WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 08:02 am BST

PDB ID	:	6FOG
Title	:	X-ray structure of homo sapiens Fumarylacetoacetate hydrolase domain containing protein 1 (FAHD1) in complex with inhibitor oxalate at 1.94A resolution.
Authors	:	Naschberger, A.; Weiss, A.K.H.
Deposited on	:	2018-02-07
Resolution	:	1.94 Å(reported)

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

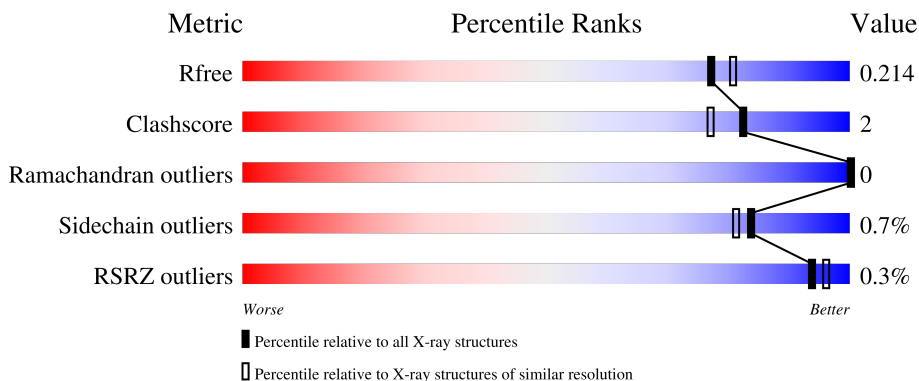|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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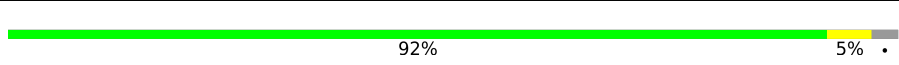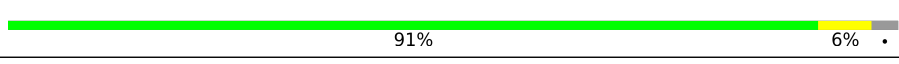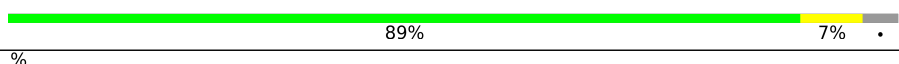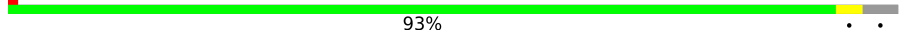*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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.
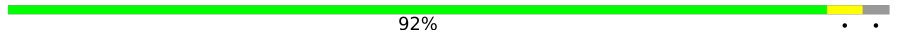
Metric	Percentile Ranks	Value
Rfree		0.214
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		0.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
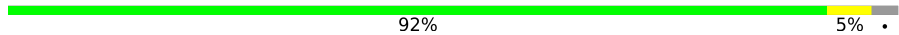
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	A	224	92% 5% ·
1	B	224	91% 6% ·
1	C	224	89% 7% ·
1	D	224	.% 93% · ·

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Mol	Chain	Length	Quality of chain
1	E	224	90% 6% •
1	F	224	88% 8% •
1	G	224	92% • •
1	H	224	92% 5% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14391 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 Acylpyruvase FAHD1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1707	1093	290	312	12			
1	G	217	Total	C	N	O	S	0	0	0
			1687	1082	285	308	12			
1	F	215	Total	C	N	O	S	0	0	0
			1674	1075	280	307	12			
1	D	215	Total	C	N	O	S	0	0	0
			1674	1075	280	307	12			
1	B	217	Total	C	N	O	S	0	1	0
			1695	1088	286	309	12			
1	C	216	Total	C	N	O	S	0	0	0
			1686	1084	281	309	12			
1	H	217	Total	C	N	O	S	0	0	0
			1687	1082	285	308	12			
1	E	215	Total	C	N	O	S	0	0	0
			1676	1076	283	305	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	G	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4) (labeled as "Ligand of Interest" by depositor).

OXL
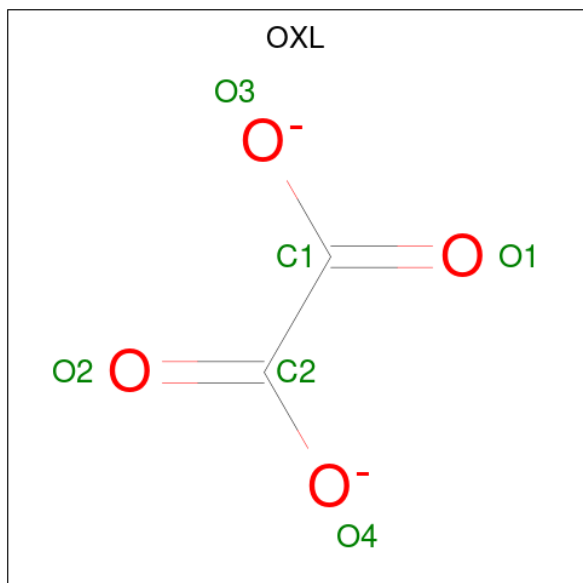
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 2	O 4	0	0
3	G	1	Total 6	C 2	O 4	0	0
3	F	1	Total 6	C 2	O 4	0	0
3	D	1	Total 6	C 2	O 4	0	0
3	B	1	Total 6	C 2	O 4	0	0
3	C	1	Total 6	C 2	O 4	0	0
3	H	1	Total 6	C 2	O 4	0	0
3	E	1	Total 6	C 2	O 4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	G	120	Total 120	O 120	0	0
5	F	108	Total 108	O 108	0	0
5	D	96	Total 96	O 96	0	0
5	B	101	Total 101	O 101	0	0
5	C	92	Total 92	O 92	0	0
5	H	98	Total 98	O 98	0	0
5	E	117	Total 117	O 117	0	0

3 Residue-property plots ⓘ

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: Acylpyruvase FAHD1, mitochondrial

Chain A:

- Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain G:

- Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain F:

- Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain D:

- Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain B:

- Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain C:

89%   7%   •

MET GLY ILE MET ALA ALA SER ARG P9 G24 R25 S36 A37 V38 V43 I59 R66 H70 E71 L101 D107 E111 P130 K147 L148 I166 Y224

• Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain H:

92%   5%   •

MET GLY ILE MET ALA A6 K18 E55 I59 E71 L101 P130 V152 E155 I205 T216 P222 GLU TYR

• Molecule 1: Acylpyruvase FAHD1, mitochondrial

Chain E:

90%   6%   •

MET GLY ILE MET ALA ALA SER R8 R35 V38 I59 R66 E71 L101 D110 L121 P130 V152 I166 E201 N202 I205 P222 GLU TYR

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.98Å 116.68Å 125.75Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	85.53 – 1.94 85.53 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.2 (85.53-1.94) 94.1 (85.53-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.208 0.186 , 0.214	Depositor DCC
R_{free} test set	7999 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 18.7	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.410 for h,-k,-l	Xtriage
Reported twinning fraction	0.392 for H, K, L 0.608 for -h,-k,l	Depositor
Outliers	0 of 154262 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9110e-03.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, CL, MG

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	0.64	0/1748	0.76	0/2368
1	B	0.64	0/1736	0.75	0/2353
1	C	0.67	0/1728	0.76	0/2342
1	D	0.66	0/1715	0.76	0/2324
1	E	0.65	0/1717	0.75	0/2327
1	F	0.61	0/1715	0.77	0/2324
1	G	0.64	0/1728	0.75	0/2342
1	H	0.62	0/1728	0.75	0/2342
All	All	0.64	0/13815	0.76	0/18722

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 ⓘ

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	1707	0	1733	9	0
1	B	1695	0	1725	8	0
1	C	1686	0	1708	15	0
1	D	1674	0	1699	5	0
1	E	1676	0	1705	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1674	0	1699	16	0
1	G	1687	0	1715	5	0
1	H	1687	0	1715	7	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	109	0	0	2	0
5	B	101	0	0	2	0
5	C	92	0	0	4	0
5	D	96	0	0	0	0
5	E	117	0	0	2	0
5	F	108	0	0	4	0
5	G	120	0	0	0	0
5	H	98	0	0	1	0
All	All	14391	0	13699	67	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.

The worst 5 of 67 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:24:GLY:HA3	1:C:43:VAL:CG2	2.16	0.75
1:A:175:TYR:OH	1:F:66:ARG:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HD22	5:C:412:HOH:O	1.95	0.66
1:C:24:GLY:CA	1:C:43:VAL:CG2	2.78	0.61
1:A:175:TYR:OH	1:F:66:ARG:CD	2.49	0.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/224 (97%)	214 (99%)	3 (1%)	0	100	100
1	B	216/224 (96%)	213 (99%)	3 (1%)	0	100	100
1	C	214/224 (96%)	211 (99%)	3 (1%)	0	100	100
1	D	213/224 (95%)	210 (99%)	3 (1%)	0	100	100
1	E	213/224 (95%)	211 (99%)	2 (1%)	0	100	100
1	F	213/224 (95%)	211 (99%)	2 (1%)	0	100	100
1	G	215/224 (96%)	213 (99%)	2 (1%)	0	100	100
1	H	215/224 (96%)	212 (99%)	3 (1%)	0	100	100
All	All	1716/1792 (96%)	1695 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/190 (98%)	185 (99%)	2 (1%)	73	67
1	B	186/190 (98%)	185 (100%)	1 (0%)	88	88
1	C	185/190 (97%)	182 (98%)	3 (2%)	62	52
1	D	184/190 (97%)	184 (100%)	0	100	100
1	E	184/190 (97%)	183 (100%)	1 (0%)	88	88
1	F	184/190 (97%)	183 (100%)	1 (0%)	88	88
1	G	185/190 (97%)	183 (99%)	2 (1%)	73	67
1	H	185/190 (97%)	184 (100%)	1 (0%)	88	88
All	All	1480/1520 (97%)	1469 (99%)	11 (1%)	84	81

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	147	LYS
1	C	148	LEU
1	E	35	ARG
1	H	155	GLU
1	F	21	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	153	ASN
1	F	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	OXL	A	302	2	5,5,5	1.71	2 (40%)	6,6,6	1.60	2 (33%)
3	OXL	H	302	2	5,5,5	1.59	1 (20%)	6,6,6	0.71	0
3	OXL	E	302	2	5,5,5	1.71	1 (20%)	6,6,6	0.80	0
3	OXL	B	302	2	5,5,5	1.76	2 (40%)	6,6,6	2.34	2 (33%)
3	OXL	C	302	2	5,5,5	1.41	0	6,6,6	2.35	2 (33%)
3	OXL	F	303	2	5,5,5	1.87	2 (40%)	6,6,6	0.87	0
3	OXL	G	302	2	5,5,5	1.75	2 (40%)	6,6,6	1.05	0
3	OXL	D	303	2	5,5,5	1.65	1 (20%)	6,6,6	0.86	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
3	OXL	A	302	2	-	0/4/4/4	-
3	OXL	H	302	2	-	0/4/4/4	-
3	OXL	E	302	2	-	1/4/4/4	-
3	OXL	B	302	2	-	1/4/4/4	-
3	OXL	C	302	2	-	0/4/4/4	-
3	OXL	F	303	2	-	0/4/4/4	-
3	OXL	G	302	2	-	1/4/4/4	-
3	OXL	D	303	2	-	2/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	OXL	C2-C1	-2.59	1.47	1.54
3	F	303	OXL	O3-C1	-2.56	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	OXL	O3-C1	-2.50	1.23	1.30
3	F	303	OXL	C2-C1	-2.41	1.47	1.54
3	E	302	OXL	C2-C1	-2.40	1.47	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	OXL	O3-C1-C2	3.70	124.14	113.16
3	C	302	OXL	O4-C2-C1	3.67	124.06	113.16
3	C	302	OXL	O3-C1-C2	3.29	122.93	113.16
3	B	302	OXL	O4-C2-C1	3.28	122.91	113.16
3	A	302	OXL	O4-C2-C1	2.54	120.70	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	303	OXL	O3-C1-C2-O4
3	D	303	OXL	O1-C1-C2-O2
3	G	302	OXL	O3-C1-C2-O4
3	B	302	OXL	O3-C1-C2-O4
3	E	302	OXL	O3-C1-C2-O4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
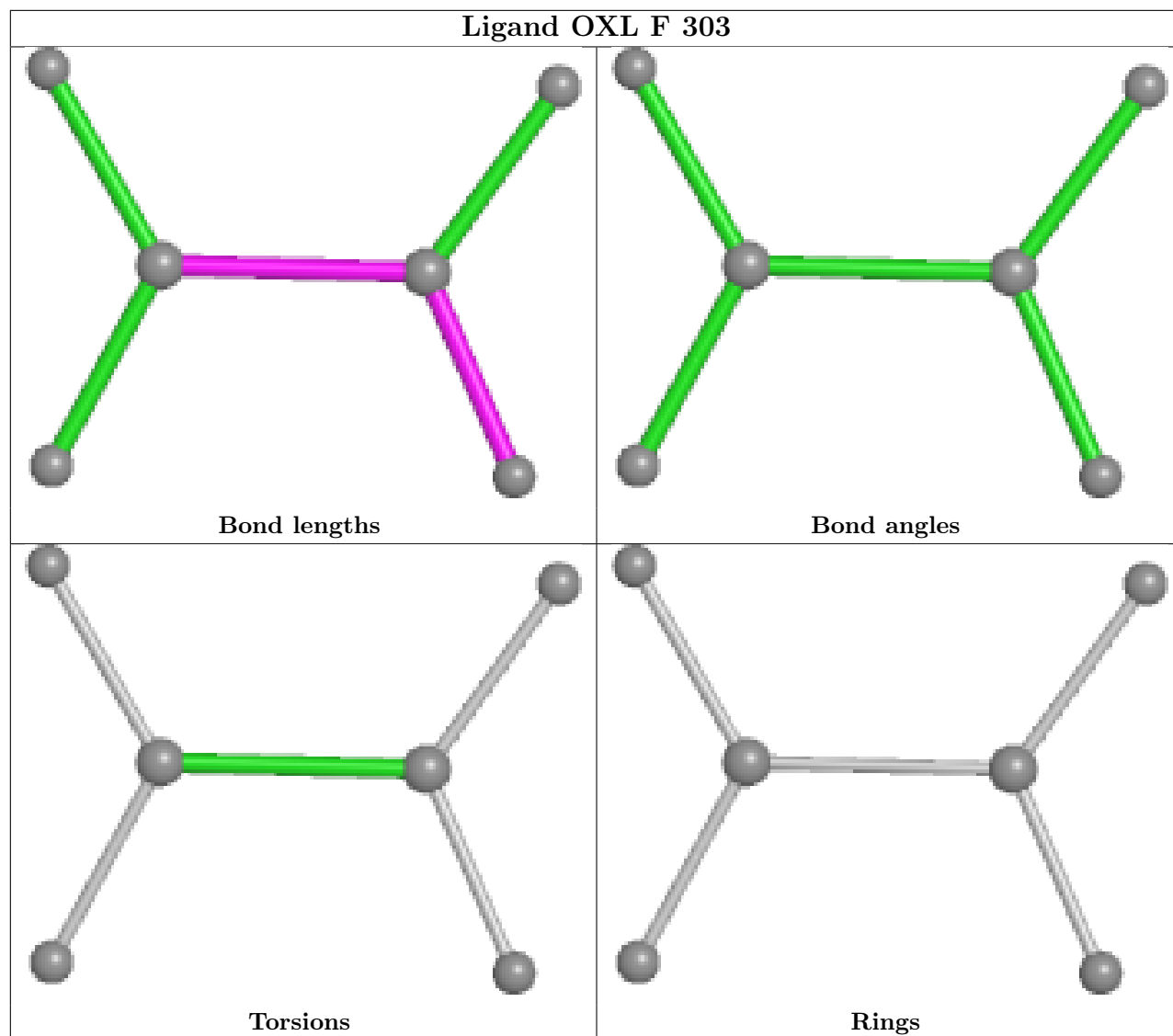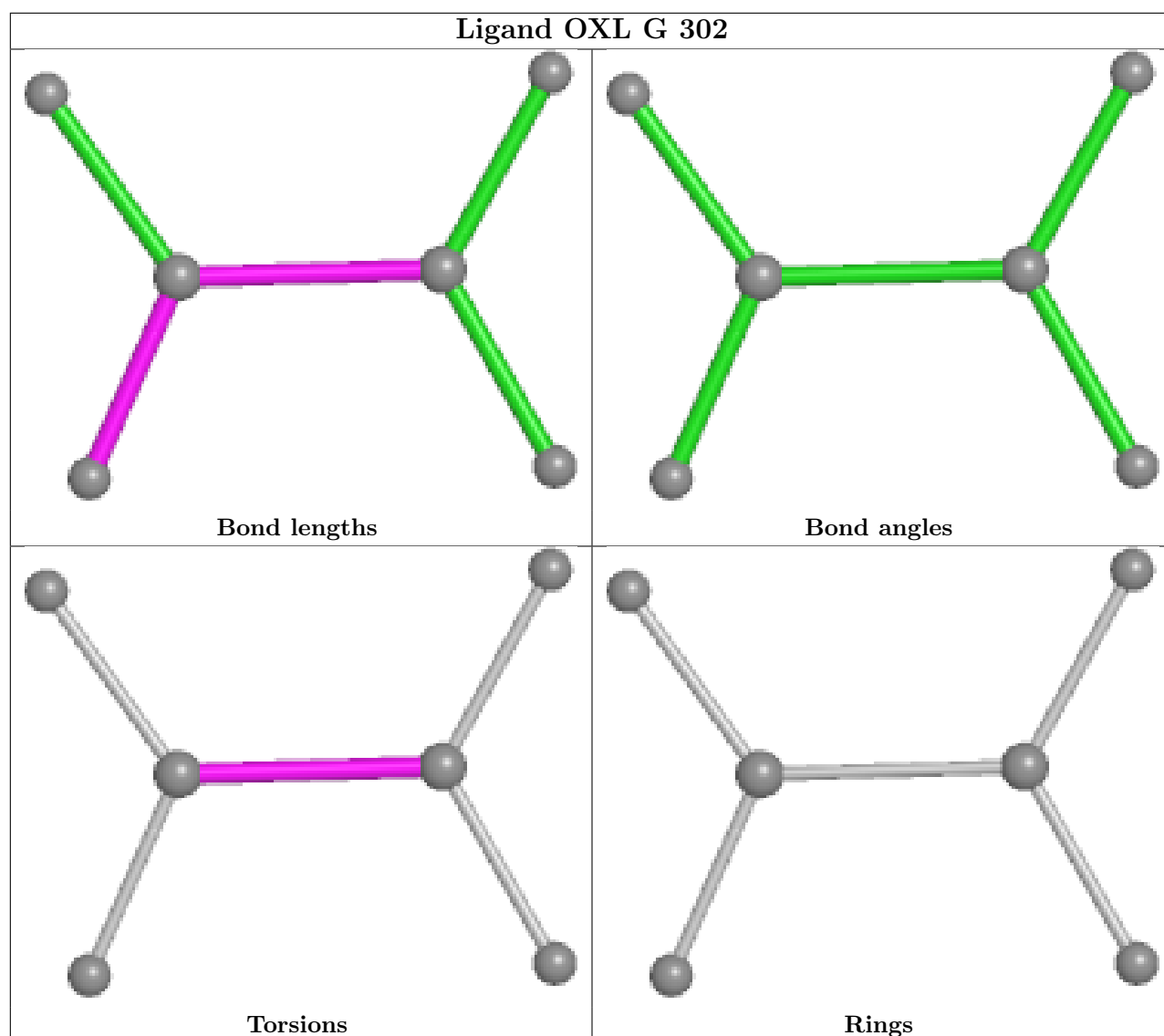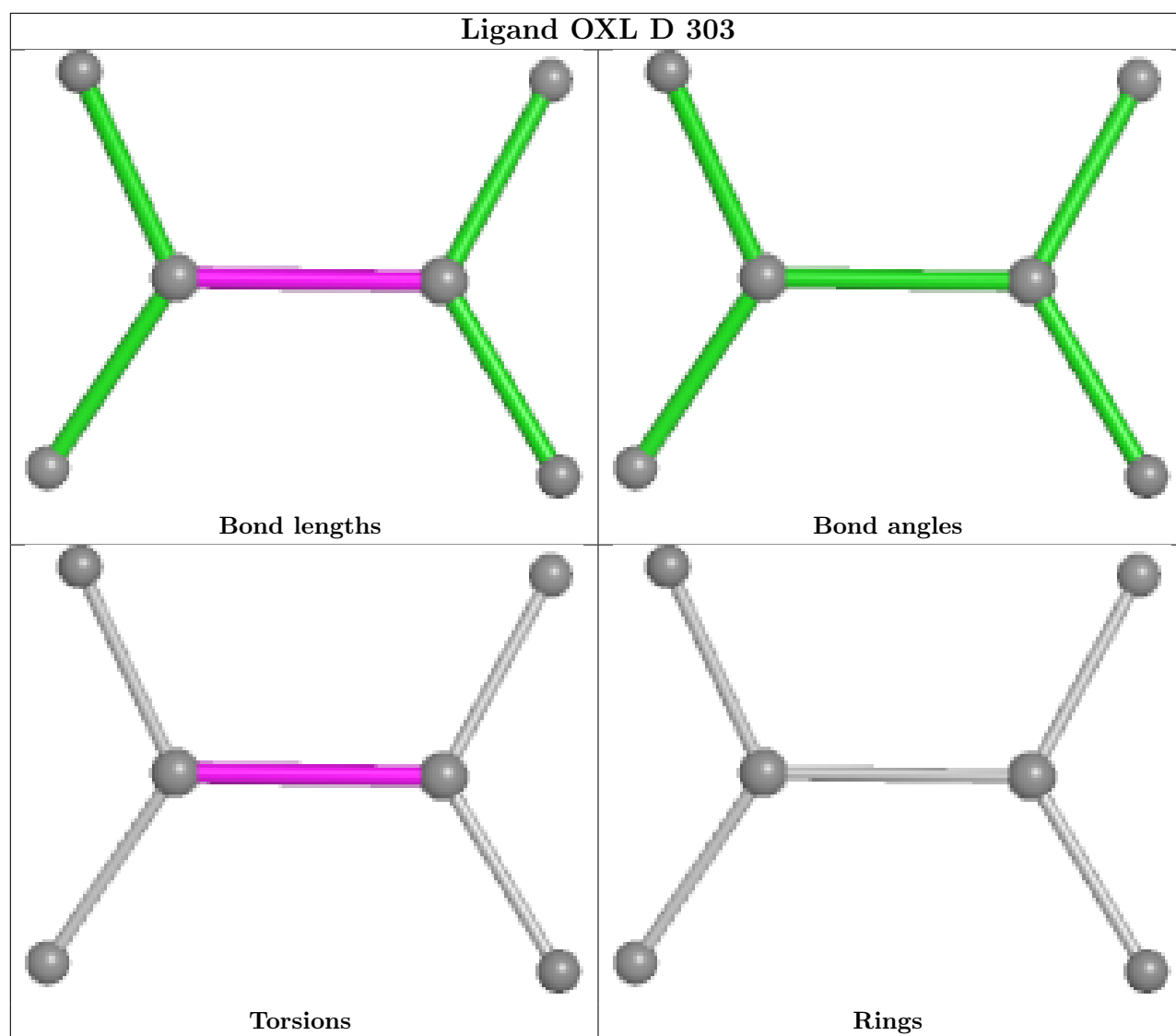
Ligand OXL A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL H 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL G 302

Bond lengths

Bond angles

Torsions

Rings

Ligand OXL D 303

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

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, 95th 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^2)	Q<0.9
1	A	218/224 (97%)	-0.51	0	100　100	18, 26, 43, 58	0
1	B	217/224 (96%)	-0.46	1 (0%)	91　93	17, 27, 44, 62	0
1	C	216/224 (96%)	-0.45	1 (0%)	91　93	15, 26, 49, 63	0
1	D	215/224 (95%)	-0.48	2 (0%)	84　87	16, 26, 44, 81	0
1	E	215/224 (95%)	-0.51	1 (0%)	91　93	17, 26, 44, 71	0
1	F	215/224 (95%)	-0.41	1 (0%)	91　93	19, 30, 50, 66	0
1	G	217/224 (96%)	-0.46	0	100　100	15, 28, 46, 64	0
1	H	217/224 (96%)	-0.37	0	100　100	18, 32, 53, 65	0
All	All	1730/1792 (96%)	-0.46	6 (0%)	94　96	15, 27, 48, 81	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	VAL	3.5
1	D	223	GLU	2.8
1	F	39	LEU	2.6
1	E	38	VAL	2.3
1	B	6	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

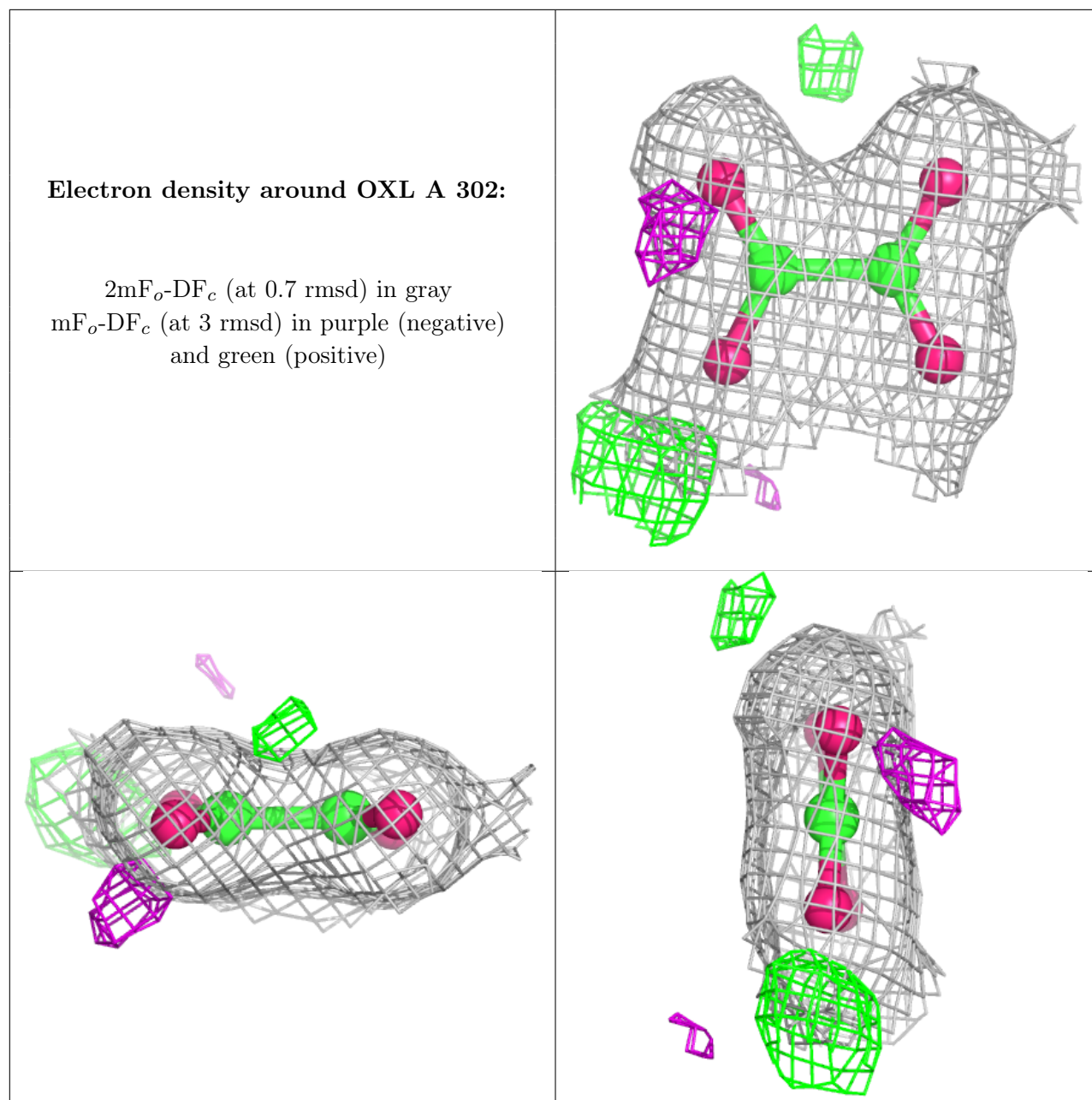There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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, 95th 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^2)	Q<0.9
3	OXL	A	302	6/6	0.93	0.09	21,24,25,27	0
3	OXL	F	303	6/6	0.93	0.12	20,24,29,35	0
3	OXL	G	302	6/6	0.94	0.12	18,26,32,37	0
3	OXL	D	303	6/6	0.94	0.11	15,19,24,24	6
3	OXL	E	302	6/6	0.94	0.10	20,28,30,35	6
3	OXL	B	302	6/6	0.95	0.09	15,20,22,25	0
2	MG	H	301	1/1	0.95	0.04	26,26,26,26	0
3	OXL	H	302	6/6	0.96	0.10	26,34,40,48	0
3	OXL	C	302	6/6	0.97	0.10	16,25,31,31	6
2	MG	A	301	1/1	0.98	0.07	21,21,21,21	0
2	MG	A	304	1/1	0.98	0.06	29,29,29,29	0
2	MG	D	301	1/1	0.98	0.06	26,26,26,26	0
2	MG	G	301	1/1	0.99	0.05	21,21,21,21	0
2	MG	D	302	1/1	0.99	0.06	30,30,30,30	0
2	MG	B	301	1/1	0.99	0.04	23,23,23,23	0
2	MG	C	301	1/1	0.99	0.09	23,23,23,23	0
2	MG	G	303	1/1	0.99	0.04	17,17,17,17	0
2	MG	E	301	1/1	0.99	0.08	21,21,21,21	0
2	MG	F	301	1/1	0.99	0.08	21,21,21,21	0
4	CL	A	303	1/1	0.99	0.05	26,26,26,26	0
4	CL	B	303	1/1	0.99	0.05	29,29,29,29	0
4	CL	E	303	1/1	0.99	0.05	28,28,28,28	0
2	MG	F	302	1/1	1.00	0.07	19,19,19,19	0
4	CL	F	304	1/1	1.00	0.03	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.
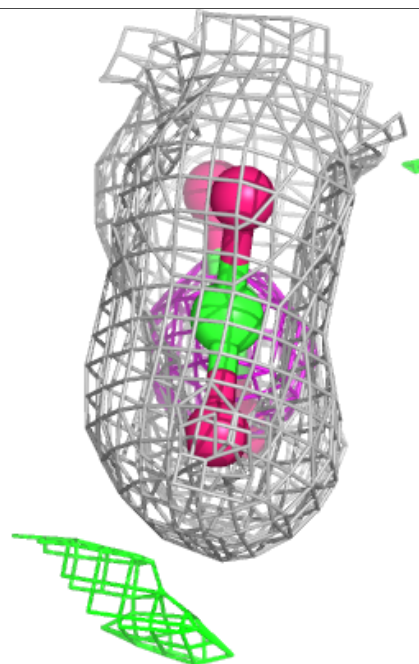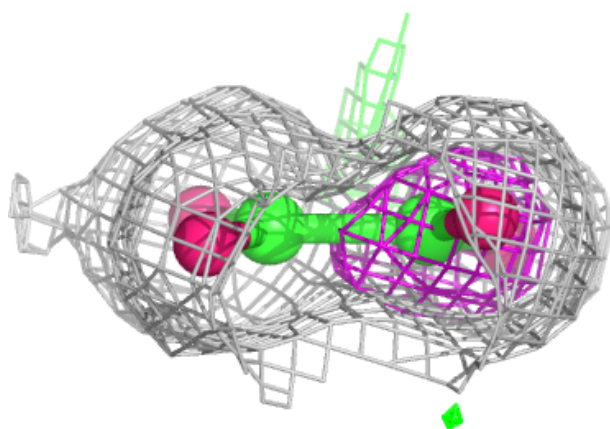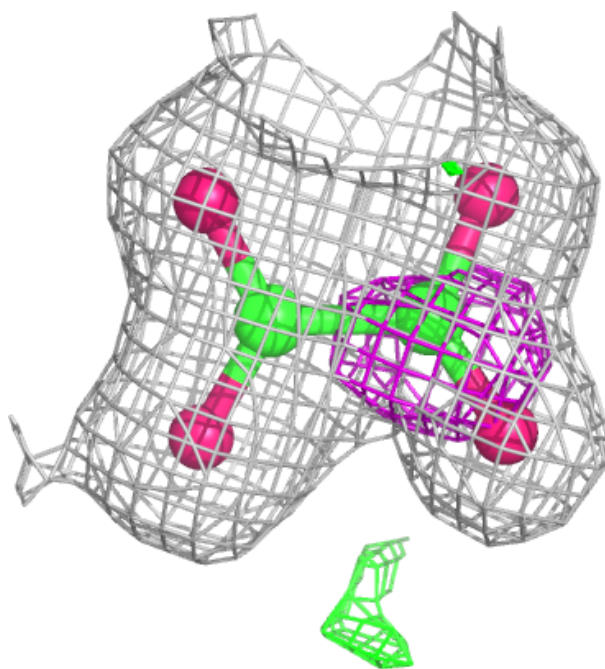
Electron density around OXL A 302:

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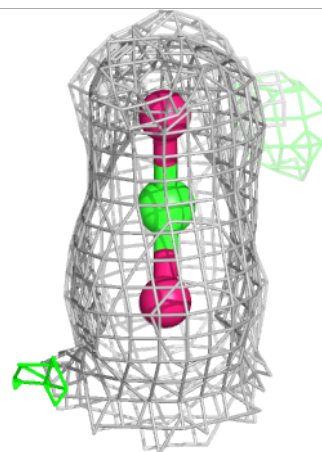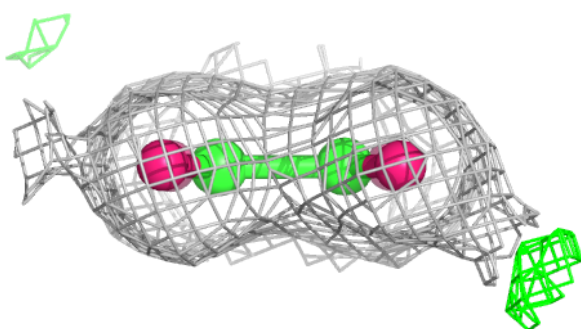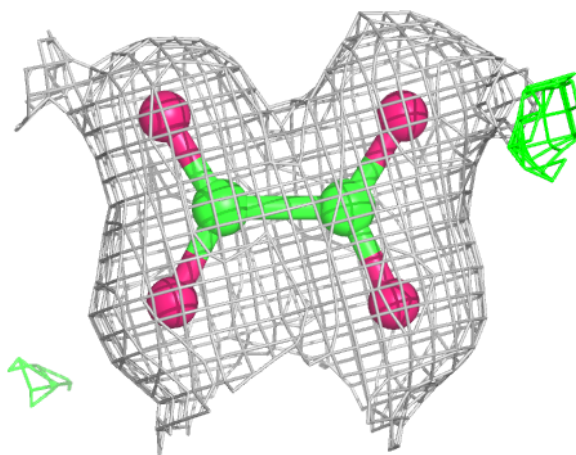and green (positive)

Electron density around OXL F 303:

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

Electron density around OXL G 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
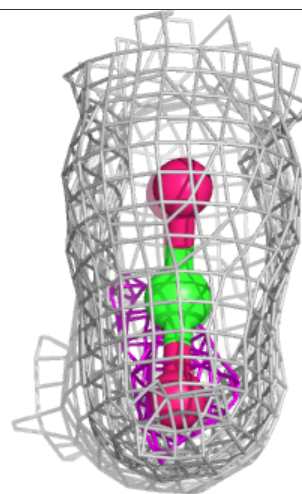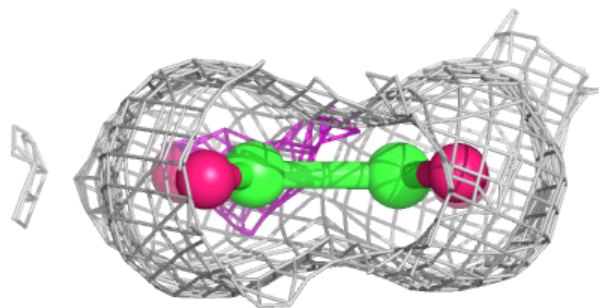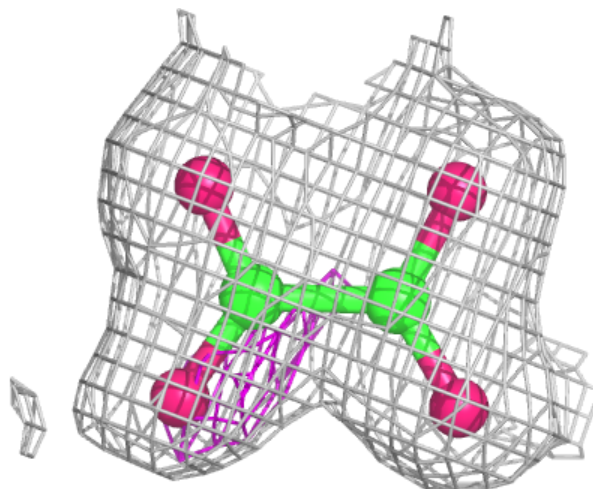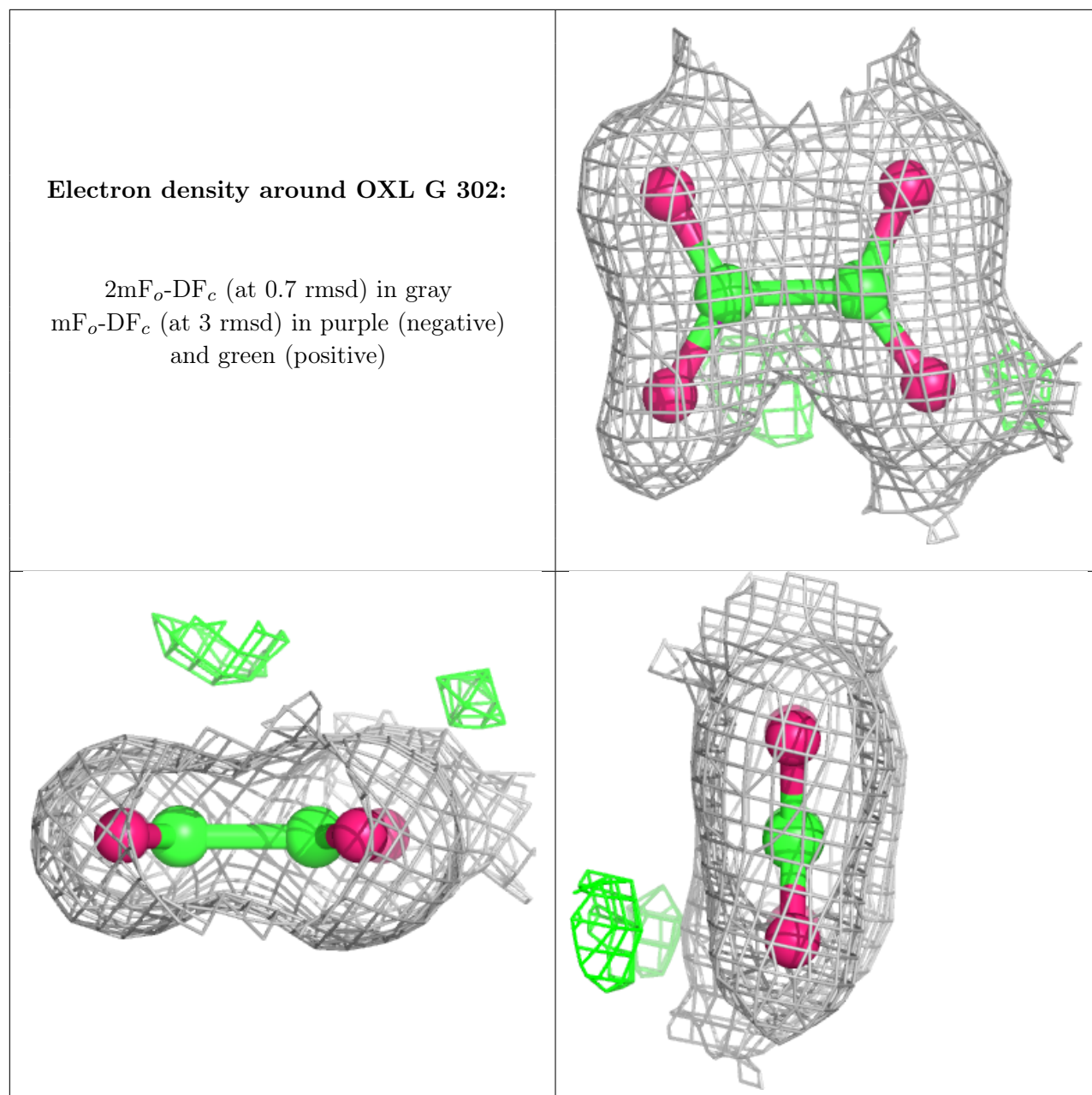
Electron density around OXL D 303:

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

Electron density around OXL E 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 OXL 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 OXL H 302:

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

Electron density around OXL C 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
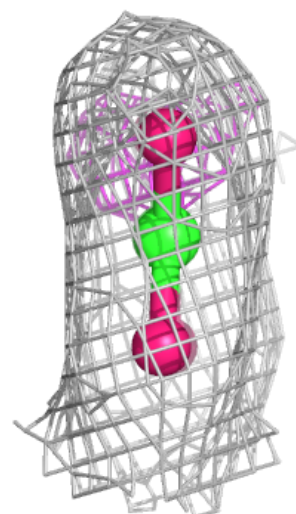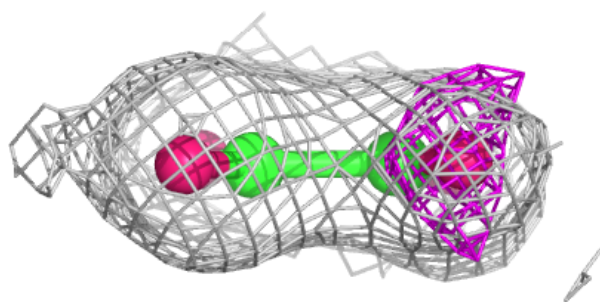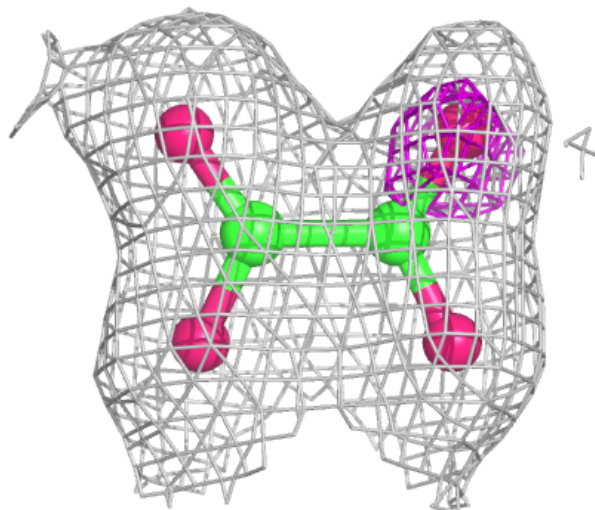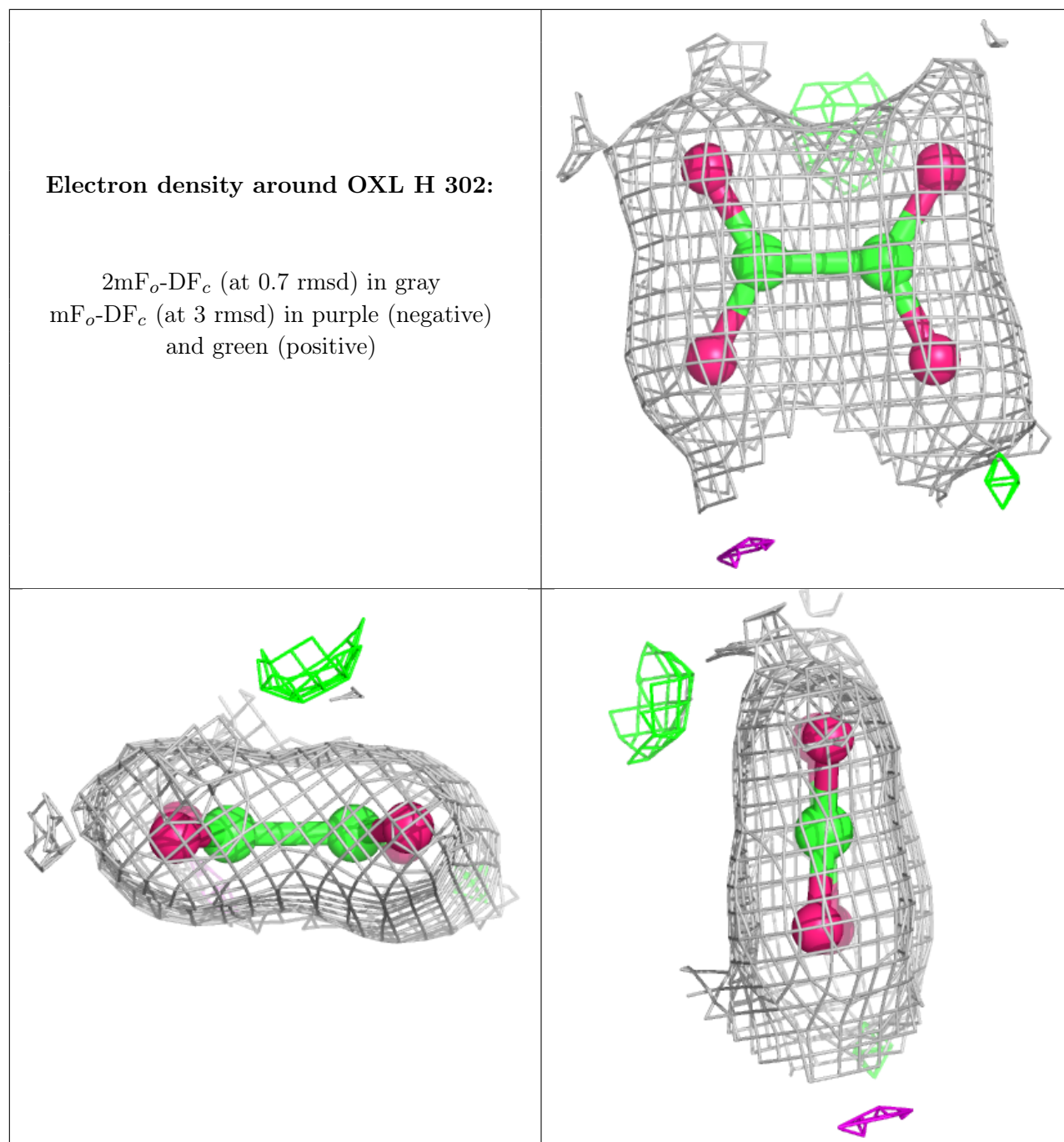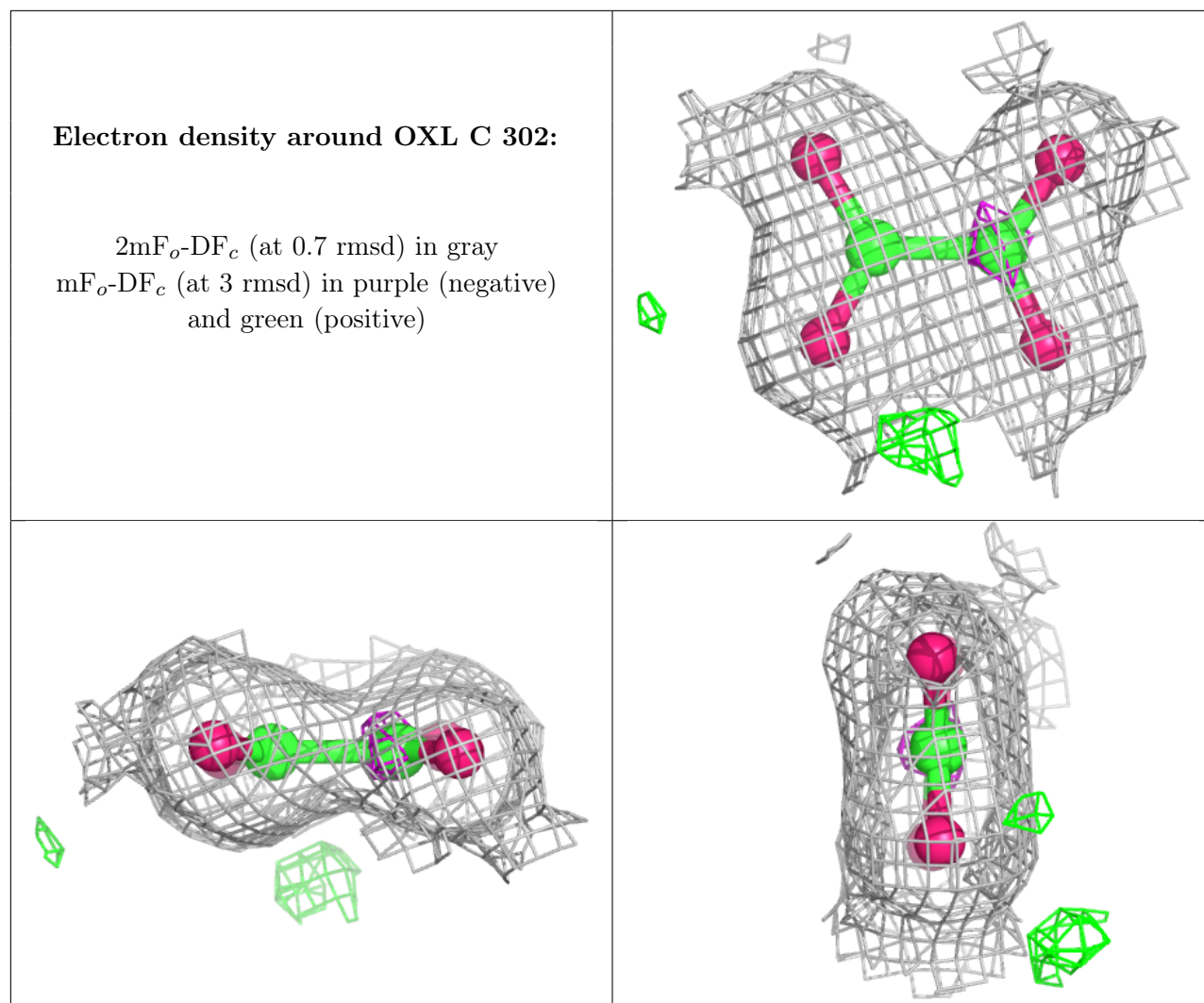
6.5 Other polymers (i)

There are no such residues in this entry.