C4-O4
9	B	313	EDO	O1-C1-C2-O2
6	B	307	PEG	O1-C1-C2-O2
9	C	313	EDO	O1-C1-C2-O2
6	C	307	PEG	C4-C3-O2-C2
7	B	310	PG4	C5-C6-O4-C7
7	B	310	PG4	C8-C7-O4-C6
5	B	306	TRS	N-C-C3-O3
5	C	303	TRS	N-C-C3-O3
6	C	305	PEG	C1-C2-O2-C3
9	C	312	EDO	O1-C1-C2-O2
7	B	310	PG4	C3-C4-O3-C5
6	B	307	PEG	C4-C3-O2-C2
7	B	310	PG4	C1-C2-O2-C3
5	B	306	TRS	C2-C-C3-O3
5	C	303	TRS	C2-C-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

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

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	B	199/205 (97%)	0.03	5 (2%) 57 65	31, 46, 75, 92	5 (2%)
1	C	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%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	3.7
1	B	106	HIS	3.4
1	C	2	SER	2.9
1	B	105	ALA	2.6
1	B	108	PRO	2.6
1	C	108	PRO	2.4
1	C	101	ARG	2.1
1	C	165	TYR	2.1
1	B	102	LEU	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,

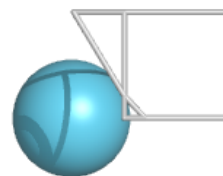
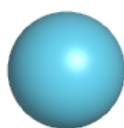
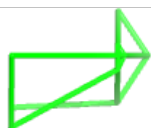
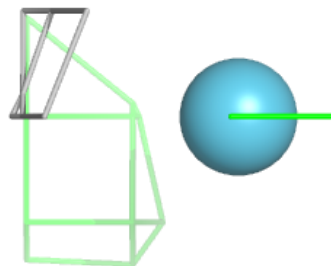
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

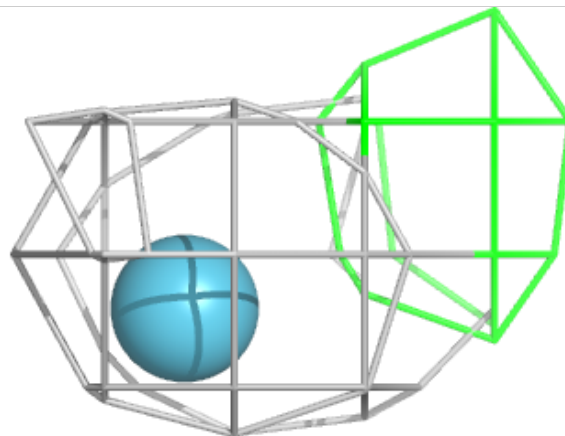
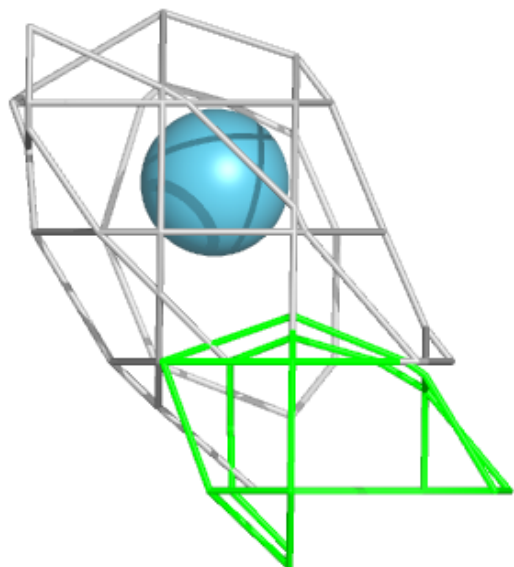
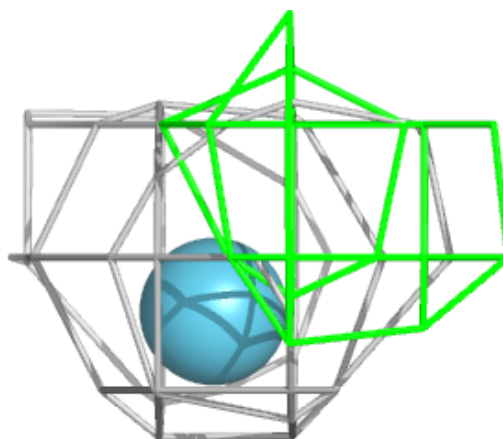
**Electron density around KR C 309:**

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



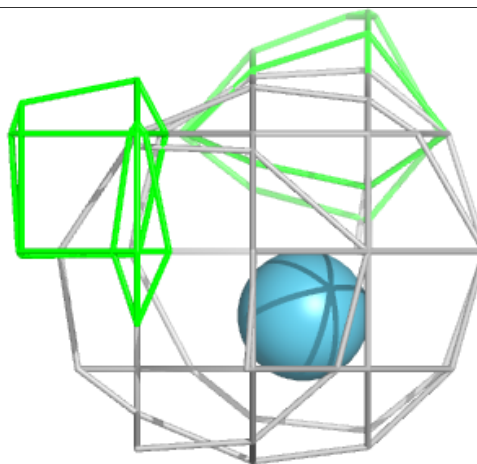
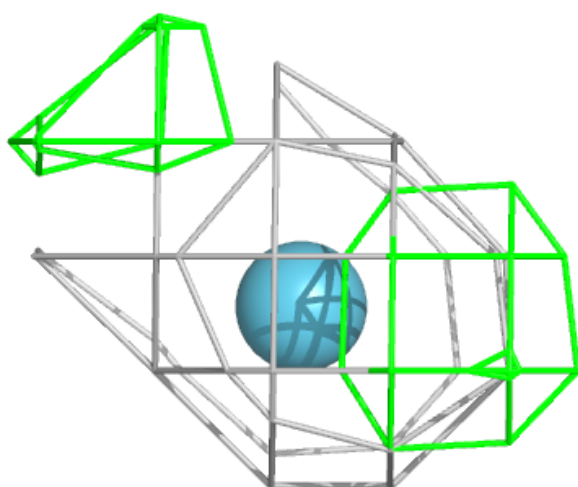
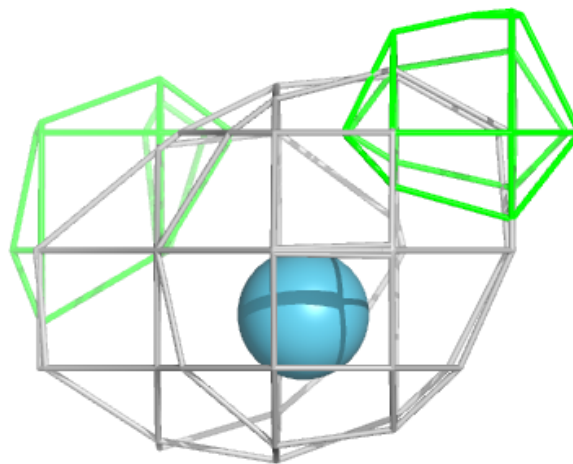
**Electron density around KR B 311:**

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



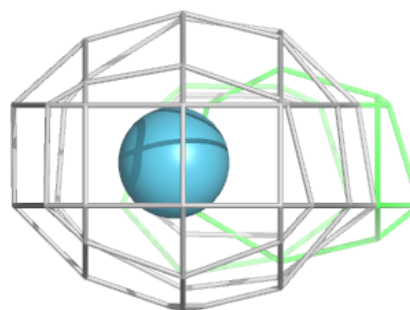
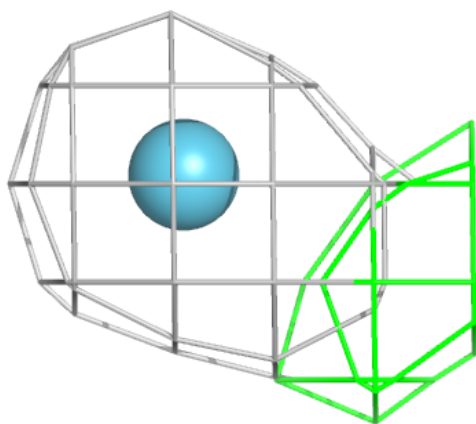
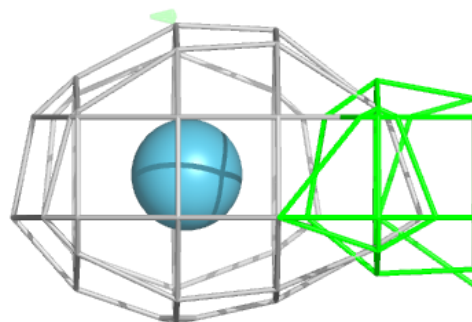
**Electron density around KR C 308:**

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



**Electron density around KR C 311:**

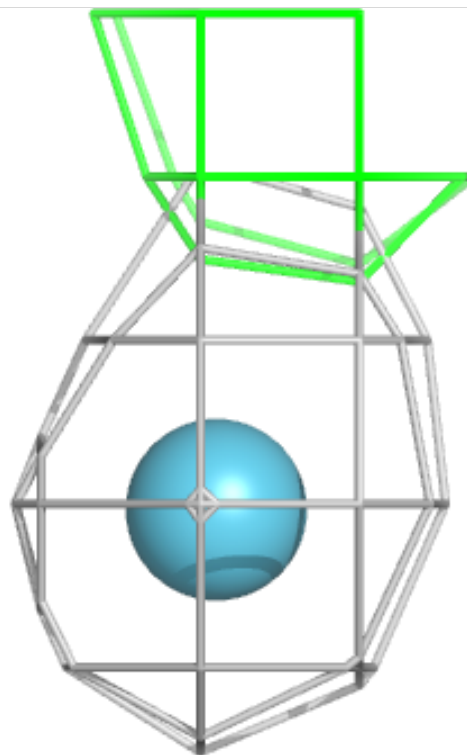
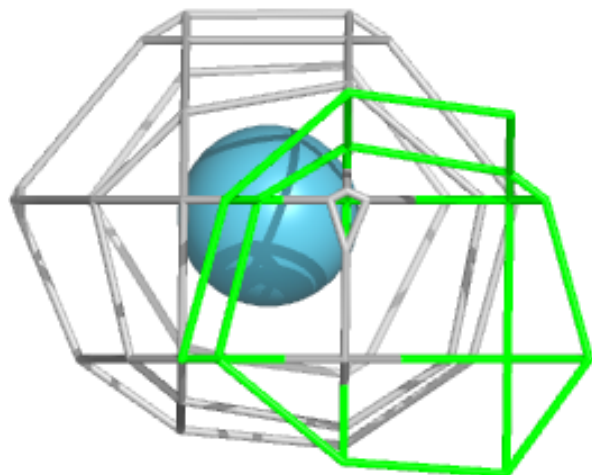
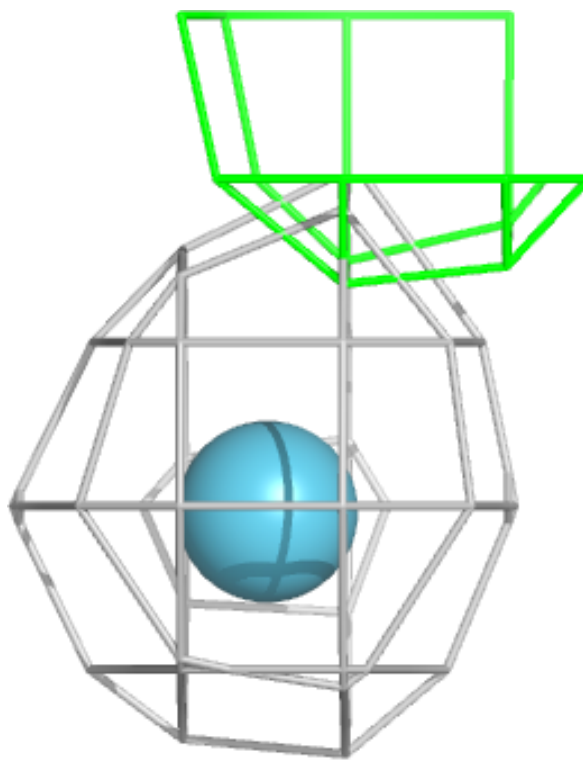
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





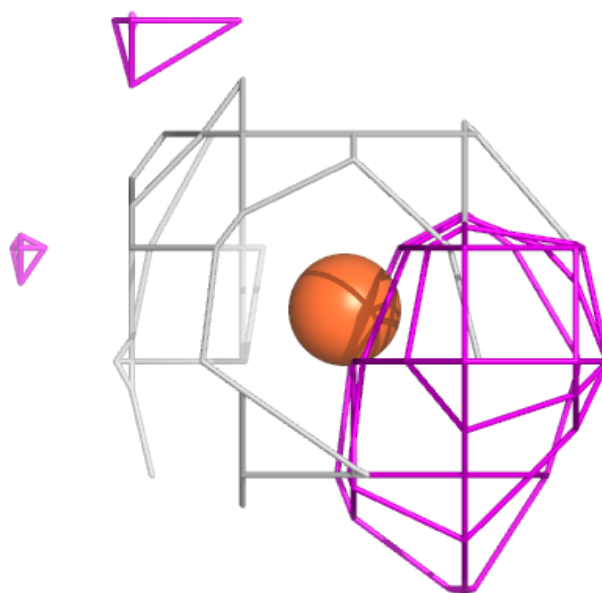
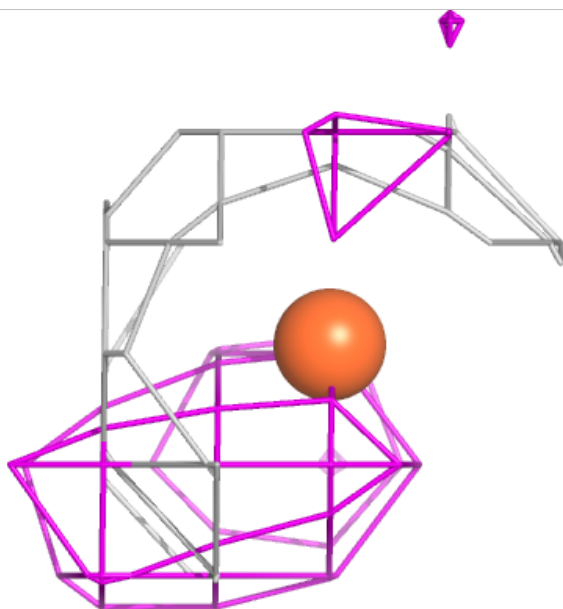
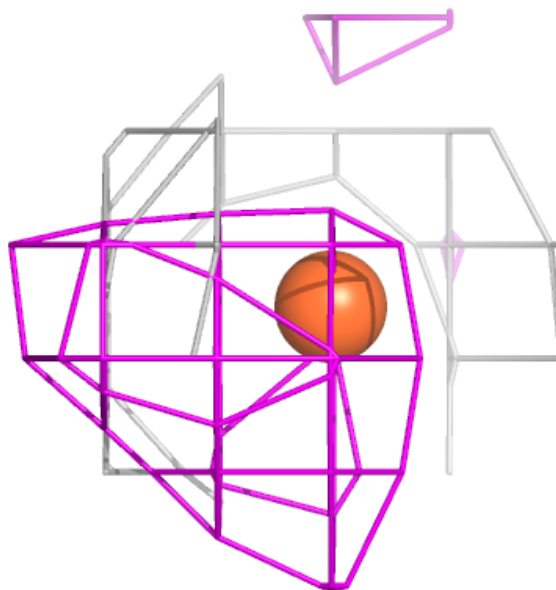
**Electron density around KR B 312:**

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



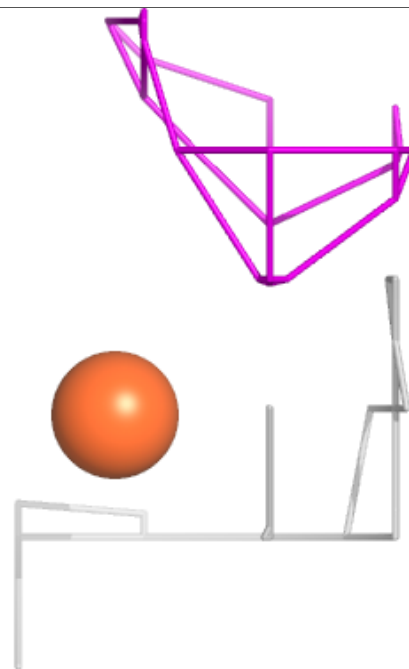
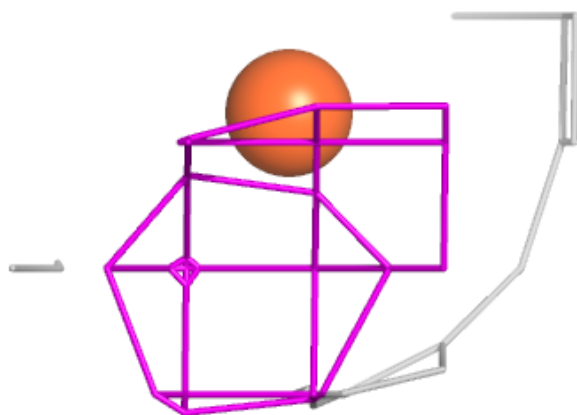
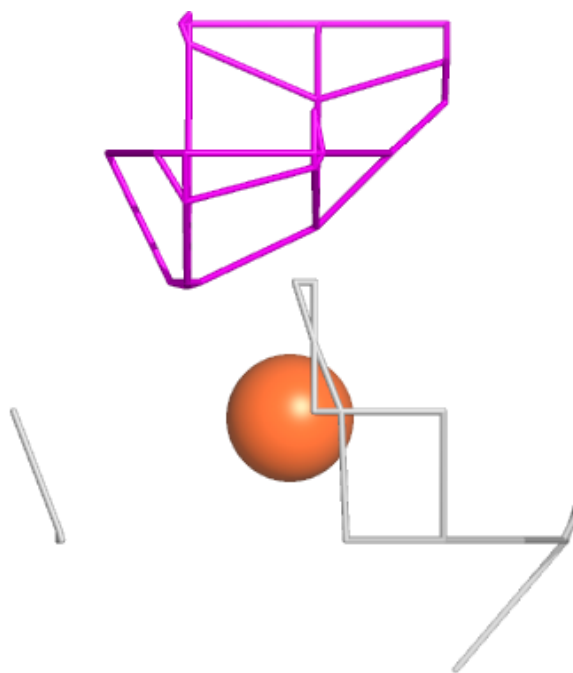
**Electron density around FE B 302:**

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



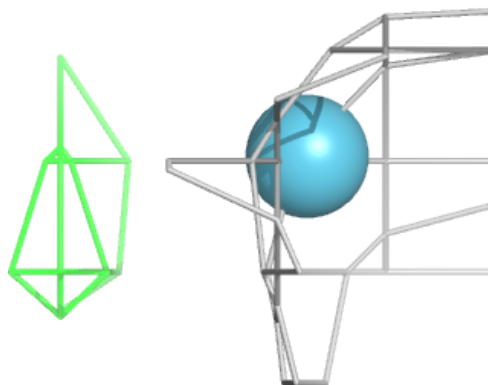
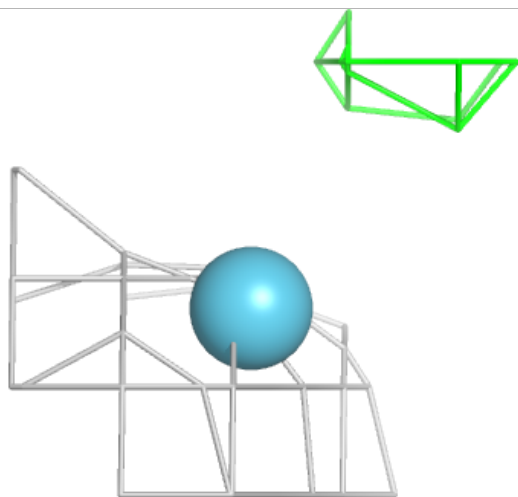
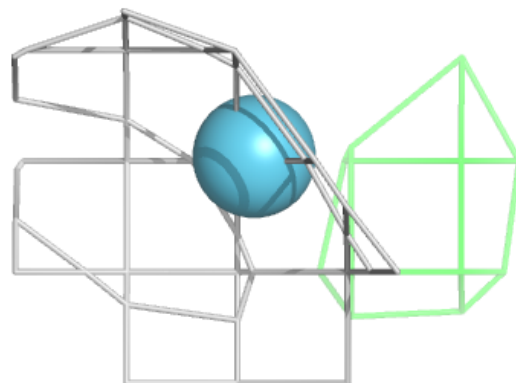
**Electron density around FE B 301:**

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



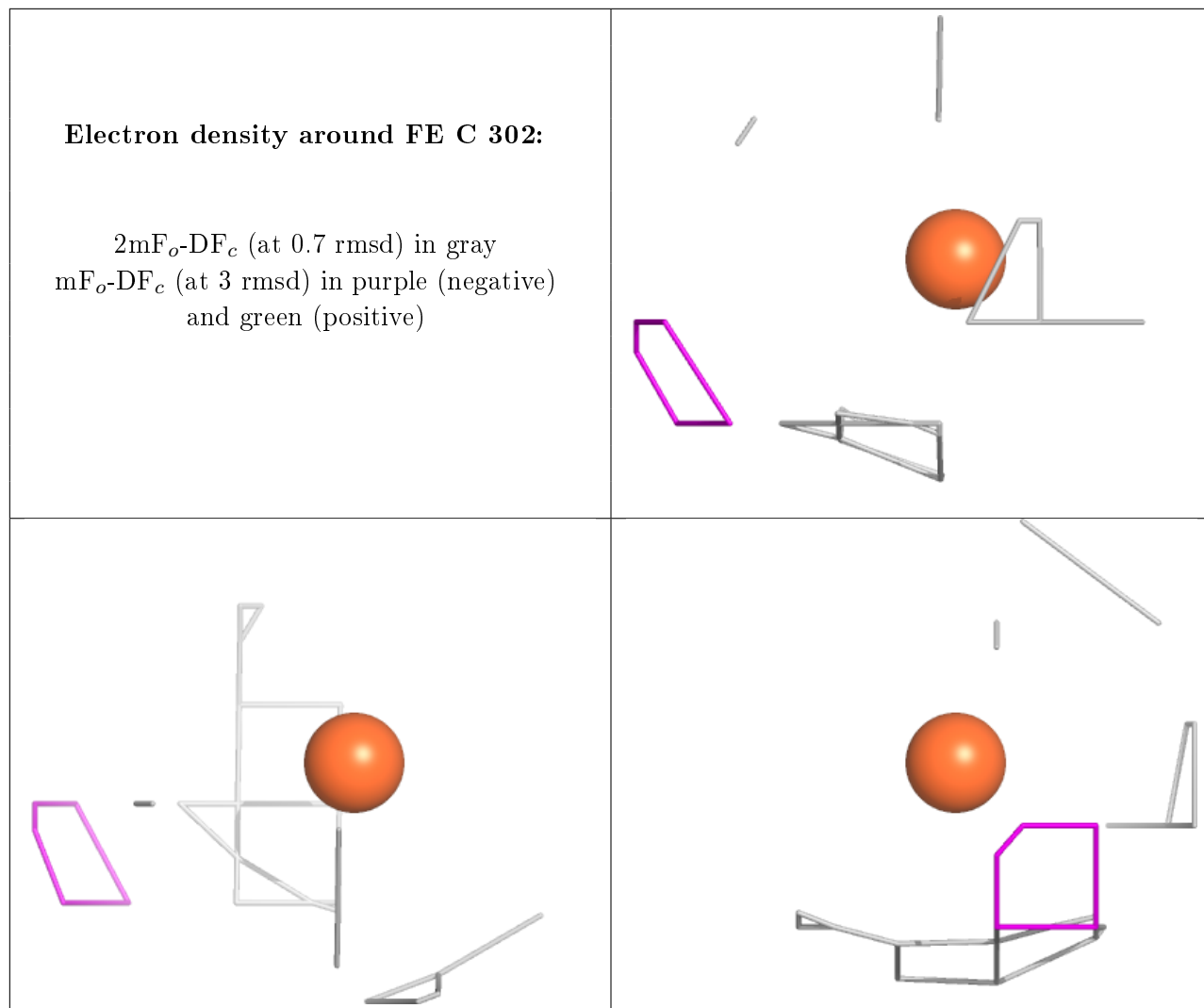
**Electron density around KR C 310:**

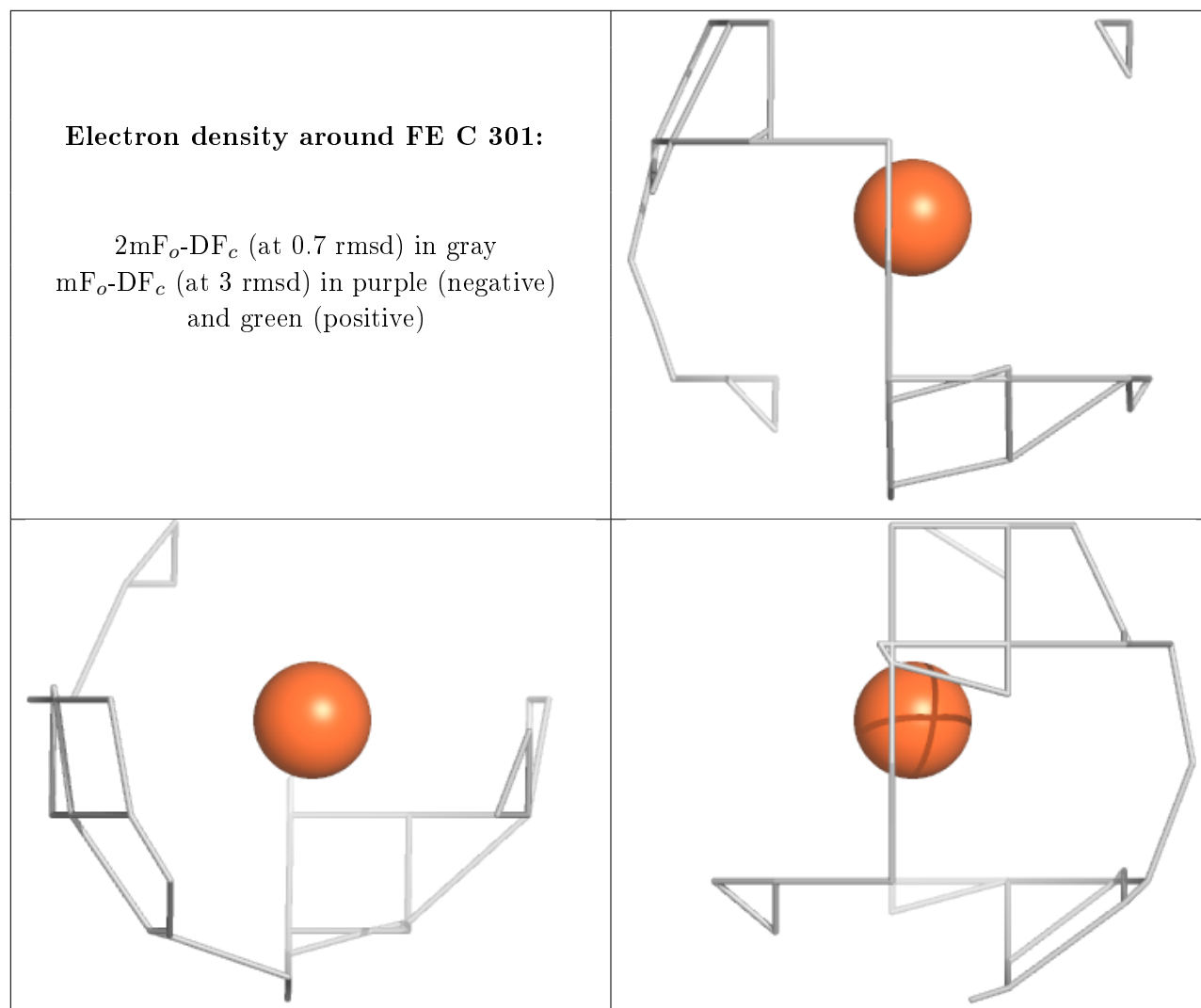
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE C 302:**

$2mF_o-DF_c$  (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.