



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2025 – 11:09 am BST

PDB ID : 9QM5 / pdb\_00009qm5  
Title : Krypton-pressurized Methyl-Coenzyme M reductase of an ANME-2c isolated from a microbial enrichment  
Authors : Mueller, M.-C.; Wagner, T.  
Deposited on : 2025-03-21  
Resolution : 1.80 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	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

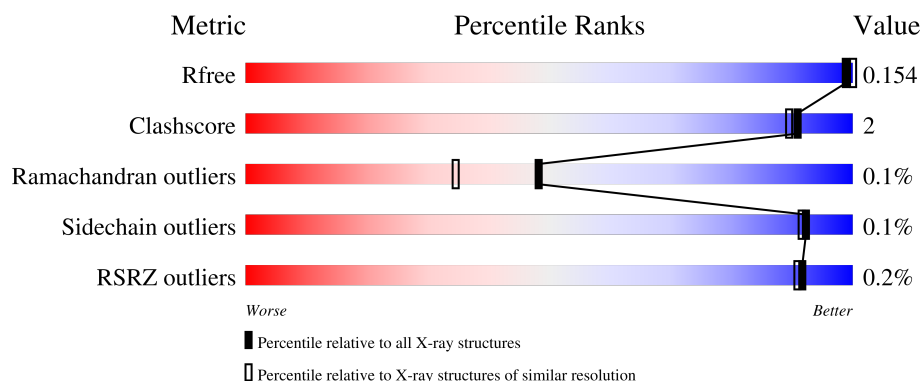
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	561	94% 5% .
1	D	561	94% 5% .
1	G	561	94% 5% .
1	J	561	95% 5% .
2	B	434	98% .

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Mol	Chain	Length	Quality of chain
2	E	434	 97% .
2	H	434	 96% .
2	K	434	 97% .
3	C	265	 97% .
3	F	265	 96% .
3	I	265	 97% .
3	L	265	 97% .

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
4	KR	A	606	-	-	X	-
4	KR	G	608	-	-	X	-
4	KR	J	607	-	-	X	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 80668 atoms, of which 37351 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 Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	558	Total	C	H	N	O	S	0	0	0
			8360	2709	4054	726	832	39			
1	D	558	Total	C	H	N	O	S	0	0	0
			8360	2709	4054	726	832	39			
1	G	558	Total	C	H	N	O	S	0	0	0
			8360	2709	4054	726	832	39			
1	J	558	Total	C	H	N	O	S	0	2	0
			8377	2714	4062	727	835	39			

- Molecule 2 is a protein called Beta subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	433	Total	C	H	N	O	S	0	2	0
			6437	2015	3212	554	627	29			
2	E	433	Total	C	H	N	O	S	0	4	0
			6462	2021	3226	558	628	29			
2	H	433	Total	C	H	N	O	S	0	2	0
			6437	2015	3212	554	627	29			
2	K	433	Total	C	H	N	O	S	0	0	0
			6425	2012	3206	553	626	28			

- Molecule 3 is a protein called Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	264	Total	C	H	N	O	S	0	2	0
			4044	1270	1987	376	396	15			
3	F	264	Total	C	H	N	O	S	0	0	0
			4022	1264	1974	374	395	15			
3	I	264	Total	C	H	N	O	S	0	4	0
			4053	1274	1987	376	401	15			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	264	Total 4038	C 1269	H 1981	N 375	O 398	S 15	0	2	0

- Molecule 4 is KRYPTON (CCD ID: KR) (formula: Kr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	Kr 8	0	2
4	B	1	Total 1	Kr 1	0	0
4	C	1	Total 1	Kr 1	0	0
4	D	6	Total 6	Kr 6	0	3
4	E	1	Total 1	Kr 1	0	0
4	F	2	Total 2	Kr 2	0	0
4	G	7	Total 7	Kr 7	0	1
4	H	1	Total 1	Kr 1	0	0
4	I	2	Total 2	Kr 2	0	0
4	J	7	Total 7	Kr 7	0	2
4	K	1	Total 1	Kr 1	0	0
4	L	1	Total 1	Kr 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

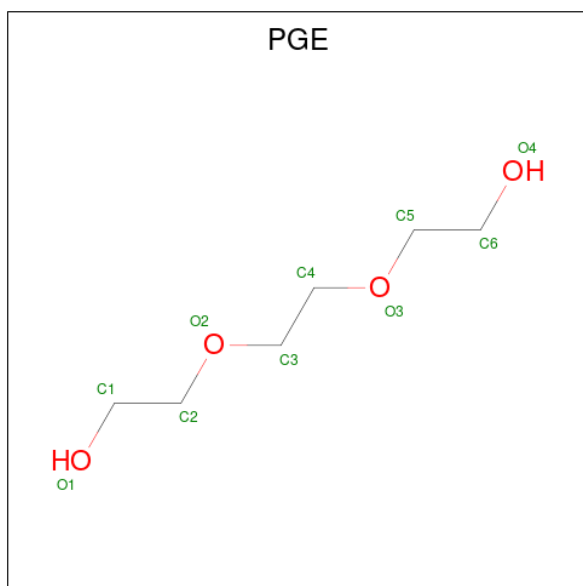
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Mg 2	0	0
5	D	1	Total 1	Mg 1	0	0
5	G	1	Total 1	Mg 1	0	0
5	J	1	Total 1	Mg 1	0	0

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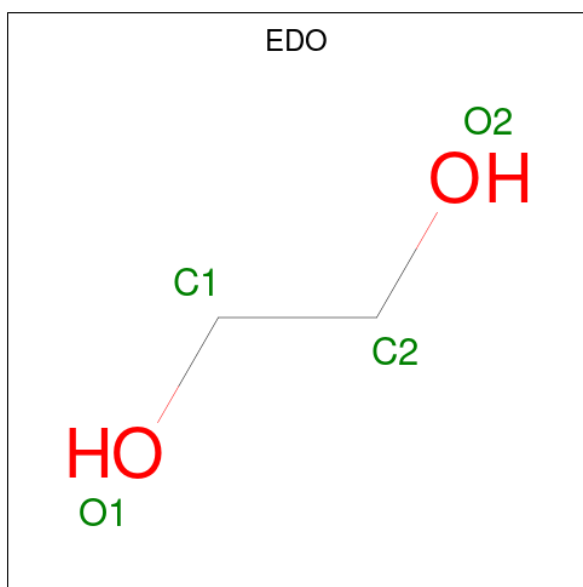
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	1	Total	Mg	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			24	6	14	4		
6	D	1	Total	C	H	O	0	0
			24	6	14	4		
6	D	1	Total	C	H	O	0	0
			24	6	14	4		
6	G	1	Total	C	H	O	0	0
			24	6	14	4		
6	G	1	Total	C	H	O	0	0
			24	6	14	4		
6	H	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	F	1	Total	C	H	O	0	0
			10	2	6	2		
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	I	1	Total	C	H	O	0	0
			10	2	6	2		
7	I	1	Total	C	H	O	0	0
			10	2	6	2		
7	J	1	Total	C	H	O	0	0
			10	2	6	2		
7	J	1	Total	C	H	O	0	0
			10	2	6	2		

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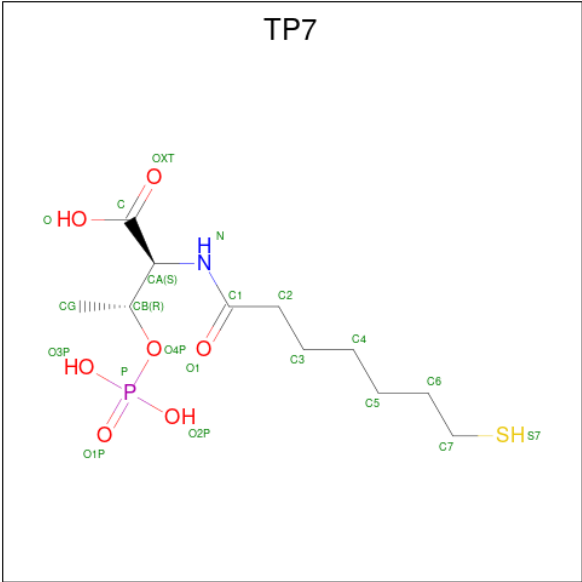
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	J	1	Total	C	H	O	0	0
			10	2	6	2		
7	K	1	Total	C	H	O	0	0
			10	2	6	2		
7	L	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

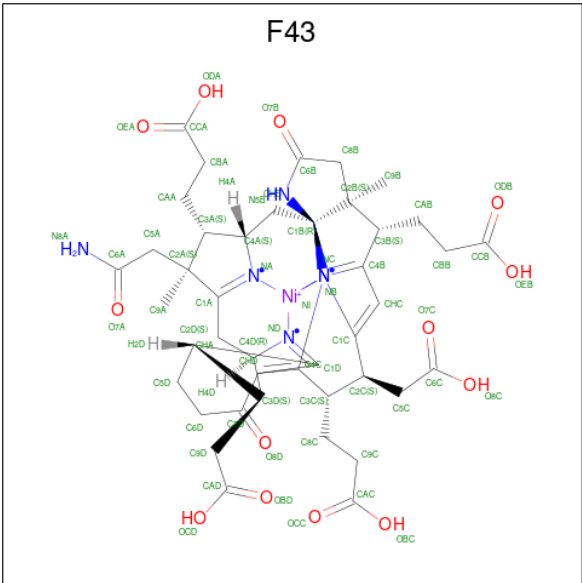
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		
8	E	1	Total	Cl	0	0
			1	1		
8	F	1	Total	Cl	0	0
			1	1		
8	G	1	Total	Cl	0	0
			1	1		
8	H	1	Total	Cl	0	0
			1	1		
8	I	1	Total	Cl	0	0
			1	1		
8	L	2	Total	Cl	0	0
			2	2		

- Molecule 9 is Coenzyme B (CCD ID: TP7) (formula: C<sub>11</sub>H<sub>22</sub>NO<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).



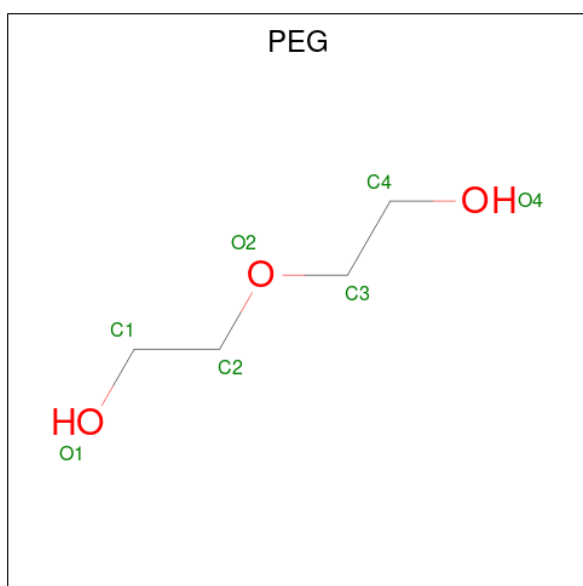
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
9	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
9	G	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
9	J	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 10 is FACTOR 430 (CCD ID: F43) (formula: C<sub>42</sub>H<sub>51</sub>N<sub>6</sub>NiO<sub>13</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
10	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
10	G	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
10	J	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	D	1	Total	C	H	O	0	0
			17	4	10	3		
11	E	1	Total	C	H	O	0	0
			17	4	10	3		
11	G	1	Total	C	H	O	0	0
			17	4	10	3		
11	G	1	Total	C	H	O	0	0
			17	4	10	3		
11	H	1	Total	C	H	O	0	0
			17	4	10	3		
11	J	1	Total	C	H	O	0	0
			17	4	10	3		
11	J	1	Total	C	H	O	0	0
			17	4	10	3		

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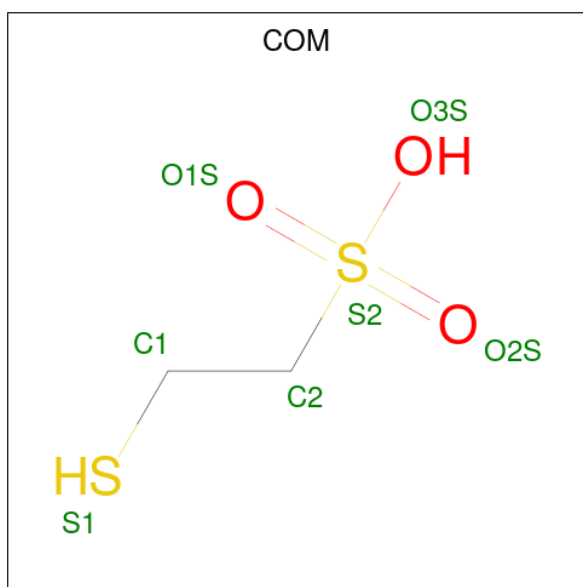
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	K	1	Total	C	H	O	0	0
			17	4	10	3		
11	L	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			14	3	8	3		
12	C	1	Total	C	H	O	0	0
			14	3	8	3		
12	C	1	Total	C	H	O	0	0
			14	3	8	3		
12	D	1	Total	C	H	O	0	0
			14	3	8	3		
12	J	1	Total	C	H	O	0	0
			14	3	8	3		
12	J	1	Total	C	H	O	0	0
			14	3	8	3		
12	J	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 13 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula:  $C_2H_6O_3S_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	S	0	0
			7	2	3	2		
13	D	1	Total	C	O	S	0	0
			7	2	3	2		
13	G	1	Total	C	O	S	0	0
			7	2	3	2		
13	J	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 14 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	1	Total	Na	0	0
			1	1		
14	K	1	Total	Na	0	0
			1	1		

- Molecule 15 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	D	1	Total	K	0	0
			1	1		
15	G	1	Total	K	0	0
			1	1		

- Molecule 16 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	497	Total 497	O 497	0	11
16	B	350	Total 350	O 350	0	19
16	C	309	Total 309	O 309	0	12
16	D	495	Total 495	O 495	0	11
16	E	331	Total 331	O 331	0	18
16	F	239	Total 239	O 239	0	11
16	G	483	Total 483	O 483	0	14
16	H	271	Total 271	O 271	0	7
16	I	283	Total 283	O 283	0	12
16	J	491	Total 491	O 491	0	12
16	K	282	Total 282	O 282	0	7
16	L	262	Total 262	O 262	0	12

### 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: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain A: 



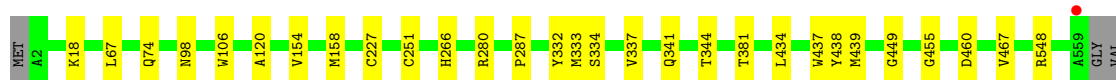
- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain D: 



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain G: 



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain J: 



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain B: 



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain E: 97%



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain H: 96%



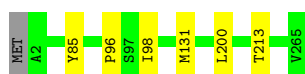
- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain K: 97%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain C: 97%



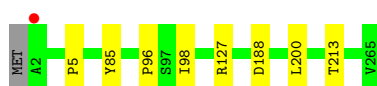
- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain F: 96%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain I: 97%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain L: 97%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.48Å 153.67Å 212.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.30 – 1.80 54.30 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.30-1.80) 100.0 (54.30-1.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.129 , 0.155 0.128 , 0.154	Depositor DCC
$R_{free}$ test set	23185 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	80668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: MGN, SMC, TRX, TP7, NA, GL3, GOL, COM, PEG, AGM, F43, EDO, K, PGE, MG, MHS, DYA, KR, 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	0.45	0/4327	0.66	0/5856
1	D	0.43	0/4327	0.65	0/5856
1	G	0.45	1/4327 (0.0%)	0.64	1/5856 (0.0%)
1	J	0.43	1/4348 (0.0%)	0.64	0/5884
2	B	0.39	0/3282	0.63	0/4447
2	E	0.38	0/3300	0.60	0/4471
2	H	0.35	0/3282	0.57	0/4447
2	K	0.37	0/3269	0.58	0/4429
3	C	0.38	0/2118	0.64	0/2870
3	F	0.40	0/2096	0.60	0/2841
3	I	0.34	0/2128	0.57	0/2884
3	L	0.39	0/2110	0.61	1/2860 (0.0%)
All	All	0.41	2/38914 (0.0%)	0.62	2/52701 (0.0%)

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	2
1	D	0	1
1	G	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	333	MET	SD-CE	-7.50	1.60	1.79
1	J	242	MET	SD-CE	6.44	1.95	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	74	GLN	N-CA-C	-5.96	104.91	111.82
3	L	6	GLN	N-CA-C	-5.58	106.60	113.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	ARG	Sidechain
1	A	548	ARG	Sidechain
1	D	450	ARG	Sidechain
1	G	548	ARG	Sidechain

## 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	4306	4054	4102	22	0
1	D	4306	4054	4102	22	0
1	G	4306	4054	4102	20	0
1	J	4315	4062	4098	20	0
2	B	3225	3212	3203	6	0
2	E	3236	3226	3207	7	0
2	H	3225	3212	3203	11	0
2	K	3219	3206	3205	8	0
3	C	2057	1987	1977	6	0
3	F	2048	1974	1973	8	0
3	I	2066	1987	1974	8	0
3	L	2057	1981	1974	5	0
4	A	8	0	0	5	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	6	0	0	1	0
4	E	1	0	0	0	0
4	F	2	0	0	1	0
4	G	7	0	0	6	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	2	0	0	1	0
4	J	7	0	0	4	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	2	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	A	10	14	14	0	0
6	D	20	28	28	0	0
6	G	20	28	28	0	0
6	H	10	14	14	0	0
7	A	12	18	18	0	0
7	B	4	6	6	0	0
7	D	12	18	18	0	0
7	F	4	6	6	0	0
7	G	8	12	12	0	0
7	I	8	12	12	0	0
7	J	12	18	18	0	0
7	K	4	6	6	0	0
7	L	4	6	6	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
8	L	2	0	0	0	0
9	A	21	0	19	1	0
9	D	21	0	19	0	0
9	G	21	0	19	0	0
9	J	21	0	19	0	0
10	A	62	0	43	3	0
10	D	62	0	43	2	0
10	G	62	0	43	3	0
10	J	62	0	43	1	0
11	A	7	10	10	0	0
11	D	7	10	10	0	0
11	E	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	14	20	20	0	0
11	H	7	10	10	0	0
11	J	14	20	20	0	0
11	K	7	10	10	0	0
11	L	7	10	10	1	0
12	A	6	8	8	0	0
12	C	12	16	16	0	0
12	D	6	8	8	0	0
12	J	18	24	24	0	0
13	A	7	0	5	0	0
13	D	7	0	5	0	0
13	G	7	0	5	0	0
13	J	7	0	5	0	0
14	C	1	0	0	0	0
14	K	1	0	0	0	0
15	D	1	0	0	0	0
15	G	1	0	0	0	0
16	A	497	0	0	0	0
16	B	350	0	0	0	0
16	C	309	0	0	0	0
16	D	495	0	0	0	0
16	E	331	0	0	0	0
16	F	239	0	0	0	0
16	G	483	0	0	0	0
16	H	271	0	0	1	0
16	I	283	0	0	0	0
16	J	491	0	0	0	0
16	K	282	0	0	0	0
16	L	262	0	0	0	0
All	All	43317	37351	37730	121	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 (121) 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:18:LYS:HG3	4:A:608:KR:KR	2.37	0.86
2:H:165:MET:HE1	1:J:275:MET:HE2	1.74	0.69
1:G:18:LYS:CG	4:G:608:KR:KR	3.06	0.65
1:G:18:LYS:HG3	4:G:608:KR:KR	2.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:VAL:HB	2:B:109:LEU:HB2	1.85	0.59
10:G:619:F43:H9A1	1:J:337:VAL:HB	1.83	0.59
1:A:154:VAL:HG22	1:D:67:LEU:HD23	1.87	0.57
1:D:337:VAL:HB	10:D:613:F43:H9A1	1.87	0.56
1:A:251:CYS:HB2	3:F:85:TYR:CZ	2.41	0.56
1:G:449:GLY:HA3	3:I:98:ILE:HD12	1.87	0.56
1:G:251:CYS:HB2	3:L:85:TYR:CE1	2.41	0.55
3:I:85:TYR:CE1	1:J:251:CYS:HB2	2.41	0.55
2:E:45:VAL:HB	2:E:109:LEU:HB2	1.88	0.55
1:A:251:CYS:HB2	3:F:85:TYR:CE1	2.42	0.54
1:D:120:ALA:HB2	4:D:603[A]:KR:KR	2.68	0.54
3:C:85:TYR:CE1	1:D:251:CYS:HB2	2.42	0.54
1:A:337:VAL:HB	10:A:615:F43:H9A1	1.89	0.53
3:I:200:LEU:HD21	4:I:301:KR:KR	2.69	0.53
1:A:449:GLY:HA3	3:C:98:ILE:HD12	1.90	0.52
1:A:381:THR:HG23	1:A:439:MET:HE3	1.92	0.51
1:D:449:GLY:HA3	3:F:98:ILE:HD12	1.92	0.51
2:H:87:LYS:NZ	16:H:607:HOH:O	2.44	0.51
1:J:380:ALA:CB	4:J:607:KR:KR	3.20	0.51
1:A:153:ILE:HG23	1:A:154:VAL:HG23	1.92	0.50
1:G:18:LYS:HG2	4:G:608:KR:KR	2.70	0.50
1:J:449:GLY:HA3	3:L:98:ILE:HD12	1.92	0.50
1:A:67:LEU:HD12	1:A:67:LEU:C	2.37	0.49
2:H:267:GLN:CD	3:I:5:PRO:HG3	2.37	0.49
3:C:96:PRO:HA	3:C:213:THR:HA	1.95	0.48
1:J:545:ARG:HH21	4:J:603[B]:KR:KR	2.57	0.48
2:E:299:MET:HE2	2:E:299:MET:HB2	1.77	0.48
1:G:251:CYS:HB2	3:L:85:TYR:CZ	2.48	0.48
1:J:158:MET:HA	1:J:158:MET:HE2	1.96	0.48
3:I:96:PRO:HA	3:I:213:THR:HA	1.96	0.48
1:A:120:ALA:HB2	4:A:602[A]:KR:KR	2.74	0.47
1:D:67:LEU:C	1:D:67:LEU:HD12	2.38	0.47
1:J:120:ALA:HB2	4:J:602:KR:KR	2.75	0.47
1:J:437:TRX:HD1	1:J:438:TYR:CD1	2.49	0.47
2:K:45:VAL:HG11	2:K:135:LEU:CD2	2.44	0.47
1:G:341:GLN:HA	1:G:344:THR:OG1	2.15	0.47
1:J:380:ALA:HB3	4:J:607:KR:KR	2.76	0.47
2:H:128:MET:HE2	2:H:174:SER:HB3	1.97	0.46
1:G:439:MET:HB2	4:G:605:KR:KR	2.77	0.46
3:C:200:LEU:HD21	4:C:301:KR:KR	2.76	0.46
1:A:380:ALA:CB	4:A:606:KR:KR	3.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:200:LEU:HD21	4:F:301:KR:KR	2.76	0.46
1:A:439:MET:HB2	4:A:606:KR:KR	2.77	0.46
2:K:45:VAL:HG11	2:K:135:LEU:HD21	1.98	0.45
3:F:96:PRO:HA	3:F:213:THR:HA	1.98	0.45
1:A:154:VAL:HG22	1:D:67:LEU:CD2	2.45	0.45
2:H:248:MET:HE1	2:H:303:TYR:CZ	2.52	0.45
3:L:96:PRO:HA	3:L:213:THR:HA	1.99	0.45
1:G:332:TYR:CZ	1:J:227:CYS:HA	2.52	0.45
2:K:240:TYR:HD2	2:K:248:MET:HE3	1.82	0.45
1:G:437:TRX:HD1	1:G:438:TYR:CD1	2.52	0.45
1:G:227:CYS:HA	1:J:332:TYR:CZ	2.53	0.44
3:I:85:TYR:CZ	1:J:251:CYS:HB2	2.52	0.44
1:A:227:CYS:HA	1:D:332:TYR:CZ	2.52	0.44
10:A:615:F43:C9A	10:A:615:F43:CBA	2.95	0.44
2:H:248:MET:HE1	2:H:303:TYR:CE1	2.53	0.44
2:H:353:THR:HG23	2:H:380:THR:HA	1.99	0.44
1:D:455:GL3:HA1	2:E:359:PHE:CB	2.48	0.44
1:J:9:LYS:HB2	1:J:12:VAL:HG23	2.00	0.43
1:D:191:ASN:ND2	1:D:194:ASP:OD2	2.51	0.43
2:H:78:LYS:HE3	2:H:143:TYR:CE1	2.54	0.43
1:D:437:TRX:HD1	1:D:438:TYR:CD1	2.53	0.43
10:G:619:F43:H3C	10:G:619:F43:O8D	2.18	0.43
1:D:219:ILE:HD13	1:D:232:THR:HA	2.01	0.43
1:J:41:ARG:NH1	1:J:44[A]:GLU:OE1	2.50	0.43
3:C:85:TYR:CZ	1:D:251:CYS:HB2	2.53	0.43
1:G:67:LEU:C	1:G:67:LEU:HD12	2.43	0.43
3:F:100:TYR:CD1	3:F:117:THR:HG21	2.54	0.43
1:A:341:GLN:HA	1:A:344:THR:OG1	2.19	0.43
2:B:152:TYR:CE2	1:D:477:CYS:HB2	2.53	0.43
1:D:381:THR:HG23	1:D:439:MET:HE3	2.01	0.43
1:G:98:ASN:HB3	4:G:606:KR:KR	2.79	0.43
2:K:183:GLU:HG3	2:K:376:ASN:O	2.19	0.43
1:A:380:ALA:HB3	4:A:606:KR:KR	2.80	0.42
2:K:233:TYR:OH	2:K:346:ASP:HA	2.19	0.42
2:E:233:TYR:OH	2:E:346:ASP:HA	2.19	0.42
1:G:337:VAL:HB	10:J:611:F43:H9A1	2.02	0.42
3:I:188:ASP:OD1	3:I:188:ASP:C	2.62	0.42
2:K:319:LEU:HD12	3:L:127:ARG:HG2	2.01	0.42
3:C:131:MET:HE3	3:C:131:MET:HB3	1.90	0.42
1:J:67:LEU:C	1:J:67:LEU:HD12	2.43	0.42
1:J:276:LEU:HD11	1:J:288:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:MET:HG2	2:H:252:MET:HE2	2.01	0.42
2:K:420:VAL:HG12	2:K:422:ILE:HG22	2.01	0.42
1:G:154:VAL:HG22	1:J:67:LEU:HD23	2.00	0.42
2:B:45:VAL:HG11	2:B:135:LEU:HD21	2.02	0.42
1:D:455:GL3:CA	2:E:359:PHE:HB2	2.50	0.42
2:H:233:TYR:OH	2:H:346:ASP:HA	2.20	0.42
1:A:437:TRX:HD1	1:A:438:TYR:CD1	2.54	0.42
2:E:319:LEU:HD12	3:F:127:ARG:HG2	2.02	0.42
1:D:89:VAL:HG12	1:D:544:MET:HE2	2.02	0.41
1:D:153:ILE:HG23	1:D:154:VAL:HG23	2.02	0.41
3:F:126:ALA:HB3	3:F:131:MET:HB2	2.01	0.41
1:D:444:HIS:CD2	1:D:444:HIS:C	2.98	0.41
1:A:332:TYR:CZ	1:D:227:CYS:HA	2.56	0.41
1:A:491:ASN:HA	9:A:614:TP7:S7	2.60	0.41
1:G:434:LEU:HG	1:G:467:VAL:HG22	2.02	0.41
2:H:319:LEU:HD12	3:I:127:ARG:HG2	2.03	0.41
2:B:45:VAL:CG1	2:B:135:LEU:HD21	2.49	0.41
1:G:120:ALA:HB2	4:G:607[A]:KR:KR	2.82	0.41
1:A:102:MET:HB3	1:A:322:MET:SD	2.60	0.41
2:B:248:MET:HE3	2:B:248:MET:HB2	1.95	0.41
10:A:615:F43:O8D	10:A:615:F43:H3C	2.21	0.41
2:B:233:TYR:OH	2:B:346:ASP:HA	2.21	0.41
1:J:41:ARG:HA	1:J:41:ARG:HD3	1.87	0.41
1:A:252:ALA:HB1	10:D:613:F43:H9B1	2.03	0.41
1:D:384:ALA:HB2	1:D:436:ALA:HB1	2.03	0.41
2:E:353:THR:HG23	2:E:380:THR:HA	2.02	0.41
1:G:106:TRP:CZ2	1:G:287:PRO:HD3	2.56	0.40
1:G:381:THR:HG23	1:G:439:MET:HE3	2.02	0.40
1:J:341:GLN:HA	1:J:344:THR:OG1	2.21	0.40
1:G:158:MET:HE2	1:G:158:MET:HA	2.03	0.40
11:L:305:PEG:H31	11:L:305:PEG:H12	1.78	0.40
1:A:113:ILE:HG23	1:A:217:VAL:HB	2.03	0.40
2:K:240:TYR:CD2	2:K:248:MET:HE3	2.57	0.40
1:D:477:CYS:SG	1:D:480:LEU:HG	2.61	0.40
10:G:619:F43:CBA	10:G:619:F43:C9A	3.00	0.40

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	549/561 (98%)	529 (96%)	19 (4%)	1 (0%)	44	31
1	D	549/561 (98%)	529 (96%)	19 (4%)	1 (0%)	44	31
1	G	549/561 (98%)	528 (96%)	20 (4%)	1 (0%)	44	31
1	J	551/561 (98%)	531 (96%)	19 (3%)	1 (0%)	44	31
2	B	433/434 (100%)	427 (99%)	6 (1%)	0	100	100
2	E	435/434 (100%)	428 (98%)	7 (2%)	0	100	100
2	H	433/434 (100%)	423 (98%)	10 (2%)	0	100	100
2	K	431/434 (99%)	423 (98%)	8 (2%)	0	100	100
3	C	264/265 (100%)	257 (97%)	7 (3%)	0	100	100
3	F	262/265 (99%)	252 (96%)	10 (4%)	0	100	100
3	I	266/265 (100%)	261 (98%)	5 (2%)	0	100	100
3	L	264/265 (100%)	256 (97%)	8 (3%)	0	100	100
All	All	4986/5040 (99%)	4844 (97%)	138 (3%)	4 (0%)	48	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	SER
1	A	334	SER
1	G	334	SER
1	J	334	SER

### 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	435/437 (100%)	435 (100%)	0	100	100
1	D	435/437 (100%)	434 (100%)	1 (0%)	92	91
1	G	435/437 (100%)	435 (100%)	0	100	100
1	J	437/437 (100%)	437 (100%)	0	100	100
2	B	341/340 (100%)	341 (100%)	0	100	100
2	E	343/340 (101%)	342 (100%)	1 (0%)	91	90
2	H	341/340 (100%)	341 (100%)	0	100	100
2	K	339/340 (100%)	339 (100%)	0	100	100
3	C	219/218 (100%)	219 (100%)	0	100	100
3	F	217/218 (100%)	217 (100%)	0	100	100
3	I	220/218 (101%)	220 (100%)	0	100	100
3	L	218/218 (100%)	217 (100%)	1 (0%)	86	86
All	All	3980/3980 (100%)	3977 (100%)	3 (0%)	92	91

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

Mol	Chain	Res	Type
1	D	282	ARG
2	E	173	LEU
3	L	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	459	GLN
2	B	56	ASN
2	B	91	GLN
2	B	234	GLN
3	C	182	ASN
1	D	74	GLN
1	D	231	ASN
1	D	271	GLN
2	E	234	GLN
2	E	402	GLN
1	G	215	GLN

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Mol	Chain	Res	Type
1	G	231	ASN
1	G	271	GLN
2	H	37	ASN
2	H	56	ASN
2	H	91	GLN
2	H	234	GLN
2	H	295	ASN
3	I	109	ASN
3	I	182	ASN
1	J	215	GLN
1	J	231	ASN
2	K	65	ASN
2	K	217	HIS
2	K	234	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	GL3	D	455	1	2,3,4	3.48	1 (50%)	1,2,4	0.19	0
1	MGN	A	410	1	6,9,10	0.68	0	5,12,14	0.21	0
1	GL3	G	455	1	2,3,4	3.84	1 (50%)	1,2,4	0.02	0
1	AGM	D	280	1	10,11,12	1.56	2 (20%)	6,13,15	0.92	0
1	SMC	D	462	1	5,6,7	0.58	0	2,6,8	0.11	0
1	SMC	J	462	1	5,6,7	0.57	0	2,6,8	0.85	0
1	TRX	J	437	1	14,16,17	0.61	0	15,22,24	0.77	0
1	GL3	A	455	1	2,3,4	3.55	1 (50%)	1,2,4	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AGM	J	280	1	10,11,12	1.30	1 (10%)	6,13,15	0.56	0
1	MHS	A	266	1	7,11,12	1.14	0	6,14,16	1.68	2 (33%)
1	TRX	G	437	1	14,16,17	0.59	0	15,22,24	0.75	0
1	MGN	G	410	1	6,9,10	0.55	0	5,12,14	0.61	0
1	AGM	A	280	1	10,11,12	1.31	1 (10%)	6,13,15	1.29	0
1	TRX	D	437	1	14,16,17	0.63	0	15,22,24	0.75	0
1	MGN	J	410	1	6,9,10	0.73	0	5,12,14	0.21	0
1	SMC	A	462	1	5,6,7	0.58	0	2,6,8	0.66	0
1	MGN	D	410	1	6,9,10	0.47	0	5,12,14	0.56	0
1	MHS	D	266	1	7,11,12	1.22	0	6,14,16	1.71	2 (33%)
1	TRX	A	437	1	14,16,17	0.64	0	15,22,24	0.73	0
1	MHS	G	266	1	7,11,12	1.27	1 (14%)	6,14,16	2.23	2 (33%)
1	DYA	G	460	1	7,7,8	2.19	2 (28%)	5,8,10	3.35	1 (20%)
1	GL3	J	455	1	2,3,4	3.53	1 (50%)	1,2,4	0.11	0
1	AGM	G	280	1	10,11,12	1.31	1 (10%)	6,13,15	0.93	0
1	MHS	J	266	1	7,11,12	1.25	1 (14%)	6,14,16	1.60	2 (33%)
1	DYA	J	460	1	7,7,8	2.17	2 (28%)	5,8,10	3.43	1 (20%)
1	SMC	G	462	1	5,6,7	0.63	0	2,6,8	0.60	0
1	DYA	D	460	1	7,7,8	2.02	2 (28%)	5,8,10	3.27	1 (20%)
1	DYA	A	460	1	7,7,8	1.99	2 (28%)	5,8,10	3.54	1 (20%)

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
1	GL3	D	455	1	-	0/1/1/2	-
1	MGN	A	410	1	-	0/7/9/12	-
1	GL3	G	455	1	-	1/1/1/2	-
1	AGM	D	280	1	-	1/10/11/13	-
1	SMC	D	462	1	-	1/3/5/7	-
1	SMC	J	462	1	-	1/3/5/7	-
1	TRX	J	437	1	-	0/4/6/8	0/2/2/2
1	GL3	A	455	1	-	0/1/1/2	-
1	AGM	J	280	1	-	2/10/11/13	-
1	MHS	A	266	1	-	0/5/6/8	0/1/1/1
1	TRX	G	437	1	-	0/4/6/8	0/2/2/2
1	MGN	G	410	1	-	0/7/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	A	280	1	-	3/10/11/13	-
1	TRX	D	437	1	-	0/4/6/8	0/2/2/2
1	MGN	J	410	1	-	0/7/9/12	-
1	SMC	A	462	1	-	1/3/5/7	-
1	MGN	D	410	1	-	0/7/9/12	-
1	MHS	D	266	1	-	0/5/6/8	0/1/1/1
1	TRX	A	437	1	-	0/4/6/8	0/2/2/2
1	MHS	G	266	1	-	0/5/6/8	0/1/1/1
1	DYA	G	460	1	-	4/4/6/8	-
1	GL3	J	455	1	-	1/1/1/2	-
1	AGM	G	280	1	-	3/10/11/13	-
1	MHS	J	266	1	-	0/5/6/8	0/1/1/1
1	DYA	J	460	1	-	4/4/6/8	-
1	SMC	G	462	1	-	1/3/5/7	-
1	DYA	D	460	1	-	4/4/6/8	-
1	DYA	A	460	1	-	4/4/6/8	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	455	GL3	C-S	-5.43	1.61	1.80
1	A	455	GL3	C-S	-5.01	1.63	1.80
1	J	455	GL3	C-S	-4.98	1.63	1.80
1	D	455	GL3	C-S	-4.91	1.63	1.80
1	G	460	DYA	C-CA	-4.81	1.37	1.45
1	J	460	DYA	C-CA	-4.74	1.37	1.45
1	A	460	DYA	C-CA	-4.22	1.38	1.45
1	D	460	DYA	C-CA	-4.20	1.38	1.45
1	D	280	AGM	CZ-NE1	3.23	1.38	1.33
1	G	280	AGM	CZ-NE1	2.83	1.38	1.33
1	G	460	DYA	OD1-CG	-2.81	1.23	1.30
1	D	460	DYA	OD1-CG	-2.75	1.23	1.30
1	J	280	AGM	CZ-NE1	2.72	1.37	1.33
1	J	460	DYA	OD1-CG	-2.70	1.23	1.30
1	A	460	DYA	OD1-CG	-2.47	1.23	1.30
1	A	280	AGM	CZ-NE1	2.33	1.37	1.33
1	D	280	AGM	CB-CA	2.16	1.56	1.53
1	J	266	MHS	CM-ND1	-2.11	1.42	1.47
1	G	266	MHS	CB-CG	-2.01	1.47	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	DYA	O-C-CA	-7.58	115.76	125.39
1	J	460	DYA	O-C-CA	-7.17	116.28	125.39
1	G	460	DYA	O-C-CA	-7.14	116.32	125.39
1	D	460	DYA	O-C-CA	-6.83	116.70	125.39
1	G	266	MHS	CB-CA-C	-4.02	103.93	111.47
1	G	266	MHS	CM-ND1-CG	3.60	129.22	124.44
1	A	266	MHS	CM-ND1-CG	3.31	128.85	124.44
1	D	266	MHS	CB-CA-C	-3.03	105.79	111.47
1	J	266	MHS	CM-ND1-CG	2.94	128.35	124.44
1	D	266	MHS	CM-ND1-CG	2.84	128.23	124.44
1	J	266	MHS	CB-CA-C	-2.44	106.89	111.47
1	A	266	MHS	CB-CA-C	-2.24	107.26	111.47

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	460	DYA	N-CA-CB-CG
1	A	460	DYA	O-C-CA-CB
1	A	462	SMC	CA-CB-SG-CS
1	D	460	DYA	N-CA-CB-CG
1	D	460	DYA	O-C-CA-CB
1	D	460	DYA	CA-CB-CG-OD1
1	D	462	SMC	CA-CB-SG-CS
1	G	460	DYA	N-CA-CB-CG
1	G	460	DYA	O-C-CA-CB
1	J	460	DYA	N-CA-CB-CG
1	J	460	DYA	O-C-CA-CB
1	J	462	SMC	CA-CB-SG-CS
1	J	460	DYA	CA-CB-CG-OD1
1	G	455	GL3	S-C-CA-N
1	A	460	DYA	CA-CB-CG-OD1
1	G	460	DYA	CA-CB-CG-OD1
1	A	460	DYA	CA-CB-CG-OD2
1	D	460	DYA	CA-CB-CG-OD2
1	G	460	DYA	CA-CB-CG-OD2
1	J	460	DYA	CA-CB-CG-OD2
1	G	462	SMC	CA-CB-SG-CS
1	J	455	GL3	S-C-CA-N
1	J	280	AGM	CE2-CD-NE1-CZ
1	G	280	AGM	NE1-CD-CG-CB
1	A	280	AGM	CE2-CD-NE1-CZ
1	G	280	AGM	CE2-CD-NE1-CZ

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Mol	Chain	Res	Type	Atoms
1	A	280	AGM	CE2-CD-CG-CB
1	A	280	AGM	NE1-CD-CG-CB
1	G	280	AGM	CE2-CD-CG-CB
1	J	280	AGM	NE1-CD-CG-CB
1	D	280	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	455	GL3	2	0
1	J	437	TRX	1	0
1	G	437	TRX	1	0
1	D	437	TRX	1	0
1	A	437	TRX	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 58 are monoatomic - leaving 52 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	$\# Z  > 2$
6	PGE	H	504	-	9,9,9	0.13	0	8,8,8	0.12	0
10	F43	D	613	1,13	61,71,71	2.12	5 (8%)	64,118,118	1.32	8 (12%)
11	PEG	A	616	-	6,6,6	0.11	0	5,5,5	0.07	0
13	COM	A	620	10	6,6,6	1.13	0	7,8,8	1.43	1 (14%)
6	PGE	G	610	-	9,9,9	0.12	0	8,8,8	0.12	0
11	PEG	K	504	-	6,6,6	0.11	0	5,5,5	0.09	0
11	PEG	J	609	-	6,6,6	0.11	0	5,5,5	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PGE	G	618	-	9,9,9	0.09	0	8,8,8	0.15	0
7	EDO	K	505	-	3,3,3	0.06	0	2,2,2	0.18	0
9	TP7	G	614	-	19,20,20	0.80	0	24,26,26	0.83	0
7	EDO	I	305	-	3,3,3	0.05	0	2,2,2	0.19	0
9	TP7	J	612	-	19,20,20	0.69	0	24,26,26	0.72	0
12	GOL	J	616	-	5,5,5	0.10	0	5,5,5	0.32	0
13	COM	J	613	10	6,6,6	1.26	1 (16%)	7,8,8	2.71	4 (57%)
7	EDO	B	503	-	3,3,3	0.05	0	2,2,2	0.31	0
11	PEG	L	305	-	6,6,6	0.12	0	5,5,5	0.07	0
7	EDO	G	611	-	3,3,3	0.06	0	2,2,2	0.19	0
6	PGE	D	610	-	9,9,9	0.13	0	8,8,8	0.12	0
7	EDO	G	617	-	3,3,3	0.06	0	2,2,2	0.18	0
7	EDO	D	615	-	3,3,3	0.08	0	2,2,2	0.18	0
7	EDO	J	619	-	3,3,3	0.11	0	2,2,2	0.14	0
9	TP7	A	614	-	19,20,20	0.89	0	24,26,26	0.74	0
9	TP7	D	611	-	19,20,20	0.79	0	24,26,26	0.81	0
11	PEG	G	616	-	6,6,6	0.10	0	5,5,5	0.07	0
11	PEG	H	503	-	6,6,6	0.10	0	5,5,5	0.08	0
12	GOL	J	614	-	5,5,5	0.09	0	5,5,5	0.37	0
12	GOL	D	609	-	5,5,5	0.09	0	5,5,5	0.32	0
6	PGE	D	614	-	9,9,9	0.13	0	8,8,8	0.13	0
7	EDO	F	304	-	3,3,3	0.06	0	2,2,2	0.18	0
12	GOL	A	619	-	5,5,5	0.09	0	5,5,5	0.32	0
7	EDO	A	612	-	3,3,3	0.06	0	2,2,2	0.38	0
7	EDO	L	304	-	3,3,3	0.06	0	2,2,2	0.19	0
11	PEG	E	503	-	6,6,6	0.11	0	5,5,5	0.07	0
7	EDO	J	617	-	3,3,3	0.06	0	2,2,2	0.18	0
11	PEG	J	610	-	6,6,6	0.11	0	5,5,5	0.08	0
7	EDO	A	617	-	3,3,3	0.06	0	2,2,2	0.19	0
6	PGE	A	611	-	9,9,9	0.12	0	8,8,8	0.13	0
13	COM	G	613	10	6,6,6	1.64	1 (16%)	7,8,8	1.20	1 (14%)
11	PEG	D	618	-	6,6,6	0.09	0	5,5,5	0.09	0
7	EDO	J	618	-	3,3,3	0.06	0	2,2,2	0.17	0
10	F43	J	611	1,13	61,71,71	2.18	13 (21%)	64,118,118	1.36	8 (12%)
7	EDO	A	618	-	3,3,3	0.06	0	2,2,2	0.19	0
10	F43	A	615	1,13	61,71,71	2.16	5 (8%)	64,118,118	1.19	7 (10%)
12	GOL	C	304	-	5,5,5	0.09	0	5,5,5	0.32	0
12	GOL	C	305	-	5,5,5	0.08	0	5,5,5	0.31	0
7	EDO	D	616	-	3,3,3	0.07	0	2,2,2	0.17	0
10	F43	G	619	1,13	61,71,71	2.12	5 (8%)	64,118,118	1.27	9 (14%)
13	COM	D	612	10	6,6,6	1.54	2 (33%)	7,8,8	1.51	2 (28%)
7	EDO	D	617	-	3,3,3	0.04	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	PEG	G	615	-	6,6,6	0.10	0	5,5,5	0.08	0
7	EDO	I	304	-	3,3,3	0.06	0	2,2,2	0.18	0
12	GOL	J	615	-	5,5,5	0.08	0	5,5,5	0.33	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	PGE	H	504	-	-	3/7/7/7	-
10	F43	D	613	1,13	-	7/28/185/185	-
11	PEG	A	616	-	-	2/4/4/4	-
13	COM	A	620	10	-	0/4/4/4	-
6	PGE	G	610	-	-	1/7/7/7	-
11	PEG	K	504	-	-	1/4/4/4	-
11	PEG	J	609	-	-	4/4/4/4	-
6	PGE	G	618	-	-	4/7/7/7	-
7	EDO	K	505	-	-	1/1/1/1	-
9	TP7	G	614	-	-	0/24/24/24	-
7	EDO	I	305	-	-	1/1/1/1	-
9	TP7	J	612	-	-	1/24/24/24	-
12	GOL	J	616	-	-	0/4/4/4	-
13	COM	J	613	10	-	1/4/4/4	-
7	EDO	B	503	-	-	1/1/1/1	-
11	PEG	L	305	-	-	3/4/4/4	-
7	EDO	G	611	-	-	1/1/1/1	-
6	PGE	D	610	-	-	0/7/7/7	-
7	EDO	G	617	-	-	1/1/1/1	-
7	EDO	D	615	-	-	0/1/1/1	-
7	EDO	J	619	-	-	1/1/1/1	-
9	TP7	A	614	-	-	1/24/24/24	-
9	TP7	D	611	-	-	0/24/24/24	-
11	PEG	G	616	-	-	2/4/4/4	-
11	PEG	H	503	-	-	3/4/4/4	-
12	GOL	J	614	-	-	4/4/4/4	-
12	GOL	D	609	-	-	2/4/4/4	-
6	PGE	D	614	-	-	3/7/7/7	-
7	EDO	F	304	-	-	0/1/1/1	-
12	GOL	A	619	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	612	-	-	0/1/1/1	-
7	EDO	L	304	-	-	0/1/1/1	-
11	PEG	E	503	-	-	1/4/4/4	-
7	EDO	J	617	-	-	1/1/1/1	-
11	PEG	J	610	-	-	1/4/4/4	-
7	EDO	A	617	-	-	1/1/1/1	-
6	PGE	A	611	-	-	2/7/7/7	-
13	COM	G	613	10	-	0/4/4/4	-
11	PEG	D	618	-	-	1/4/4/4	-
7	EDO	J	618	-	-	1/1/1/1	-
10	F43	J	611	1,13	-	5/28/185/185	-
7	EDO	A	618	-	-	1/1/1/1	-
10	F43	A	615	1,13	-	9/28/185/185	-
12	GOL	C	304	-	-	2/4/4/4	-
12	GOL	C	305	-	-	2/4/4/4	-
7	EDO	D	616	-	-	1/1/1/1	-
10	F43	G	619	1,13	-	7/28/185/185	-
13	COM	D	612	10	-	0/4/4/4	-
7	EDO	D	617	-	-	0/1/1/1	-
11	PEG	G	615	-	-	4/4/4/4	-
7	EDO	I	304	-	-	1/1/1/1	-
12	GOL	J	615	-	-	4/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	619	F43	NI-NA	9.34	2.09	1.89
10	D	613	F43	NI-NA	9.03	2.09	1.89
10	A	615	F43	NI-NB	8.32	2.07	1.89
10	A	615	F43	NI-NA	8.31	2.07	1.89
10	J	611	F43	NI-NA	7.69	2.06	1.89
10	A	615	F43	NI-ND	7.54	2.05	1.89
10	D	613	F43	NI-NB	7.34	2.05	1.89
10	J	611	F43	CHD-C1D	-7.14	1.34	1.43
10	G	619	F43	NI-ND	7.12	2.04	1.89
10	G	619	F43	NI-NB	7.10	2.04	1.89
10	D	613	F43	NI-ND	6.79	2.04	1.89
10	J	611	F43	NI-ND	6.77	2.04	1.89
10	J	611	F43	NI-NB	6.62	2.03	1.89
10	D	613	F43	CHD-C1D	-5.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	615	F43	CHD-C1D	-5.45	1.36	1.43
10	G	619	F43	CHD-C1D	-5.39	1.36	1.43
13	G	613	COM	C2-S2	3.58	1.82	1.77
10	A	615	F43	CHC-C4B	3.15	1.48	1.39
10	J	611	F43	CHB-C1B	-2.91	1.51	1.53
10	G	619	F43	CHC-C4B	2.79	1.47	1.39
10	D	613	F43	CHC-C4B	2.61	1.46	1.39
10	J	611	F43	CHC-C4B	2.55	1.46	1.39
13	D	612	COM	O2S-S2	2.43	1.52	1.45
13	D	612	COM	C2-S2	2.34	1.80	1.77
10	J	611	F43	C2B-C3B	-2.18	1.50	1.57
10	J	611	F43	C6A-N8A	-2.17	1.25	1.32
10	J	611	F43	C8B-C2B	-2.15	1.51	1.54
10	J	611	F43	CHC-C1C	-2.13	1.32	1.36
13	J	613	COM	O1S-S2	2.04	1.51	1.45
10	J	611	F43	C1C-NC	-2.03	1.32	1.37
10	J	611	F43	O8C-C6C	-2.03	1.23	1.30
10	J	611	F43	CHD-C4C	-2.00	1.35	1.40

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	613	COM	O2S-S2-C2	4.19	111.97	106.92
10	J	611	F43	O7B-C6B-C8B	-4.19	121.47	126.59
13	J	613	COM	O2S-S2-O1S	-3.66	101.30	113.95
13	J	613	COM	O1S-S2-C2	3.65	111.31	106.92
10	J	611	F43	O8D-C7D-C6D	-3.63	114.91	120.86
10	D	613	F43	O7B-C6B-C8B	-3.27	122.60	126.59
10	J	611	F43	CAB-C3B-C2B	-3.04	112.66	119.09
10	A	615	F43	O8D-C7D-C6D	-2.95	116.03	120.86
10	D	613	F43	C5D-C2D-C1D	2.82	114.25	110.45
10	D	613	F43	C6D-C7D-CHD	2.82	122.24	116.95
10	A	615	F43	O7B-C6B-C8B	-2.63	123.38	126.59
10	J	611	F43	C4D-ND-C1D	2.56	111.88	108.51
10	G	619	F43	C2C-C5C-C6C	-2.56	108.94	114.04
13	A	620	COM	O2S-S2-C2	2.52	109.95	106.92
13	D	612	COM	O3S-S2-O1S	2.48	117.32	111.27
10	A	615	F43	CAB-C3B-C2B	-2.42	113.97	119.09
10	A	615	F43	C4D-ND-C1D	2.41	111.69	108.51
10	G	619	F43	O8C-C6C-C5C	2.38	121.70	114.07
10	D	613	F43	O8D-C7D-C6D	-2.38	116.97	120.86
13	J	613	COM	O3S-S2-C2	2.30	109.49	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	619	F43	C2B-C1B-NB	2.27	105.24	101.84
10	D	613	F43	C1B-C2B-C3B	2.20	104.77	101.51
10	J	611	F43	C3A-C4A-NA	-2.19	98.97	102.30
10	G	619	F43	C9B-C2B-C8B	-2.18	104.94	110.45
10	J	611	F43	C9A-C2A-C3A	2.18	116.20	112.98
13	D	612	COM	O2S-S2-O1S	-2.18	106.41	113.95
10	G	619	F43	OBC-CAC-C9C	2.17	121.01	114.03
10	J	611	F43	C1B-C2B-C3B	2.17	104.72	101.51
10	G	619	F43	O8D-C7D-C6D	-2.15	117.34	120.86
10	D	613	F43	ODA-CCA-CBA	2.12	120.84	114.03
10	A	615	F43	C2B-C1B-NB	2.11	105.00	101.84
10	A	615	F43	C6D-C7D-CHD	2.11	120.92	116.95
13	G	613	COM	O1S-S2-C2	2.10	109.44	106.92
10	D	613	F43	CAB-C3B-C2B	-2.10	114.65	119.09
10	J	611	F43	O7B-C6B-N5B	2.09	127.86	125.13
10	G	619	F43	C4D-ND-C1D	2.06	111.22	108.51
10	G	619	F43	C6D-C7D-CHD	2.06	120.82	116.95
10	G	619	F43	O7B-C6B-C8B	-2.02	124.12	126.59
10	D	613	F43	C2C-C5C-C6C	-2.02	110.02	114.04
10	A	615	F43	C1B-C2B-C3B	2.00	104.48	101.51

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	304	GOL	O1-C1-C2-O2
12	C	304	GOL	O1-C1-C2-C3
12	J	614	GOL	O1-C1-C2-C3
12	J	614	GOL	C1-C2-C3-O3
11	L	305	PEG	C1-C2-O2-C3
6	A	611	PGE	O2-C3-C4-O3
6	H	504	PGE	O2-C3-C4-O3
12	J	614	GOL	O2-C2-C3-O3
11	G	615	PEG	O1-C1-C2-O2
11	J	610	PEG	O2-C3-C4-O4
6	G	618	PGE	O1-C1-C2-O2
11	D	618	PEG	O1-C1-C2-O2
11	G	615	PEG	O2-C3-C4-O4
11	G	616	PEG	O2-C3-C4-O4
11	J	609	PEG	O1-C1-C2-O2
12	A	619	GOL	O1-C1-C2-C3
12	C	305	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	D	609	GOL	O1-C1-C2-C3
12	J	615	GOL	C1-C2-C3-O3
6	G	618	PGE	O3-C5-C6-O4
12	J	615	GOL	O2-C2-C3-O3
7	B	503	EDO	O1-C1-C2-O2
7	D	616	EDO	O1-C1-C2-O2
7	G	611	EDO	O1-C1-C2-O2
7	I	305	EDO	O1-C1-C2-O2
7	J	618	EDO	O1-C1-C2-O2
7	J	619	EDO	O1-C1-C2-O2
6	H	504	PGE	O3-C5-C6-O4
11	H	503	PEG	O2-C3-C4-O4
11	L	305	PEG	O2-C3-C4-O4
12	J	614	GOL	O1-C1-C2-O2
11	J	609	PEG	O2-C3-C4-O4
10	G	619	F43	C3A-CAA-CBA-CCA
10	D	613	F43	C3A-CAA-CBA-CCA
12	A	619	GOL	O1-C1-C2-O2
12	D	609	GOL	O1-C1-C2-O2
7	A	617	EDO	O1-C1-C2-O2
7	A	618	EDO	O1-C1-C2-O2
11	H	503	PEG	C4-C3-O2-C2
11	G	615	PEG	C4-C3-O2-C2
11	J	609	PEG	C1-C2-O2-C3
9	A	614	TP7	CB-O4P-P-O3P
9	J	612	TP7	CB-O4P-P-O3P
12	J	615	GOL	O1-C1-C2-O2
11	G	615	PEG	C1-C2-O2-C3
10	A	615	F43	C3A-CAA-CBA-CCA
6	G	610	PGE	O2-C3-C4-O3
11	L	305	PEG	O1-C1-C2-O2
6	D	614	PGE	C1-C2-O2-C3
6	G	618	PGE	C6-C5-O3-C4
10	G	619	F43	C2C-C5C-C6C-O8C
11	K	504	PEG	O2-C3-C4-O4
11	J	609	PEG	C4-C3-O2-C2
7	J	617	EDO	O1-C1-C2-O2
6	H	504	PGE	C4-C3-O2-C2
11	G	616	PEG	C1-C2-O2-C3
11	A	616	PEG	C4-C3-O2-C2
11	E	503	PEG	C1-C2-O2-C3
12	C	305	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	D	614	PGE	C3-C4-O3-C5
10	A	615	F43	CAB-CBB-CCB-OEB
10	G	619	F43	CAA-CBA-CCA-OEA
11	A	616	PEG	C1-C2-O2-C3
10	G	619	F43	CAA-CBA-CCA-ODA
10	J	611	F43	C3A-CAA-CBA-CCA
10	D	613	F43	C2C-C5C-C6C-O8C
10	A	615	F43	CAB-CBB-CCB-ODB
10	J	611	F43	CAA-CBA-CCA-OEA
10	J	611	F43	CAB-CBB-CCB-OEB
7	I	304	EDO	O1-C1-C2-O2
7	K	505	EDO	O1-C1-C2-O2
10	D	613	F43	C2C-C5C-C6C-O7C
6	A	611	PGE	C4-C3-O2-C2
6	G	618	PGE	C3-C4-O3-C5
10	A	615	F43	CAA-CBA-CCA-ODA
11	H	503	PEG	C1-C2-O2-C3
10	G	619	F43	CAB-CBB-CCB-OEB
6	D	614	PGE	C4-C3-O2-C2
10	D	613	F43	CAA-CBA-CCA-ODA
10	A	615	F43	C2C-C5C-C6C-O7C
10	G	619	F43	C2C-C5C-C6C-O7C
10	D	613	F43	CAB-CBB-CCB-OEB
10	J	611	F43	CAB-CBB-CCB-ODB
7	G	617	EDO	O1-C1-C2-O2
10	A	615	F43	CAA-CBA-CCA-OEA
10	D	613	F43	CAB-CBB-CCB-ODB
10	J	611	F43	CAA-CBA-CCA-ODA
10	A	615	F43	C2C-C5C-C6C-O8C
10	A	615	F43	C3D-C9D-CAD-OCD
13	J	613	COM	C1-C2-S2-O2S
10	D	613	F43	CAA-CBA-CCA-OEA
10	G	619	F43	CAB-CBB-CCB-ODB
12	J	615	GOL	O1-C1-C2-C3
10	A	615	F43	C3D-C9D-CAD-OB

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	613	F43	2	0
11	L	305	PEG	1	0

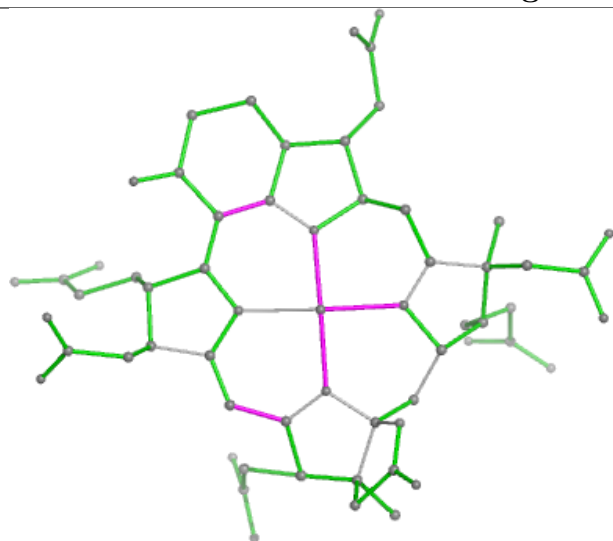
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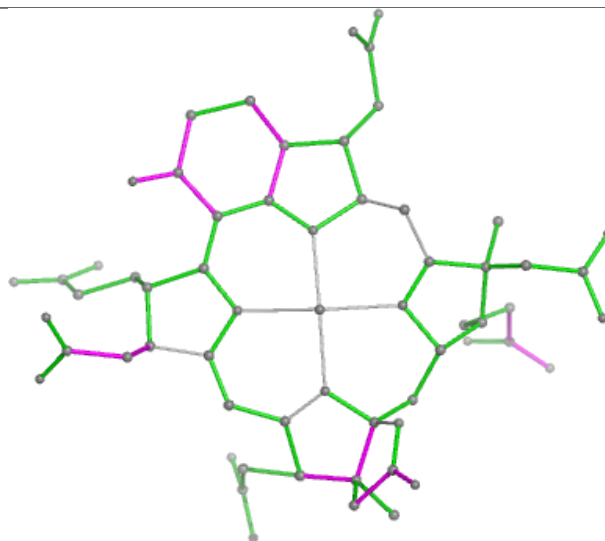
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	614	TP7	1	0
10	J	611	F43	1	0
10	A	615	F43	3	0
10	G	619	F43	3	0

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 than 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.

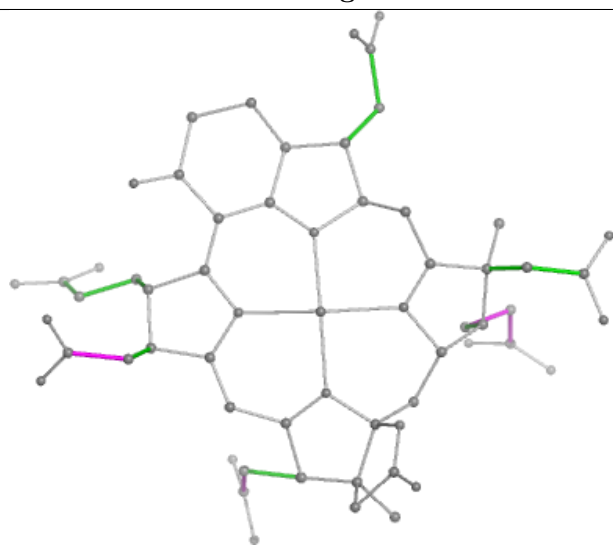
## Ligand F43 D 613



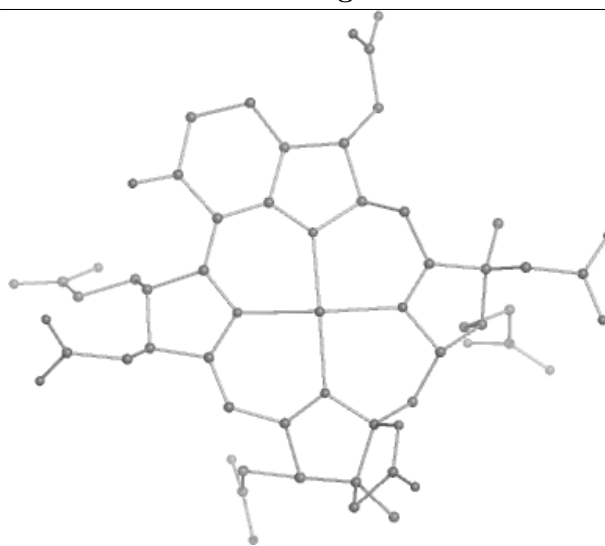
Bond lengths



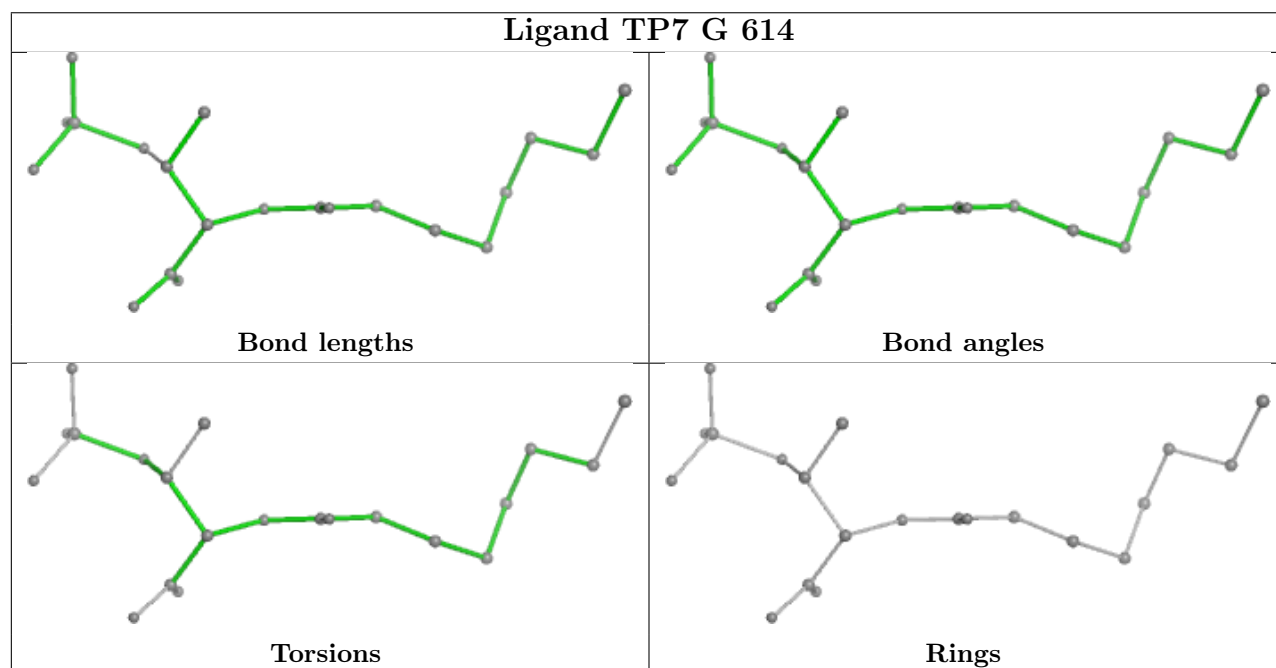
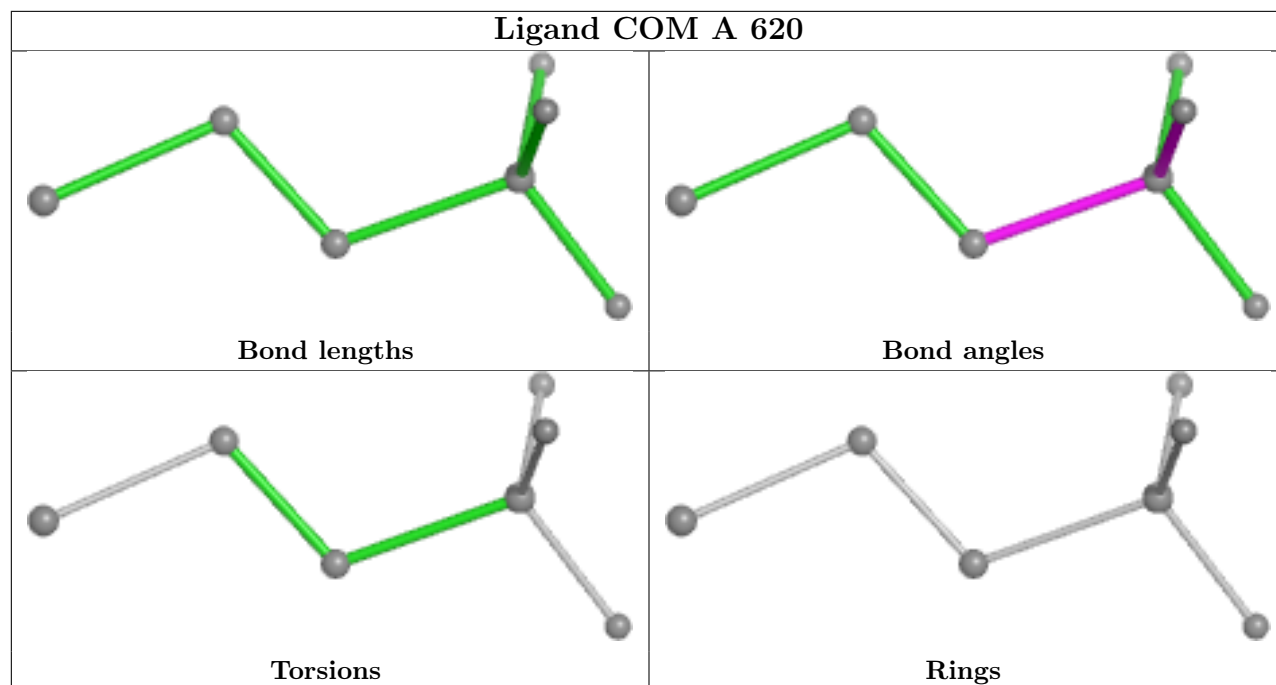
Bond angles

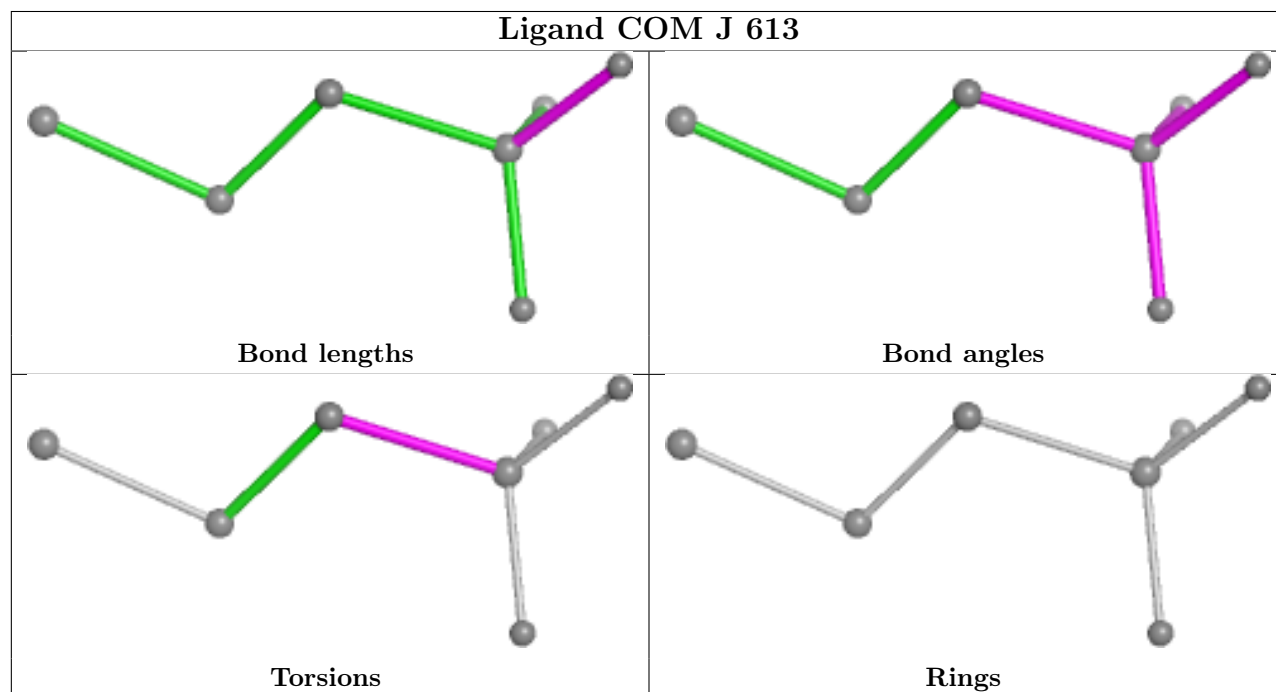
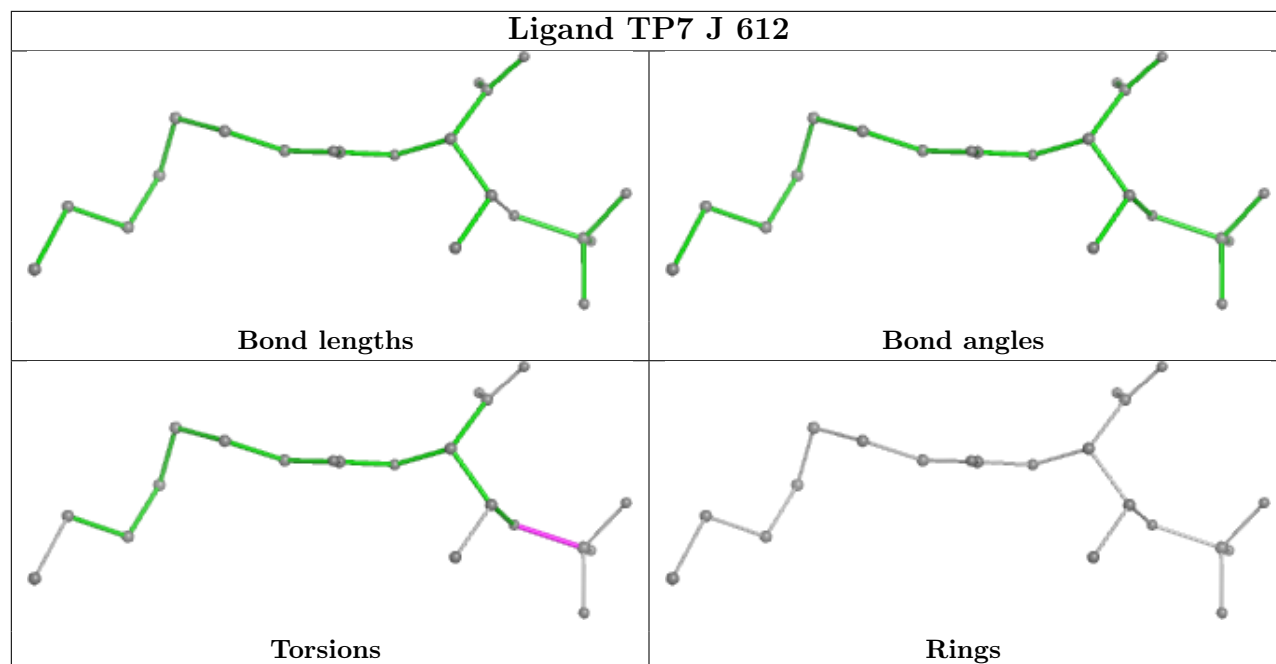


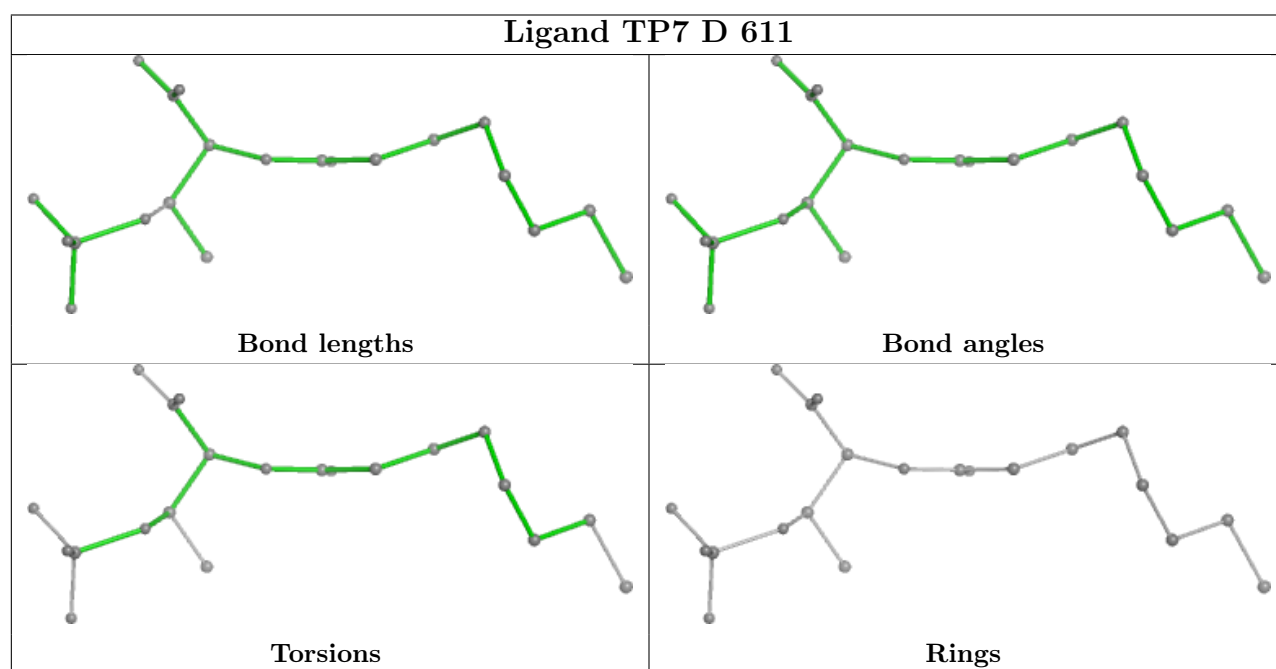
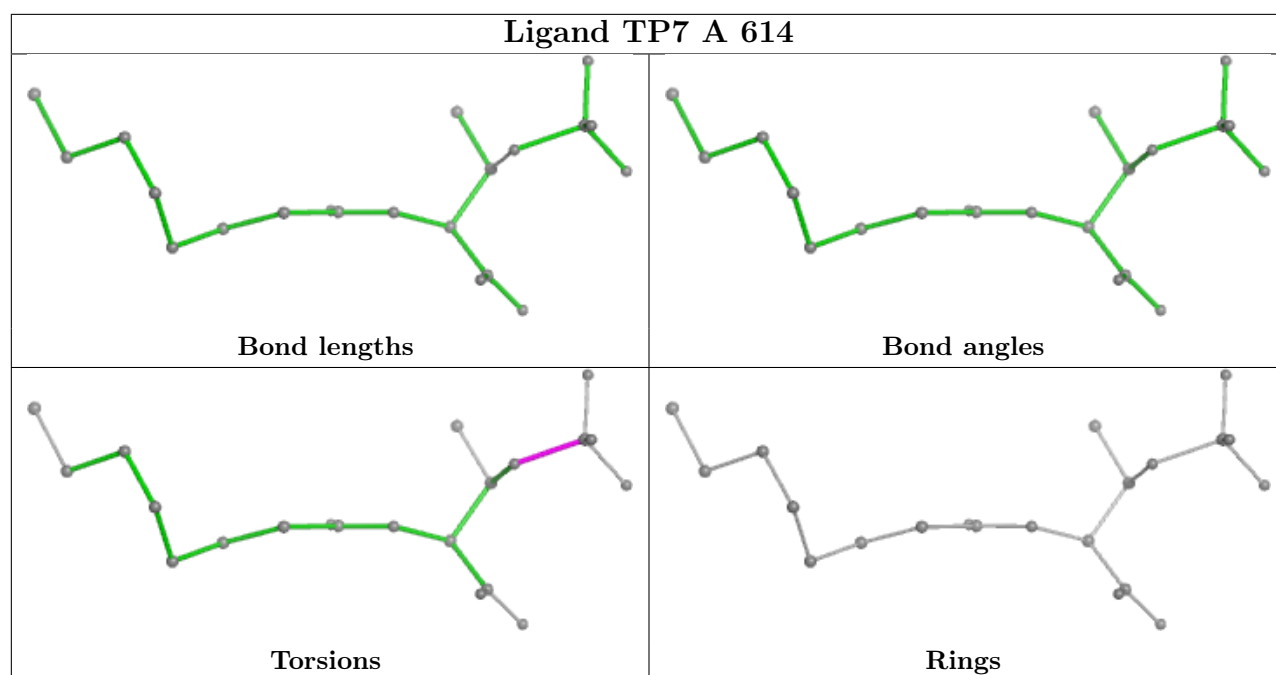
Torsions

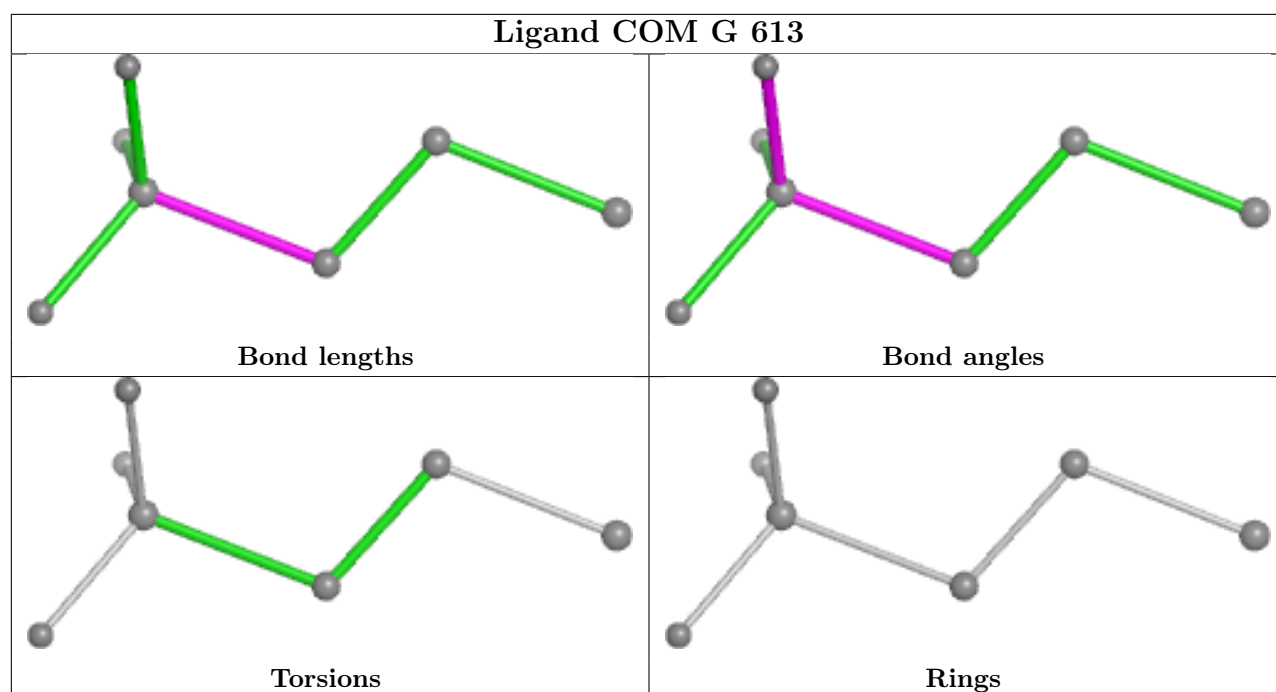


Rings



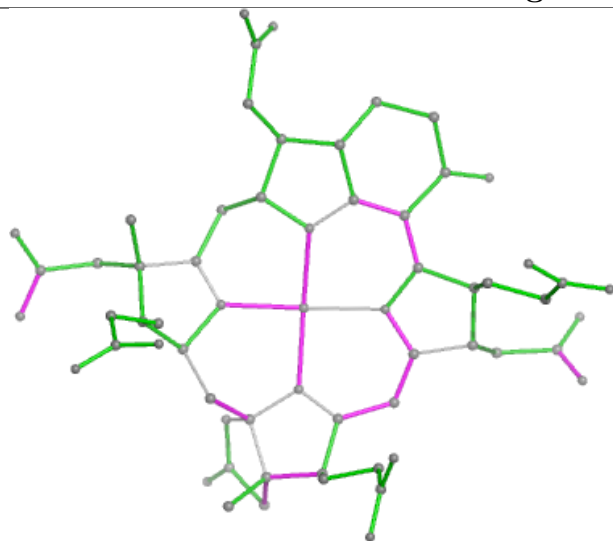




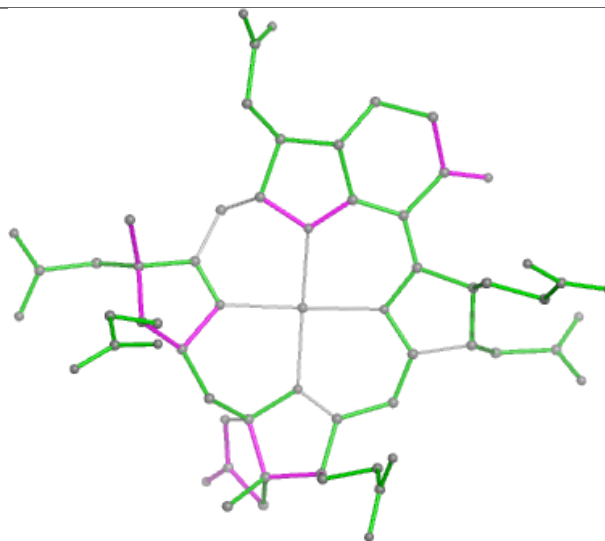




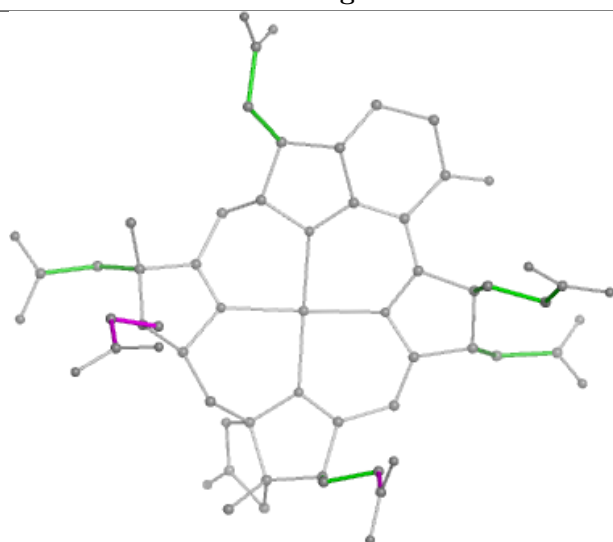
## Ligand F43 J 611



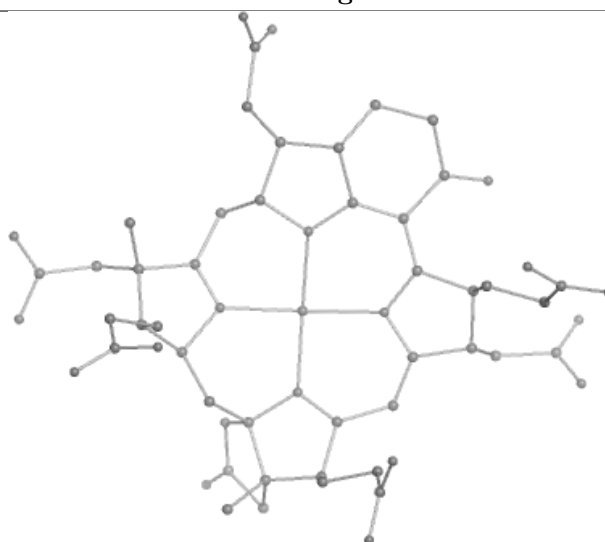
Bond lengths



Bond angles

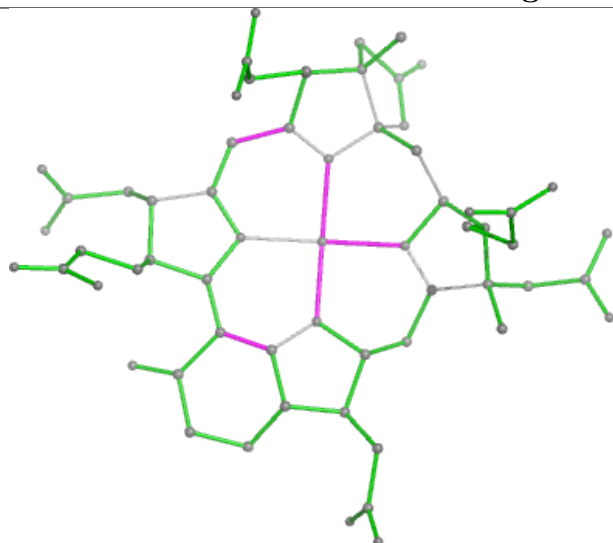


Torsions

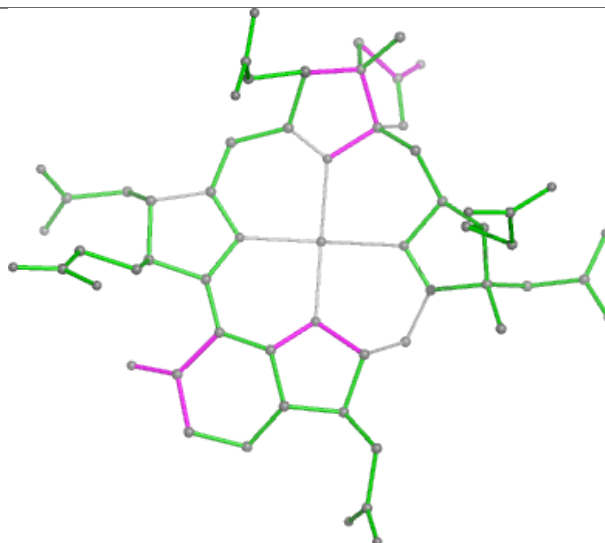


Rings

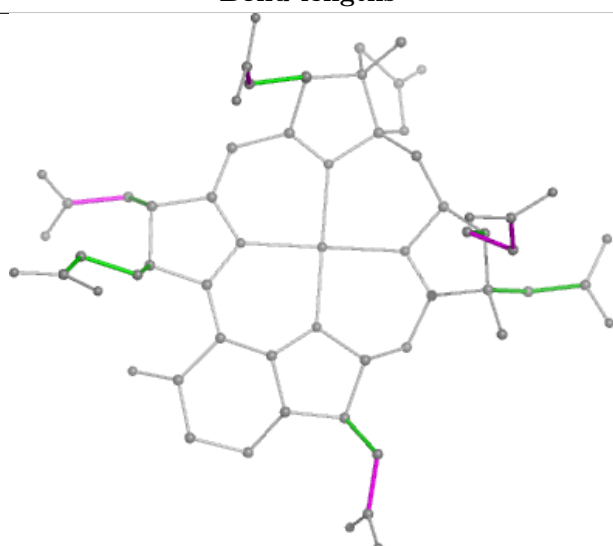
## Ligand F43 A 615



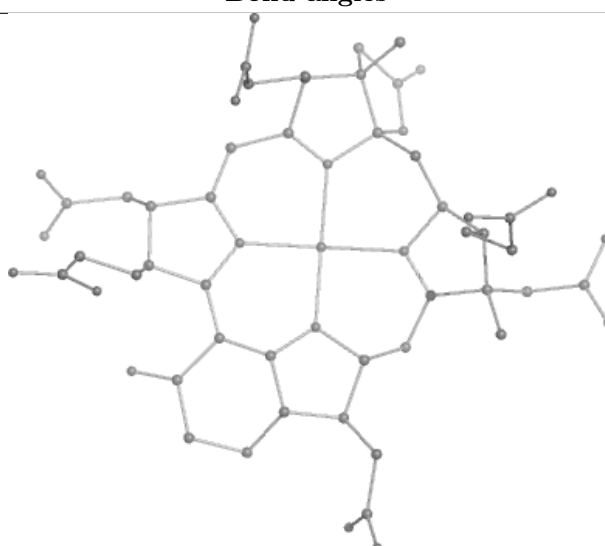
Bond lengths



Bond angles

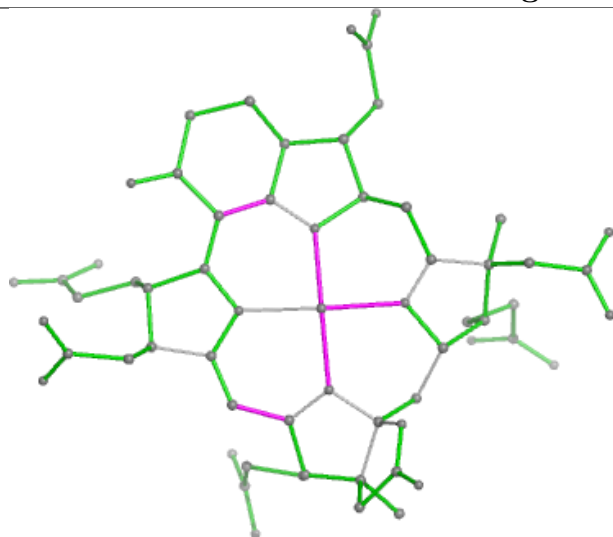


Torsions

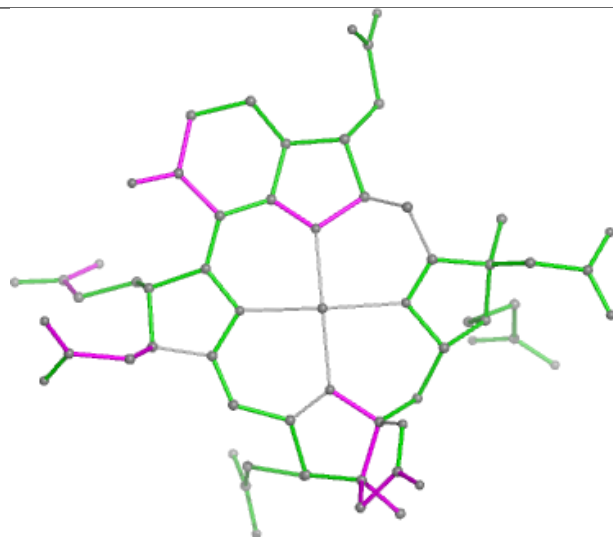


Rings

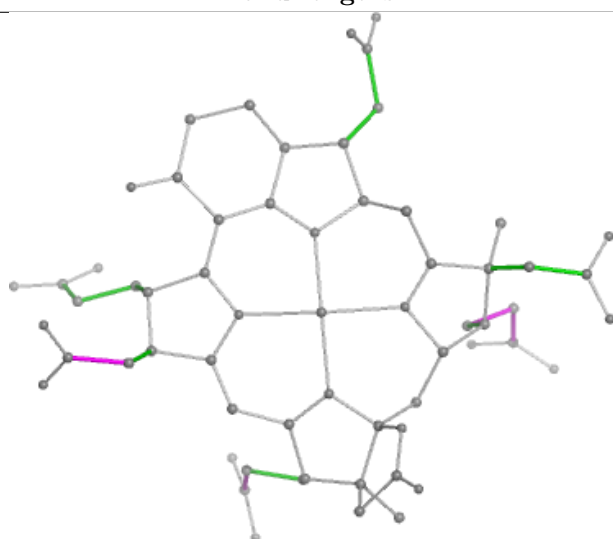
## Ligand F43 G 619



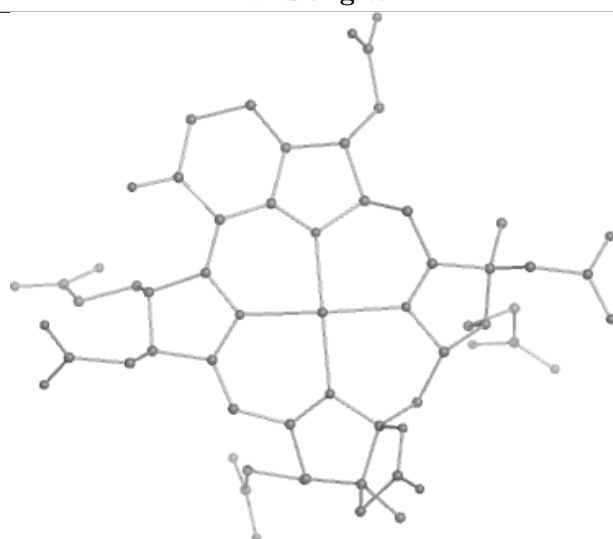
Bond lengths



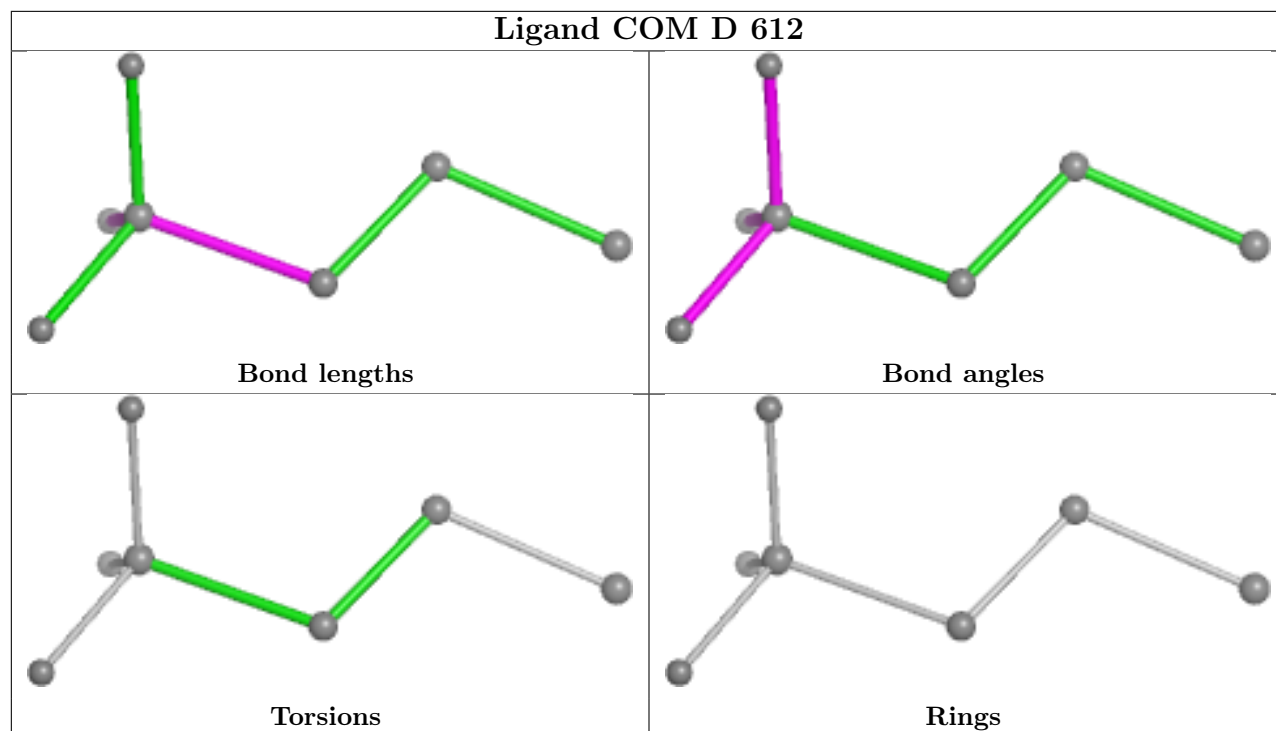
Bond angles



Torsions



Rings



## 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	551/561 (98%)	-1.02	1 (0%) 92 91	19, 25, 38, 69	0
1	D	551/561 (98%)	-1.01	1 (0%) 92 91	19, 26, 39, 60	0
1	G	551/561 (98%)	-1.02	1 (0%) 92 91	21, 26, 38, 58	0
1	J	551/561 (98%)	-0.98	1 (0%) 92 91	15, 27, 40, 60	1 (0%)
2	B	433/434 (99%)	-0.94	1 (0%) 92 91	14, 28, 41, 71	1 (0%)
2	E	433/434 (99%)	-0.84	0 100 100	14, 30, 43, 67	2 (0%)
2	H	433/434 (99%)	-0.70	1 (0%) 92 91	18, 34, 55, 79	1 (0%)
2	K	433/434 (99%)	-0.72	0 100 100	24, 35, 52, 85	0
3	C	264/265 (99%)	-0.99	0 100 100	17, 28, 40, 51	1 (0%)
3	F	264/265 (99%)	-0.63	3 (1%) 77 77	26, 38, 57, 73	0
3	I	264/265 (99%)	-0.88	1 (0%) 89 88	16, 31, 45, 76	2 (0%)
3	L	264/265 (99%)	-0.69	1 (0%) 89 88	22, 36, 52, 75	1 (0%)
All	All	4992/5040 (99%)	-0.89	11 (0%) 92 91	14, 29, 47, 85	9 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	559	ALA	3.1
3	L	2	ALA	2.8
1	A	559	ALA	2.7
1	D	559	ALA	2.6
1	G	559	ALA	2.6
3	F	181	GLY	2.6
3	I	2	ALA	2.5
2	B	2	ALA	2.5
2	H	2	ALA	2.5
3	F	2	ALA	2.3
3	F	180	GLY	2.1

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

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
1	MGN	J	410	10/11	0.95	0.07	20,21,24,25	0
1	TRX	D	437	15/16	0.96	0.07	19,22,24,25	0
1	MHS	J	266	11/12	0.96	0.07	22,24,27,28	0
1	TRX	A	437	15/16	0.96	0.06	17,19,21,21	0
1	MHS	D	266	11/12	0.97	0.07	19,21,23,24	0
1	MGN	D	410	10/11	0.97	0.06	20,22,24,24	0
1	MGN	A	410	10/11	0.97	0.06	17,19,20,21	0
1	DYA	D	460	8/9	0.97	0.05	22,24,25,26	0
1	MHS	G	266	11/12	0.97	0.08	23,24,27,29	0
1	AGM	G	280	12/13	0.97	0.07	19,22,23,24	0
1	TRX	G	437	15/16	0.97	0.05	19,21,22,22	0
1	DYA	G	460	8/9	0.97	0.04	19,21,24,25	0
1	MHS	A	266	11/12	0.97	0.05	22,25,26,26	0
1	DYA	A	460	8/9	0.97	0.04	17,21,21,24	0
1	DYA	J	460	8/9	0.97	0.06	22,25,27,27	0
1	AGM	D	280	12/13	0.98	0.06	19,20,22,23	0
1	AGM	A	280	12/13	0.98	0.07	17,19,21,22	0
1	AGM	J	280	12/13	0.98	0.06	19,22,24,24	0
1	MGN	G	410	10/11	0.98	0.06	17,18,20,20	0
1	TRX	J	437	15/16	0.98	0.05	20,23,25,25	0
1	SMC	D	462	7/8	0.98	0.05	22,23,24,27	0
1	GL3	G	455	4/5	0.99	0.04	21,21,21,21	0
1	SMC	A	462	7/8	0.99	0.06	18,20,22,22	0
1	SMC	G	462	7/8	0.99	0.05	21,23,25,25	0
1	GL3	J	455	4/5	0.99	0.04	20,21,22,23	0
1	GL3	D	455	4/5	0.99	0.04	22,23,23,24	0
1	SMC	J	462	7/8	0.99	0.05	22,23,27,27	0
1	GL3	A	455	4/5	1.00	0.04	16,17,18,20	0

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	GOL	C	305	6/6	0.55	0.23	45,54,65,71	0
12	GOL	J	615	6/6	0.61	0.16	59,71,76,78	0
7	EDO	A	618	4/4	0.64	0.18	43,51,55,64	0
12	GOL	J	614	6/6	0.69	0.16	51,61,71,77	0
11	PEG	E	503	7/7	0.70	0.16	43,52,62,62	0
7	EDO	J	617	4/4	0.70	0.13	50,60,68,68	0
7	EDO	D	615	4/4	0.72	0.13	43,51,59,67	0
6	PGE	G	618	10/10	0.72	0.14	50,60,69,71	0
7	EDO	D	617	4/4	0.73	0.16	34,45,54,65	0
5	MG	A	610	1/1	0.74	0.25	57,57,57,57	0
7	EDO	K	505	4/4	0.75	0.12	53,64,71,71	0
7	EDO	B	503	4/4	0.77	0.14	50,60,71,71	0
7	EDO	A	612	4/4	0.77	0.14	46,56,61,67	0
11	PEG	G	615	7/7	0.77	0.14	44,54,67,72	0
11	PEG	L	305	7/7	0.78	0.13	51,62,66,71	0
11	PEG	H	503	7/7	0.78	0.14	52,62,70,74	0
12	GOL	D	609	6/6	0.79	0.14	42,53,66,66	0
11	PEG	G	616	7/7	0.80	0.14	42,50,60,68	0
12	GOL	A	619	6/6	0.80	0.13	39,55,67,67	0
6	PGE	D	614	10/10	0.80	0.13	47,62,72,75	0
6	PGE	H	504	10/10	0.81	0.12	45,58,66,76	0
7	EDO	L	304	4/4	0.81	0.11	53,63,69,72	0
11	PEG	A	616	7/7	0.82	0.13	46,57,64,74	0
14	NA	C	302	1/1	0.82	0.14	54,54,54,54	0
12	GOL	C	304	6/6	0.83	0.10	48,60,72,74	0
7	EDO	J	618	4/4	0.83	0.11	42,51,63,63	0
12	GOL	J	616	6/6	0.83	0.12	42,54,64,73	0
7	EDO	F	304	4/4	0.83	0.11	56,67,73,77	0
11	PEG	J	609	7/7	0.84	0.12	42,51,63,67	0
6	PGE	A	611	10/10	0.84	0.11	45,56,73,76	0
6	PGE	G	610	10/10	0.85	0.11	43,53,64,77	0
7	EDO	G	611	4/4	0.85	0.11	43,54,54,65	0
11	PEG	K	504	7/7	0.85	0.11	49,59,69,71	0
11	PEG	D	618	7/7	0.86	0.10	41,53,68,73	0
6	PGE	D	610	10/10	0.86	0.11	44,56,69,71	0
7	EDO	I	304	4/4	0.86	0.10	49,59,60,66	0
7	EDO	J	619	4/4	0.86	0.10	43,51,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	KR	D	603[A]	1/1	0.87	0.17	43,43,43,43	1
11	PEG	J	610	7/7	0.87	0.11	41,52,63,70	0
7	EDO	G	617	4/4	0.87	0.10	40,48,53,63	0
4	KR	J	602	1/1	0.88	0.18	48,48,48,48	1
7	EDO	I	305	4/4	0.89	0.08	48,58,63,65	0
7	EDO	D	616	4/4	0.89	0.09	39,47,53,64	0
4	KR	G	608	1/1	0.89	0.27	26,26,26,26	1
7	EDO	A	617	4/4	0.91	0.09	40,48,58,59	0
4	KR	A	608	1/1	0.91	0.20	44,44,44,44	1
4	KR	A	607	1/1	0.92	0.21	42,42,42,42	1
4	KR	G	606	1/1	0.92	0.16	39,39,39,39	1
4	KR	A	602[A]	1/1	0.93	0.12	46,46,46,46	1
8	CL	L	303	1/1	0.93	0.09	37,37,37,37	0
4	KR	J	606[A]	1/1	0.94	0.16	32,32,32,32	1
4	KR	D	606[A]	1/1	0.94	0.13	31,31,31,31	1
5	MG	K	502	1/1	0.94	0.07	47,47,47,47	0
4	KR	D	607[A]	1/1	0.94	0.14	33,33,33,33	1
4	KR	F	301	1/1	0.94	0.10	56,56,56,56	1
14	NA	K	503	1/1	0.94	0.12	46,46,46,46	0
8	CL	L	302	1/1	0.95	0.07	37,37,37,37	0
4	KR	G	605	1/1	0.95	0.28	63,63,63,63	1
4	KR	J	603[B]	1/1	0.95	0.13	42,42,42,42	1
4	KR	G	607[A]	1/1	0.96	0.15	31,31,31,31	1
4	KR	A	605[A]	1/1	0.96	0.17	32,32,32,32	1
4	KR	H	501	1/1	0.96	0.10	43,43,43,43	1
8	CL	I	303	1/1	0.96	0.10	36,36,36,36	0
4	KR	F	302	1/1	0.96	0.11	36,36,36,36	1
5	MG	D	608	1/1	0.97	0.05	42,42,42,42	0
5	MG	J	608	1/1	0.97	0.06	46,46,46,46	0
4	KR	A	606	1/1	0.97	0.27	25,25,25,25	1
4	KR	J	607	1/1	0.97	0.24	26,26,26,26	1
4	KR	L	301	1/1	0.97	0.11	53,53,53,53	1
4	KR	B	501	1/1	0.97	0.10	36,36,36,36	1
5	MG	A	609	1/1	0.98	0.04	38,38,38,38	0
4	KR	C	301	1/1	0.98	0.11	31,31,31,31	1
8	CL	E	502	1/1	0.98	0.05	31,31,31,31	0
8	CL	H	502	1/1	0.98	0.06	35,35,35,35	0
4	KR	D	605	1/1	0.98	0.11	31,31,31,31	1
5	MG	G	609	1/1	0.98	0.05	42,42,42,42	0
4	KR	J	605	1/1	0.98	0.12	25,25,25,25	1
9	TP7	D	611	21/21	0.98	0.06	18,22,25,26	0
9	TP7	J	612	21/21	0.98	0.06	19,22,25,27	0

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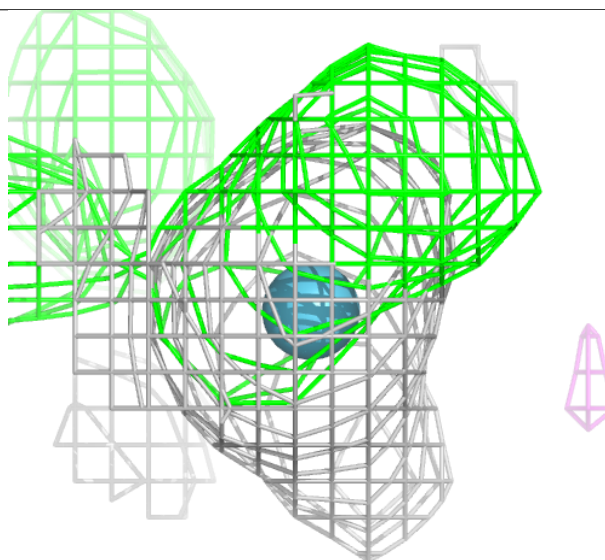
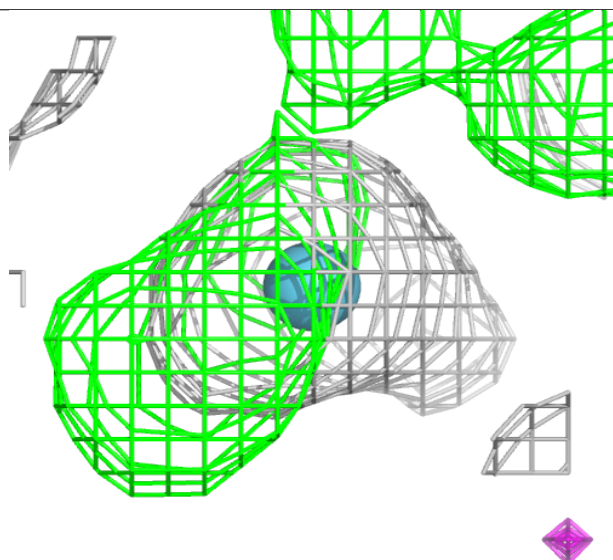
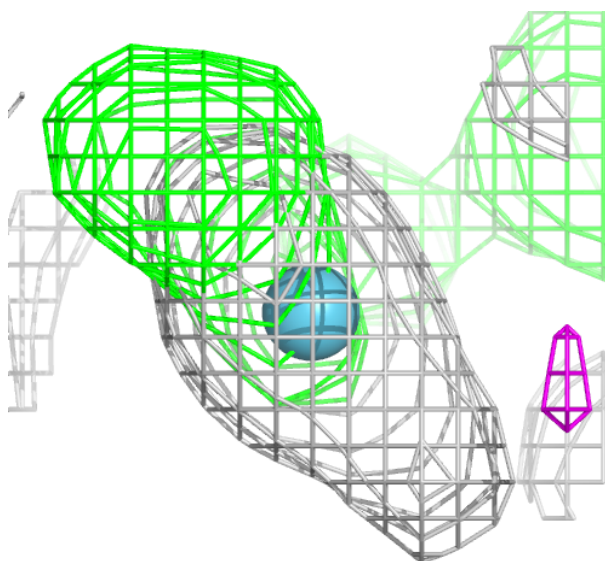
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	F43	D	613	62/62	0.98	0.05	17,21,24,28	0
10	F43	J	611	62/62	0.98	0.06	16,20,24,26	0
4	KR	G	604	1/1	0.98	0.10	35,35,35,35	1
4	KR	E	501	1/1	0.98	0.12	39,39,39,39	1
13	COM	J	613	7/7	0.98	0.05	19,21,23,24	0
4	KR	K	501	1/1	0.98	0.09	41,41,41,41	1
4	KR	I	301	1/1	0.98	0.14	38,38,38,38	1
4	KR	A	604	1/1	0.99	0.12	23,23,23,23	1
4	KR	D	604	1/1	0.99	0.09	23,23,23,23	1
4	KR	I	302	1/1	0.99	0.12	33,33,33,33	1
4	KR	J	601	1/1	0.99	0.09	37,37,37,37	1
9	TP7	A	614	21/21	0.99	0.04	18,19,21,23	0
4	KR	G	603	1/1	0.99	0.07	30,30,30,30	1
9	TP7	G	614	21/21	0.99	0.04	18,22,25,26	0
4	KR	D	602	1/1	0.99	0.07	32,32,32,32	1
10	F43	A	615	62/62	0.99	0.04	14,17,21,24	0
8	CL	A	613	1/1	0.99	0.04	30,30,30,30	0
10	F43	G	619	62/62	0.99	0.05	18,21,24,26	0
8	CL	B	502	1/1	0.99	0.03	31,31,31,31	0
8	CL	C	303	1/1	0.99	0.09	31,31,31,31	0
13	COM	A	620	7/7	0.99	0.04	17,20,20,21	0
13	COM	D	612	7/7	0.99	0.04	21,23,24,25	0
13	COM	G	613	7/7	0.99	0.04	21,21,22,24	0
4	KR	J	604	1/1	0.99	0.09	32,32,32,32	1
8	CL	F	303	1/1	0.99	0.03	32,32,32,32	0
8	CL	G	612	1/1	0.99	0.05	33,33,33,33	0
4	KR	A	603	1/1	1.00	0.08	27,27,27,27	1
4	KR	G	602	1/1	1.00	0.06	41,41,41,41	0
4	KR	A	601	1/1	1.00	0.09	30,30,30,30	1
15	K	D	601	1/1	1.00	0.03	19,19,19,19	0
15	K	G	601	1/1	1.00	0.02	20,20,20,20	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.

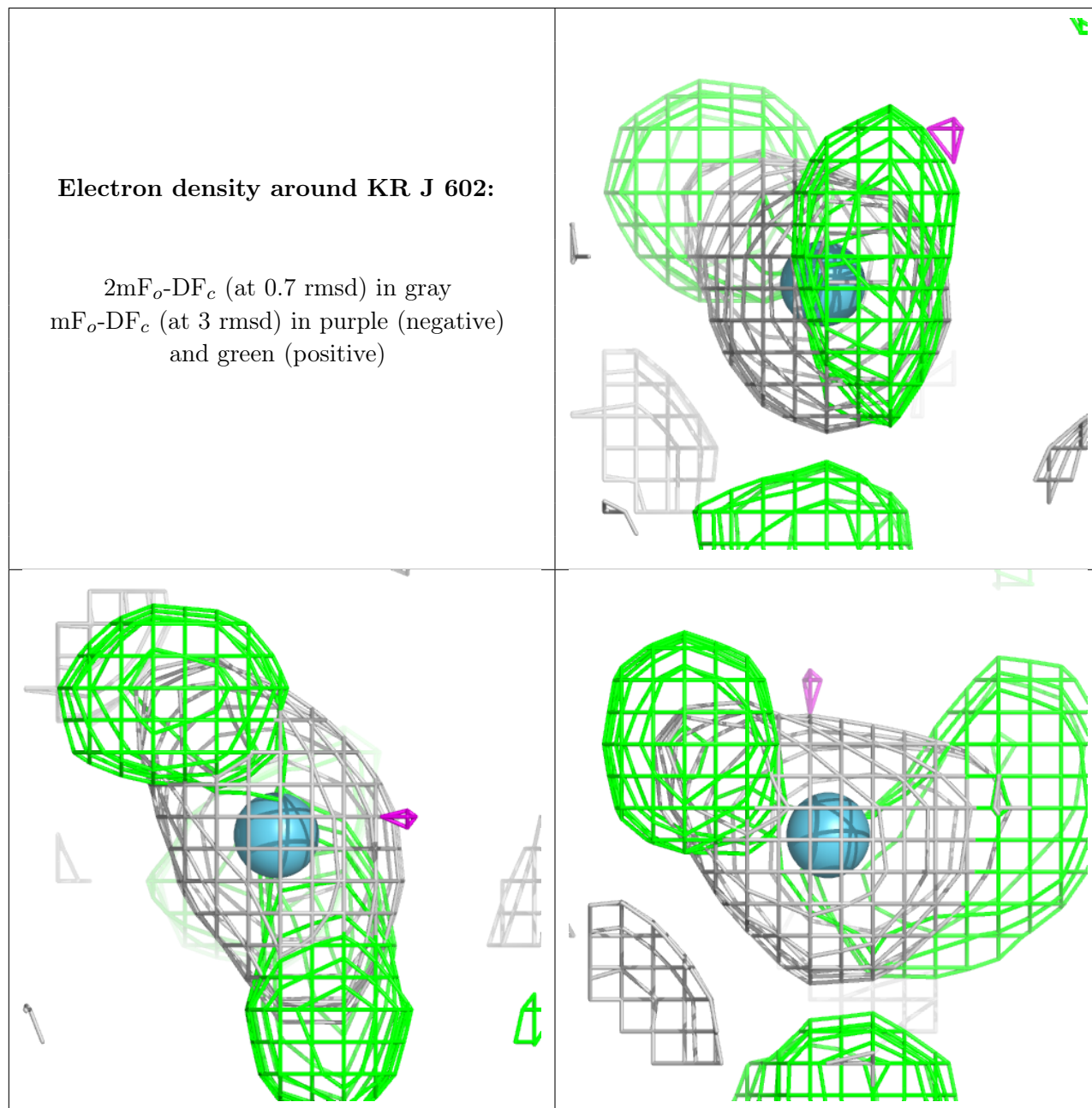
**Electron density around KR D 603 (A):**

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



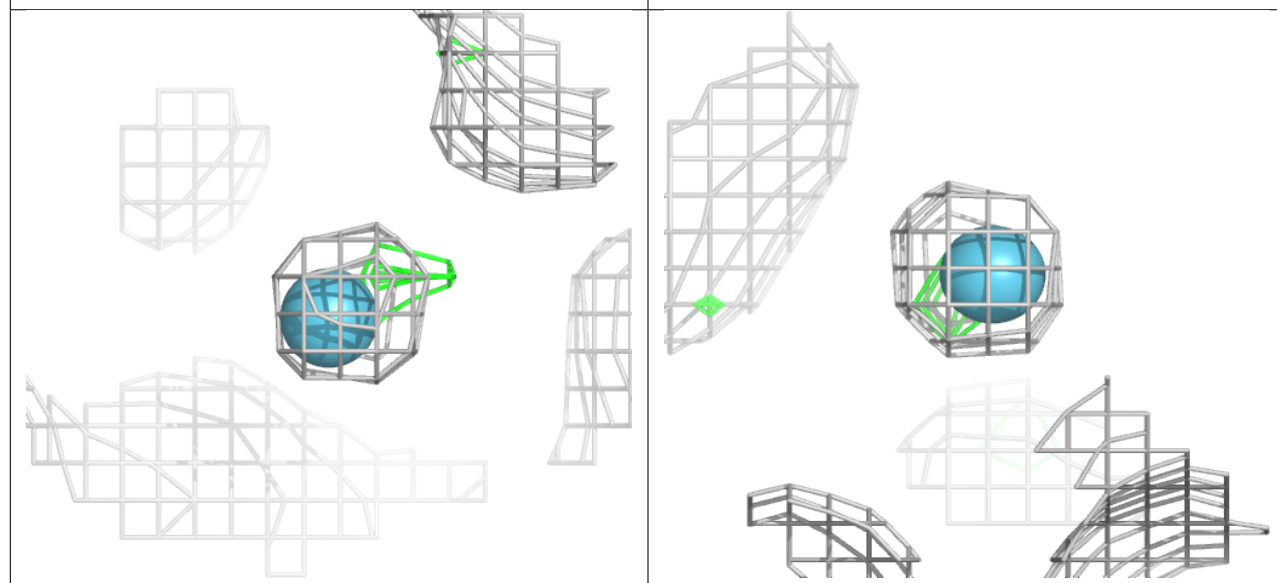
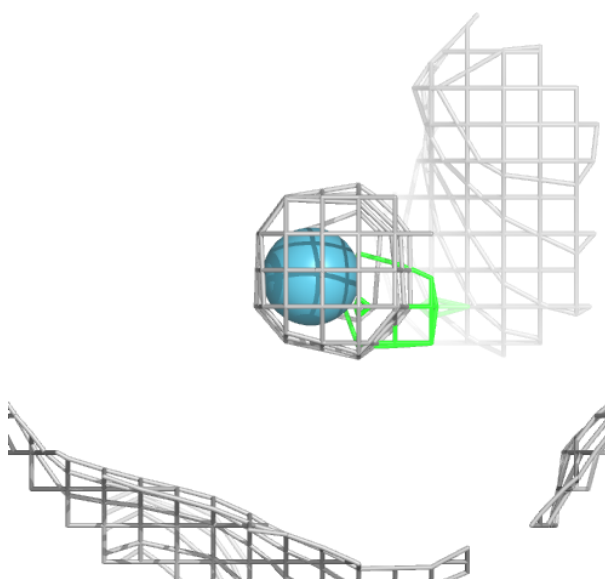
**Electron density around KR J 602:**

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



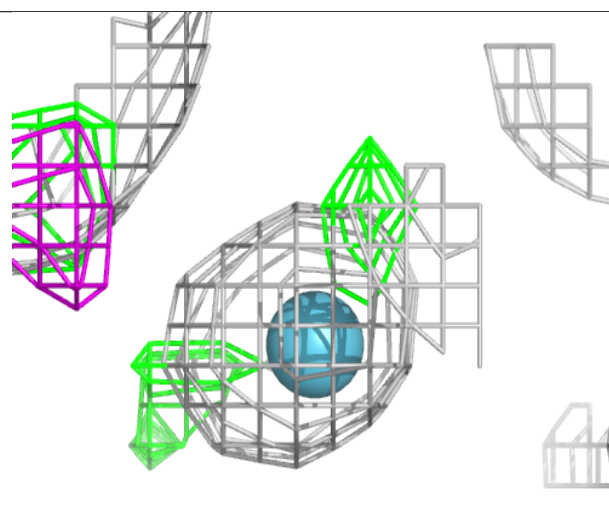
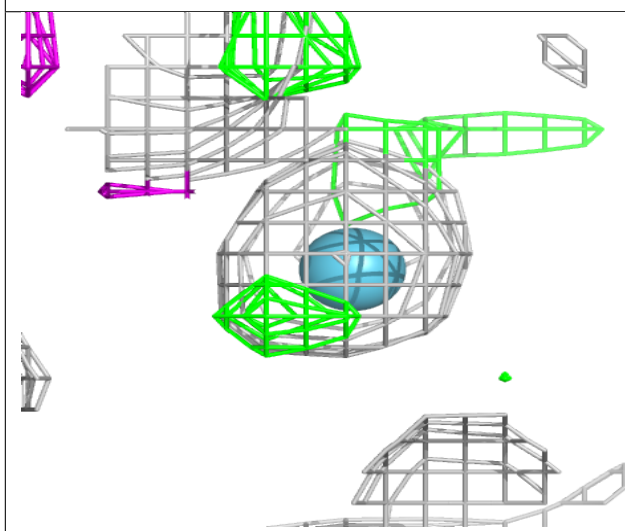
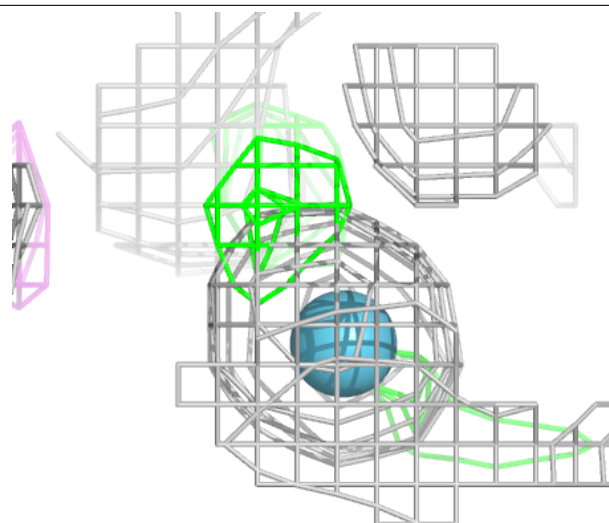
**Electron density around KR G 608:**

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



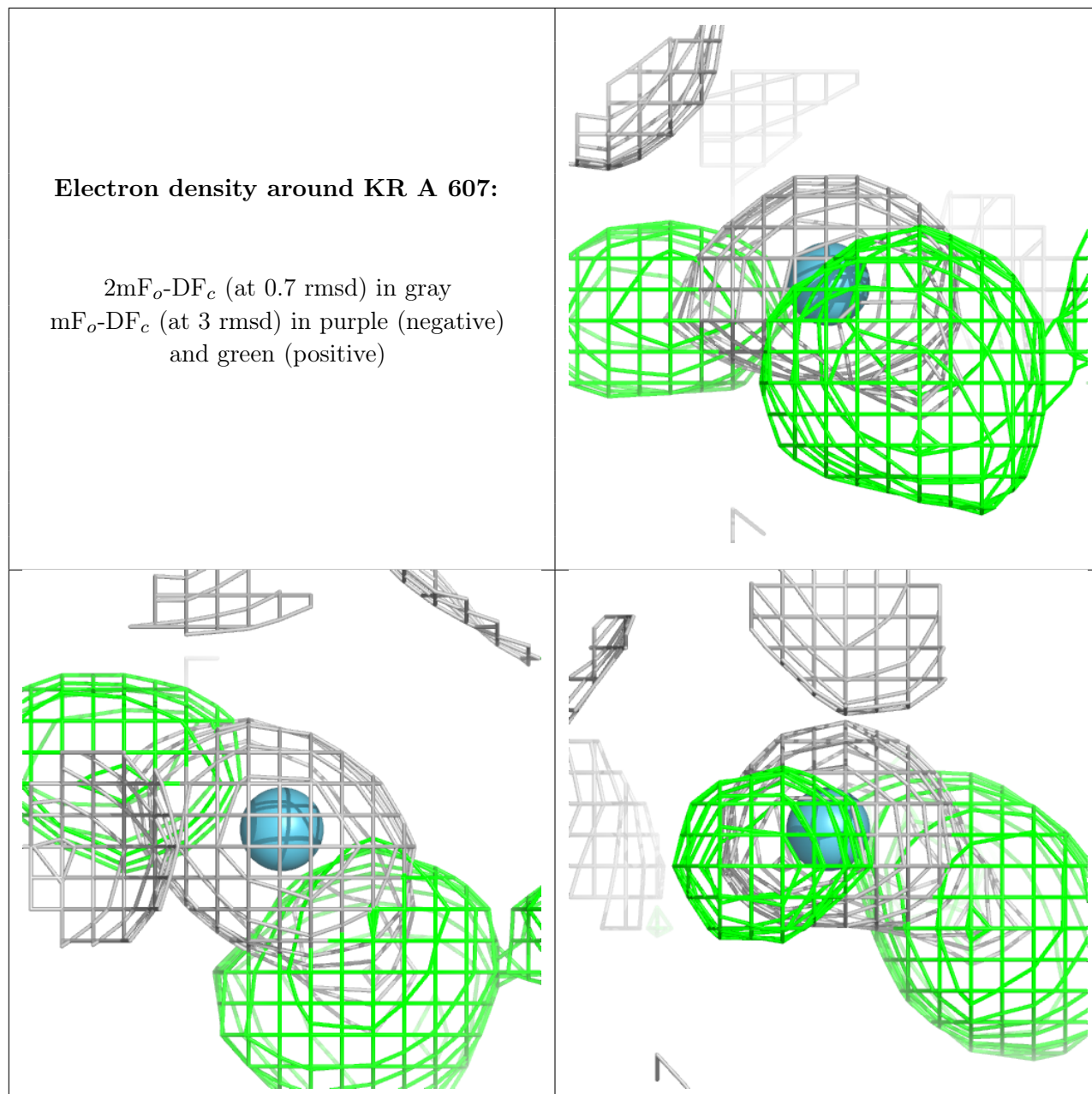
**Electron density around KR A 608:**

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



**Electron density around KR A 607:**

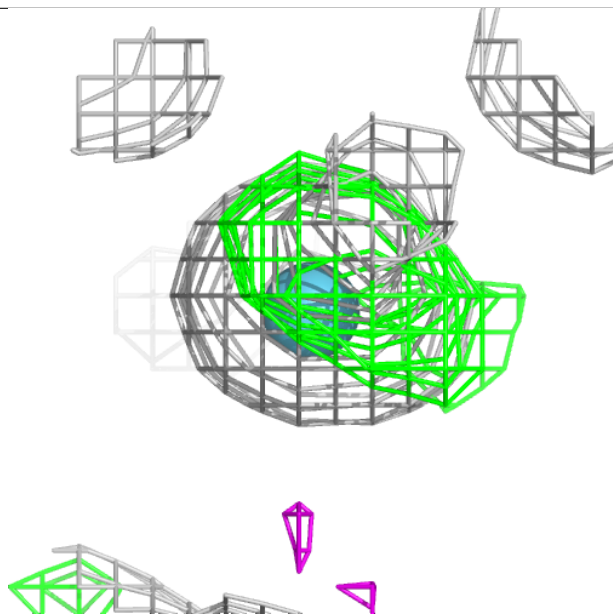
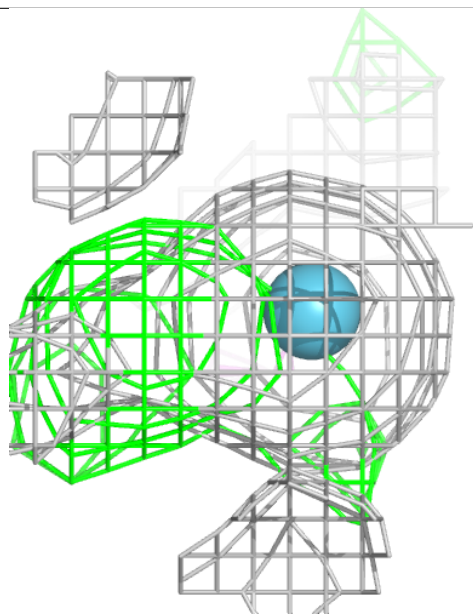
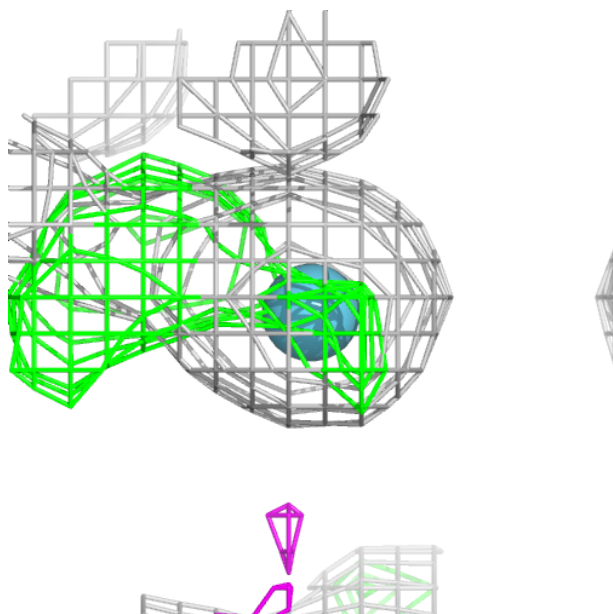
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





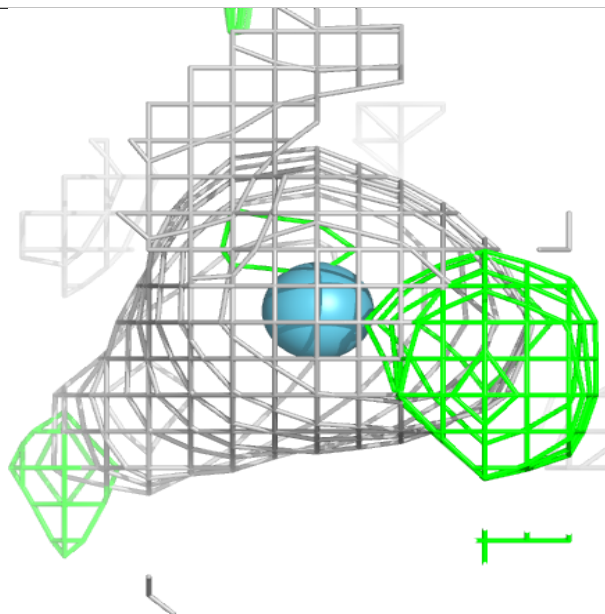
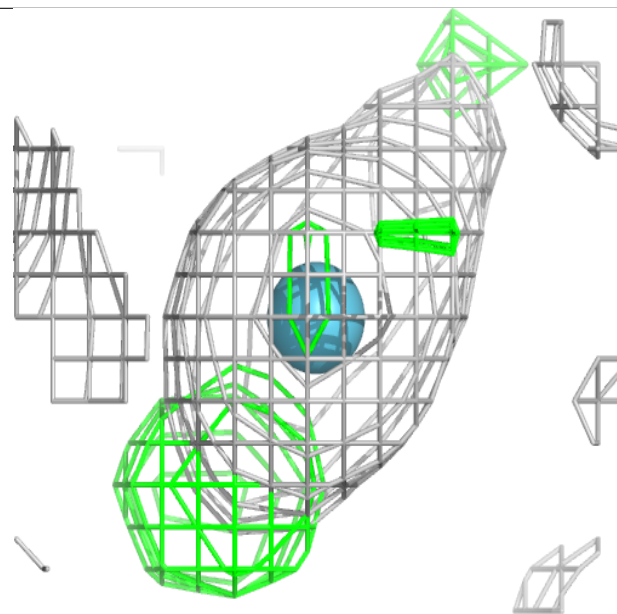
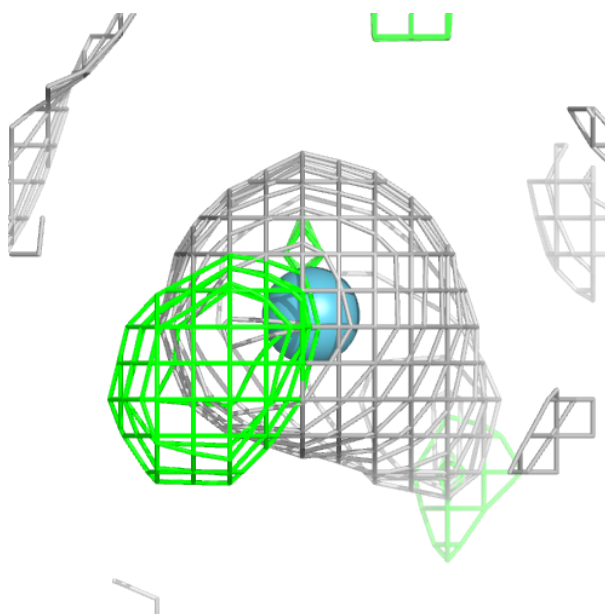
**Electron density around KR G 606:**

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



**Electron density around KR A 602 (A):**

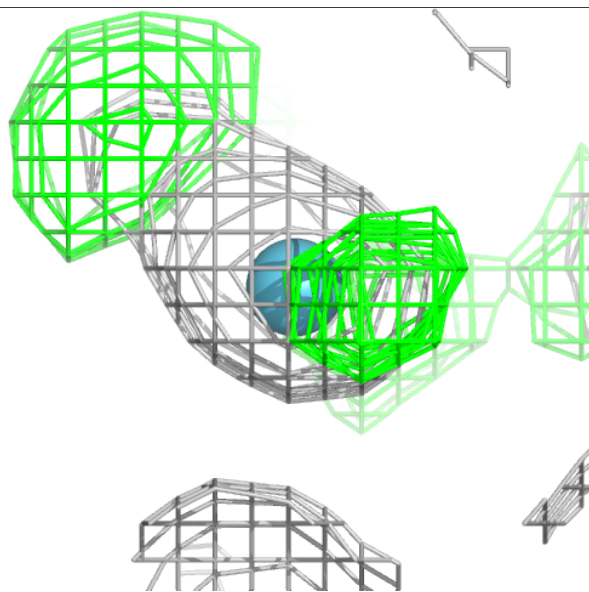
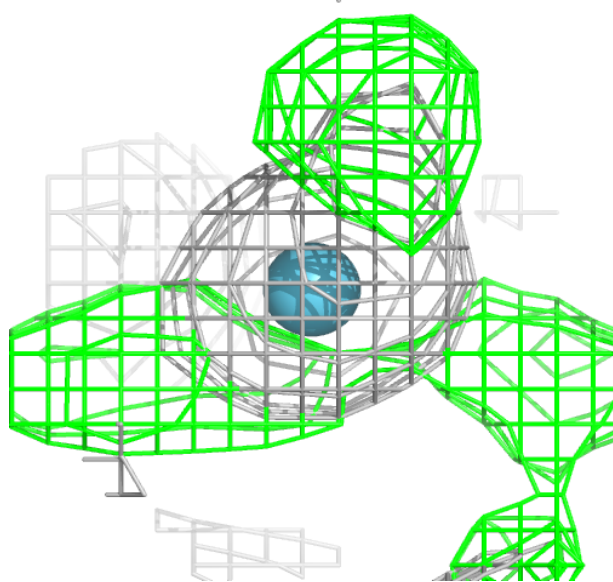
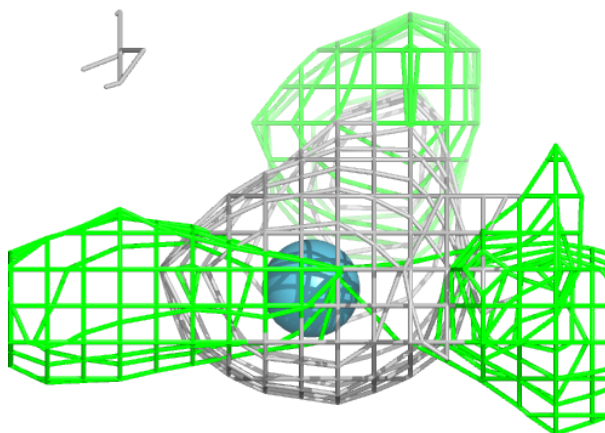
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





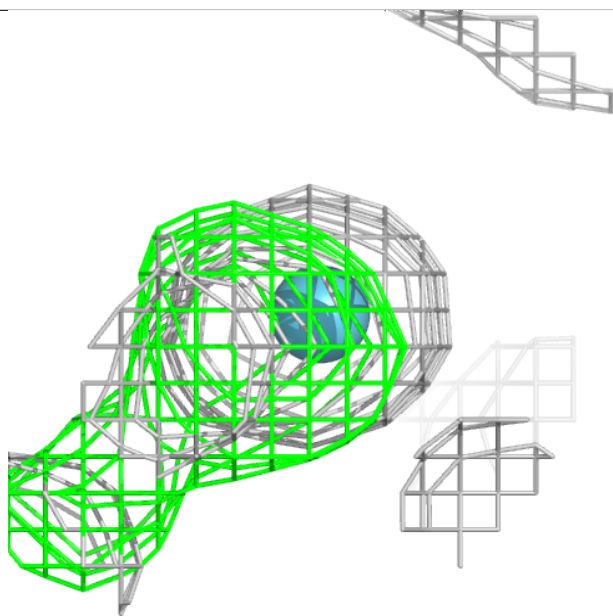
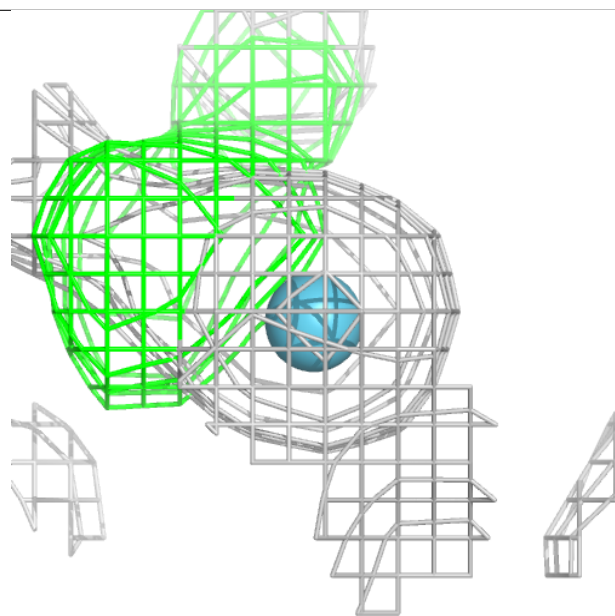
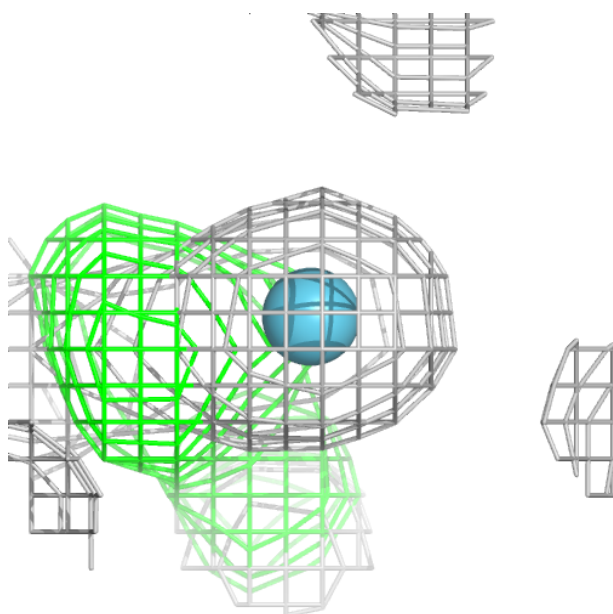
**Electron density around KR J 606 (A):**

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



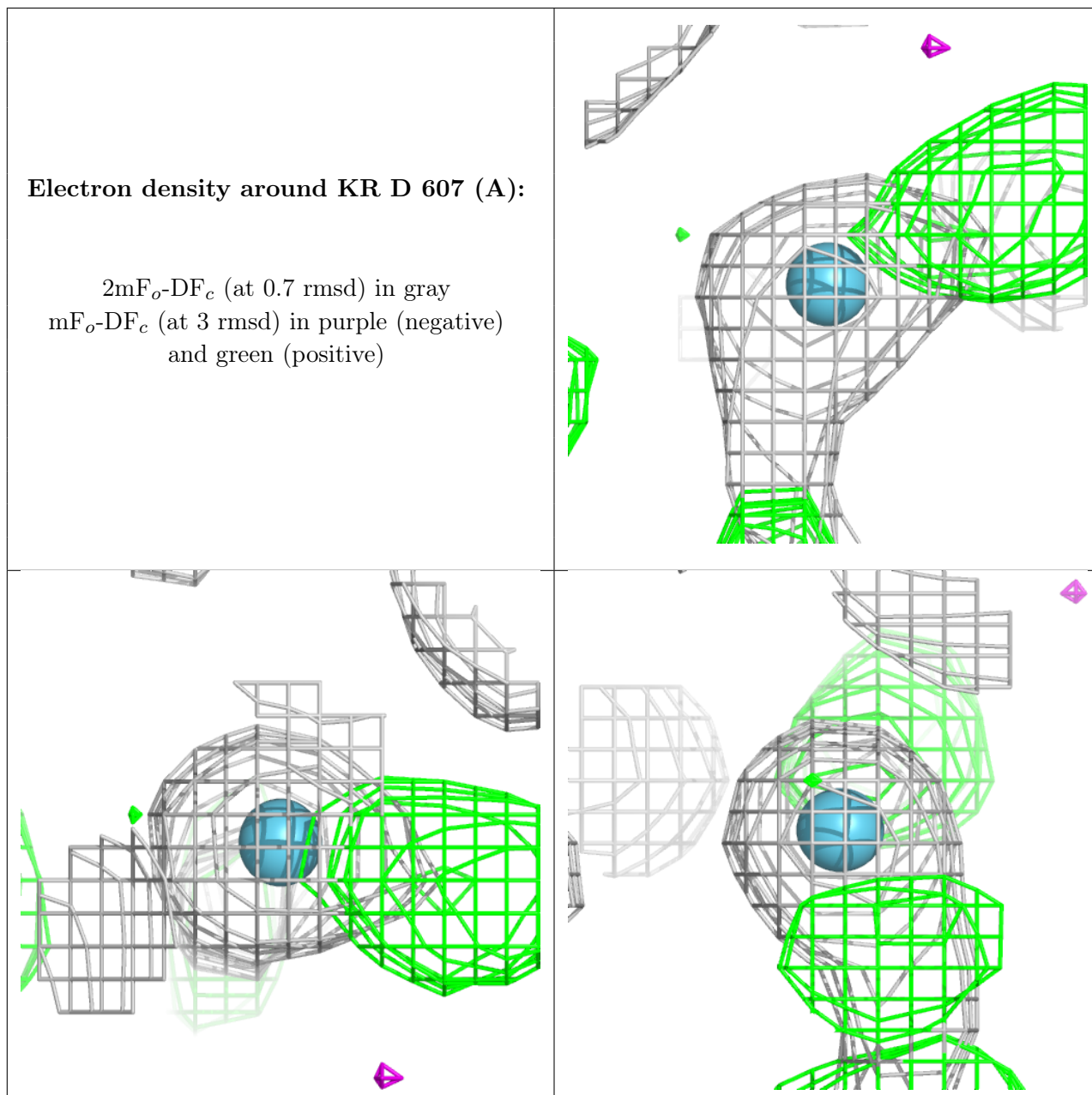
**Electron density around KR D 606 (A):**

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



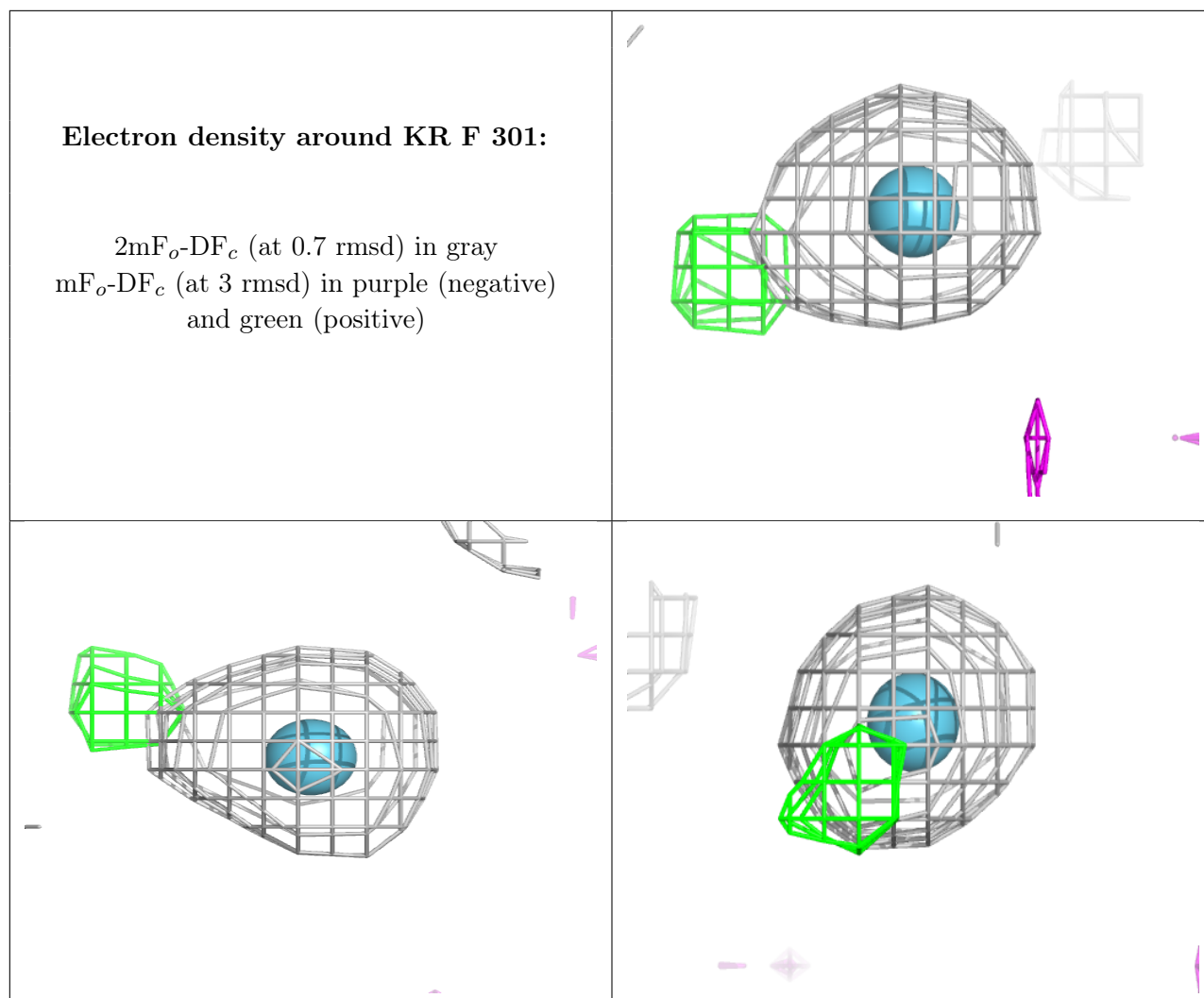
**Electron density around KR D 607 (A):**

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



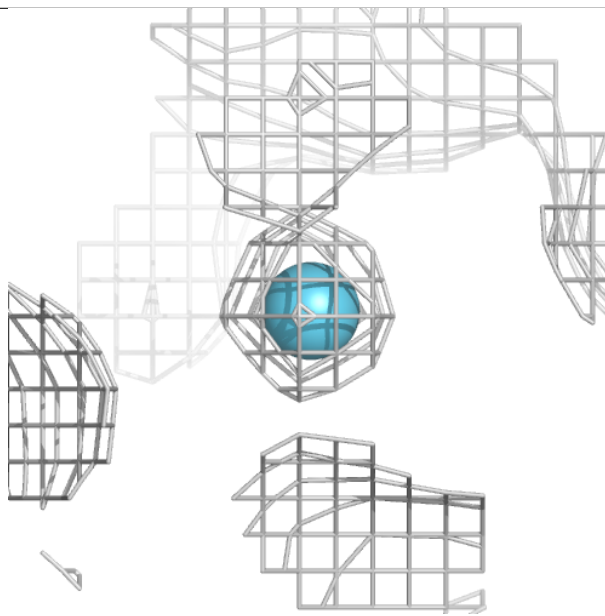
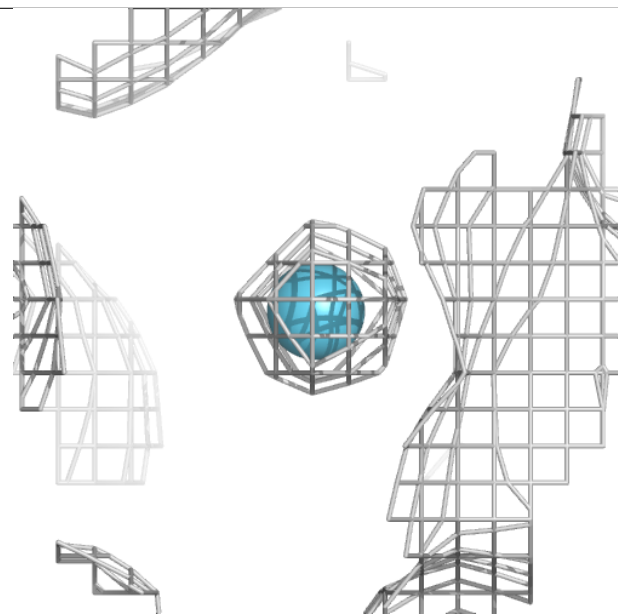
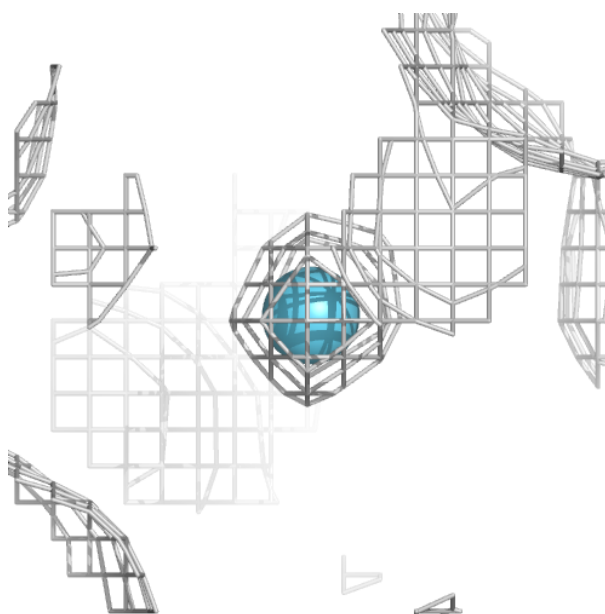
**Electron density around KR F 301:**

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



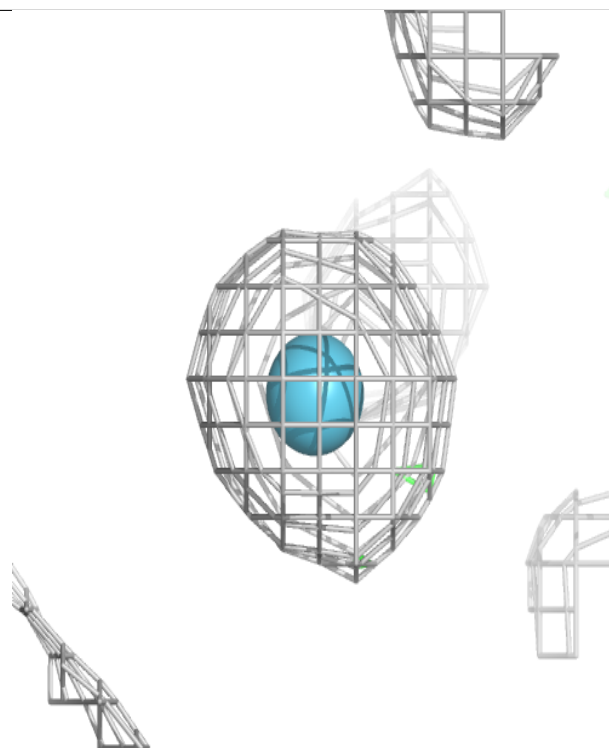
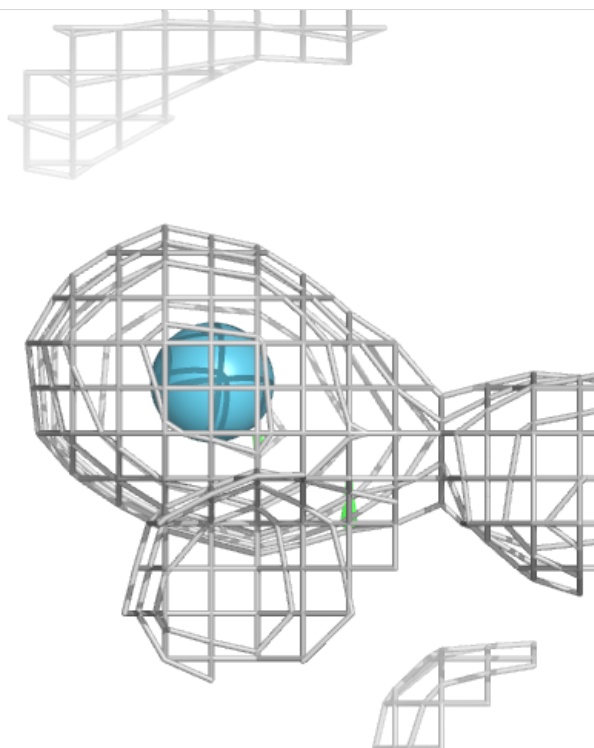
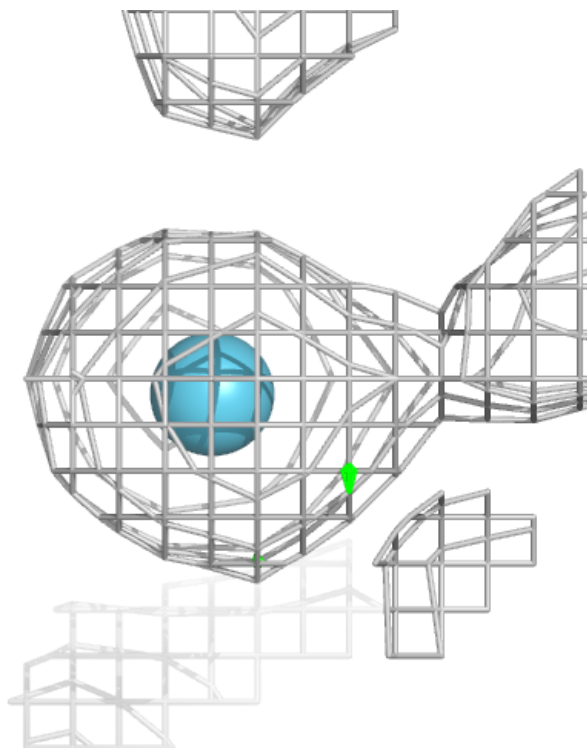
**Electron density around KR G 605:**

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



**Electron density around KR J 603 (B):**

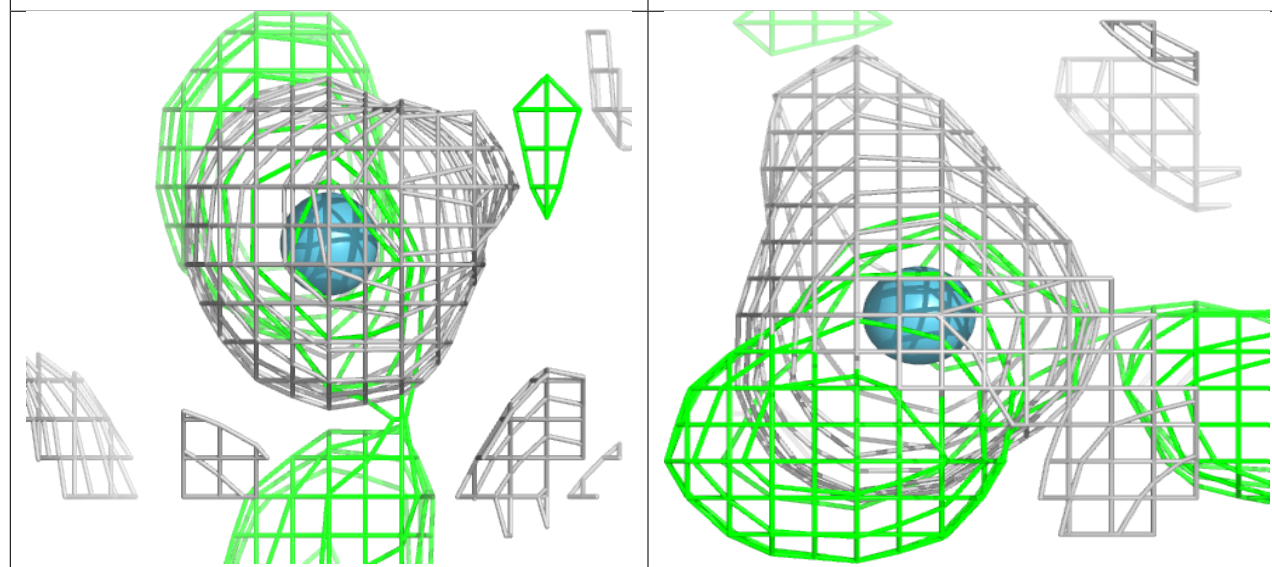
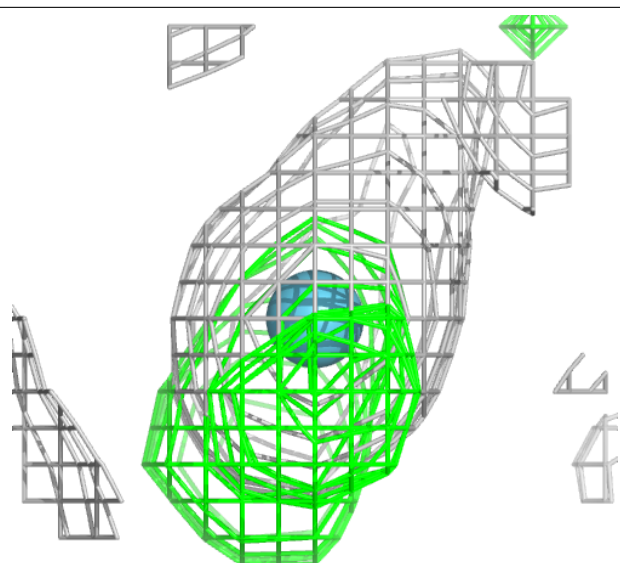
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





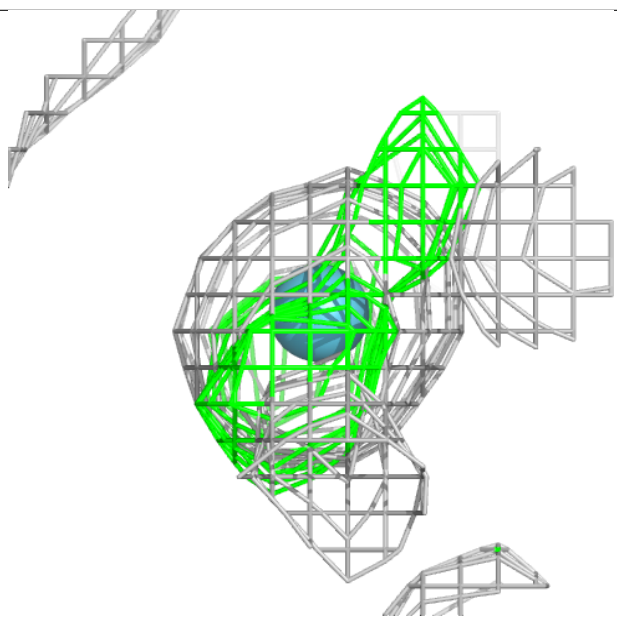
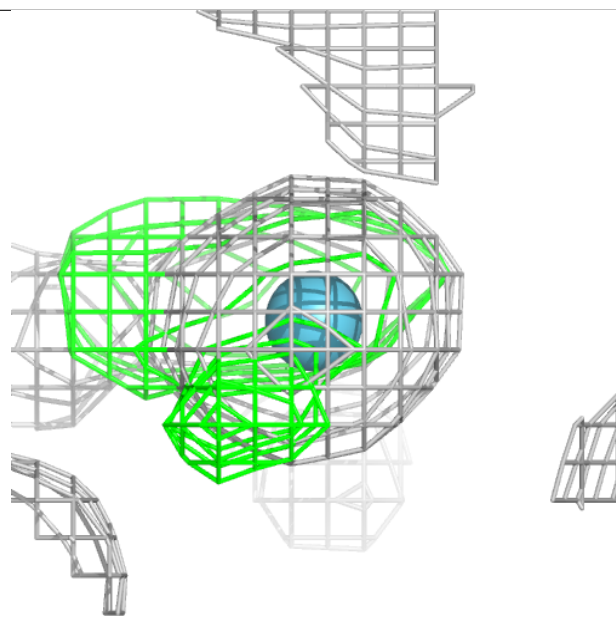
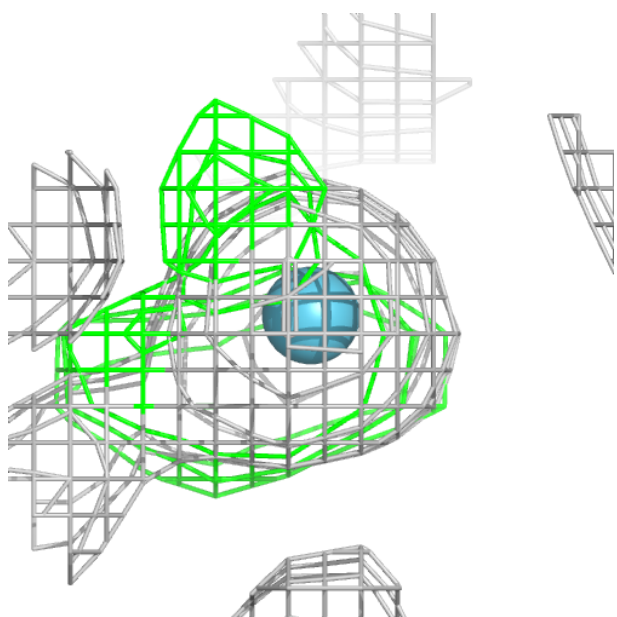
**Electron density around KR G 607 (A):**

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



**Electron density around KR A 605 (A):**

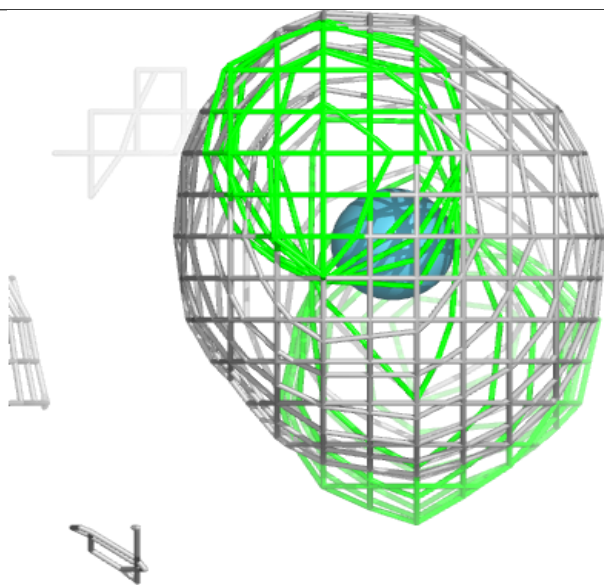
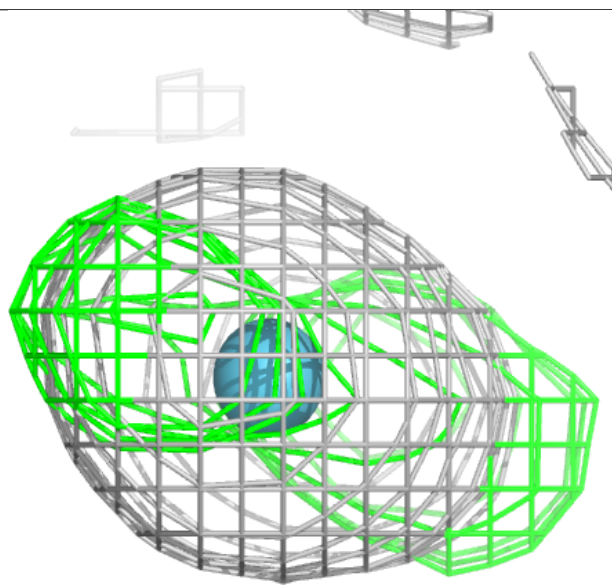
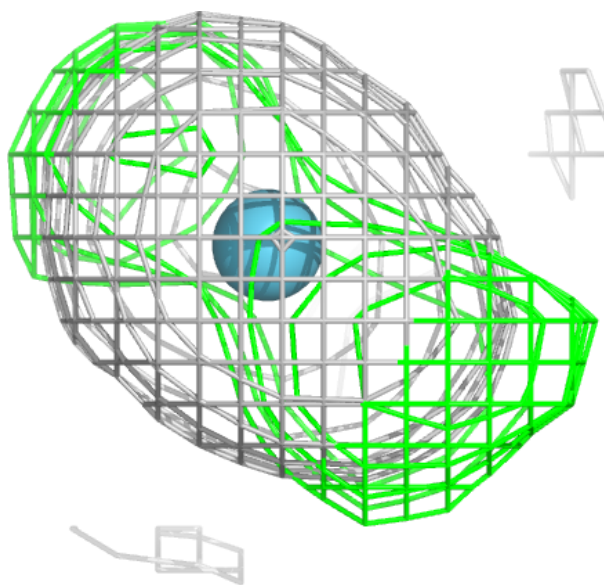
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





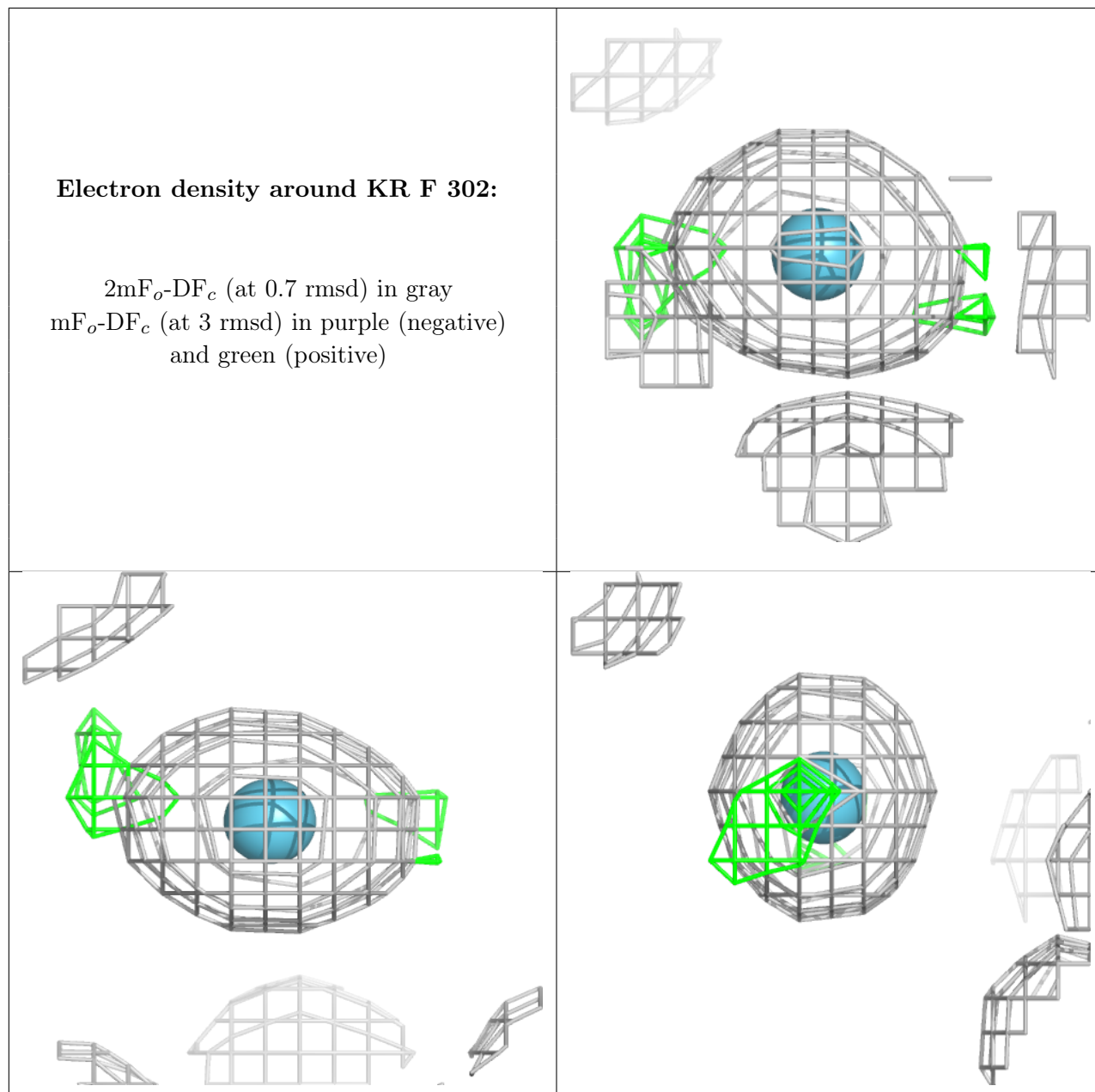
**Electron density around KR H 501:**

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



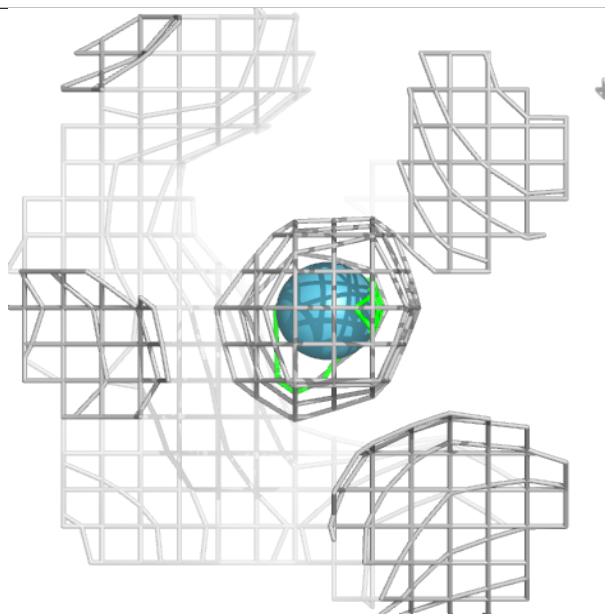
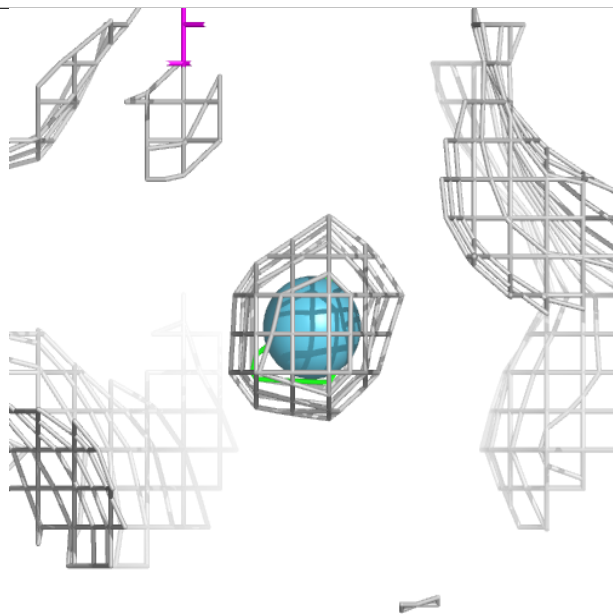
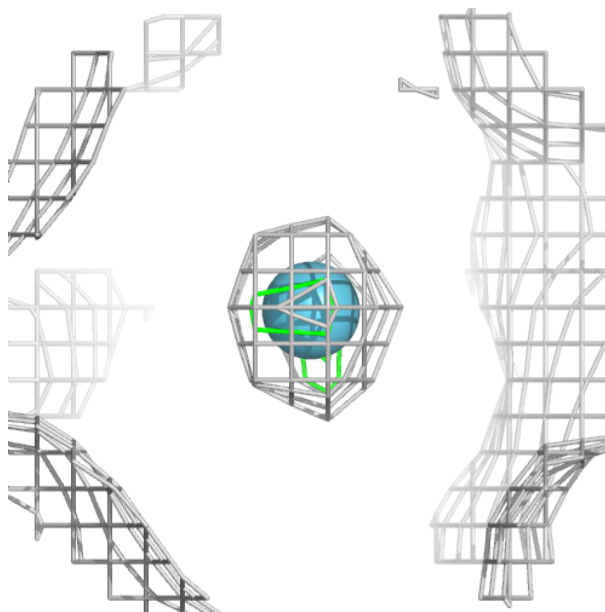
**Electron density around KR F 302:**

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



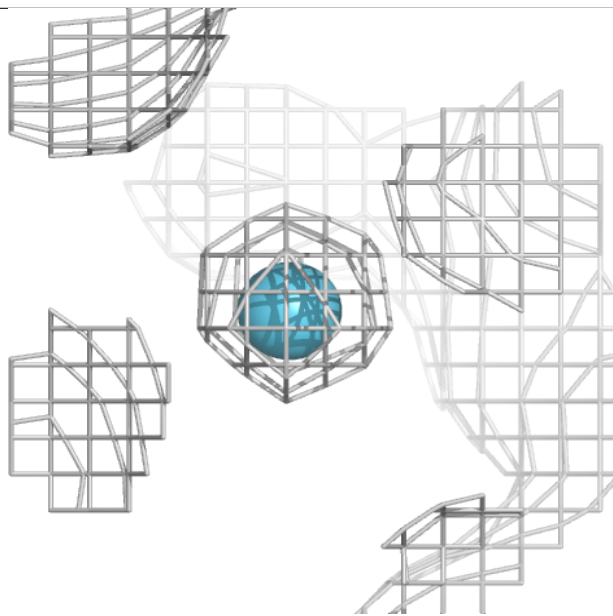
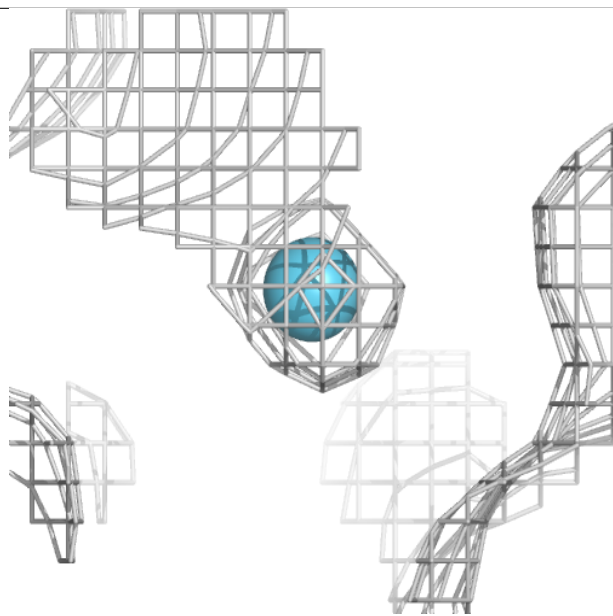
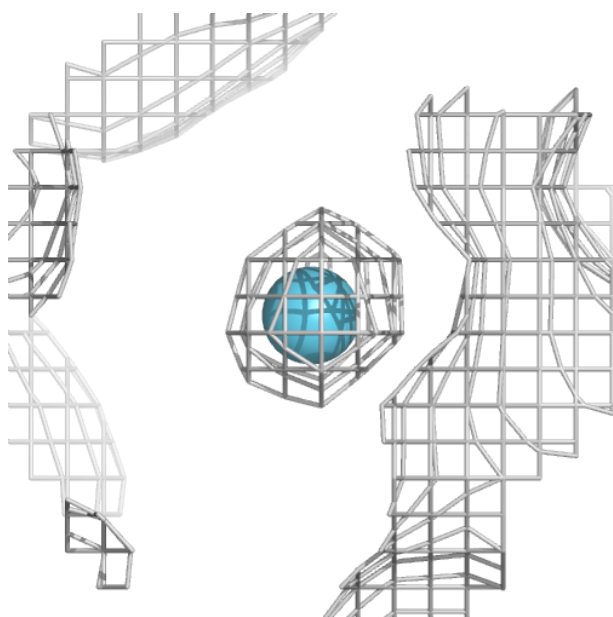
**Electron density around KR A 606:**

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



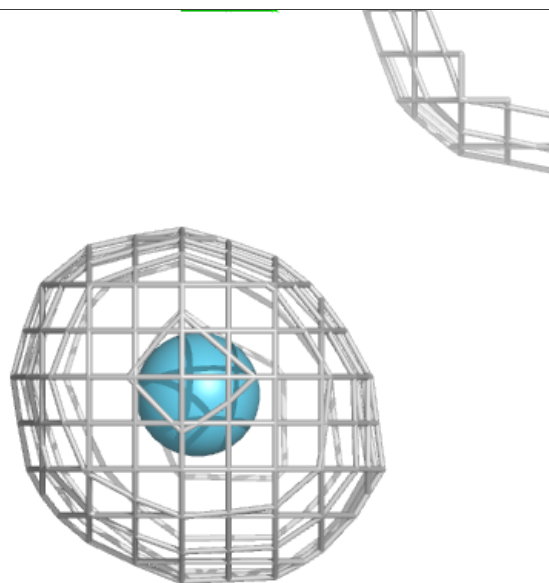
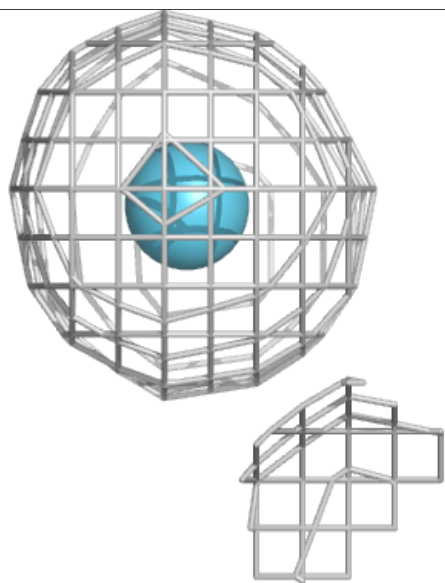
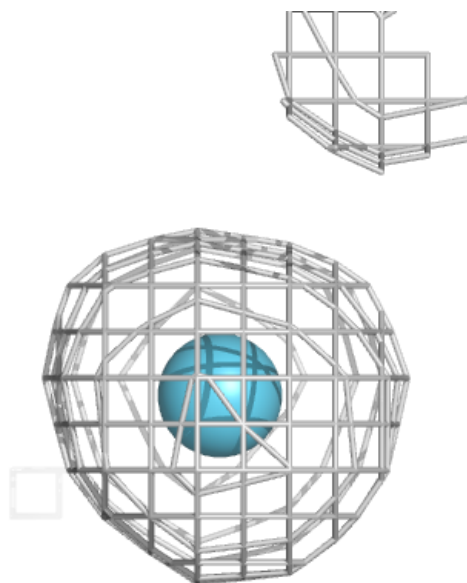
**Electron density around KR J 607:**

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



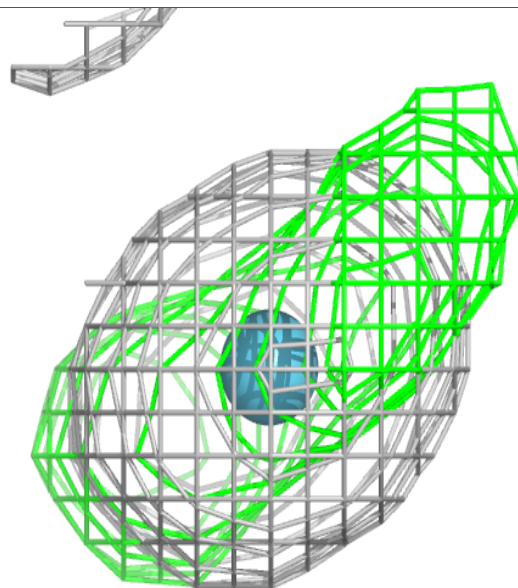
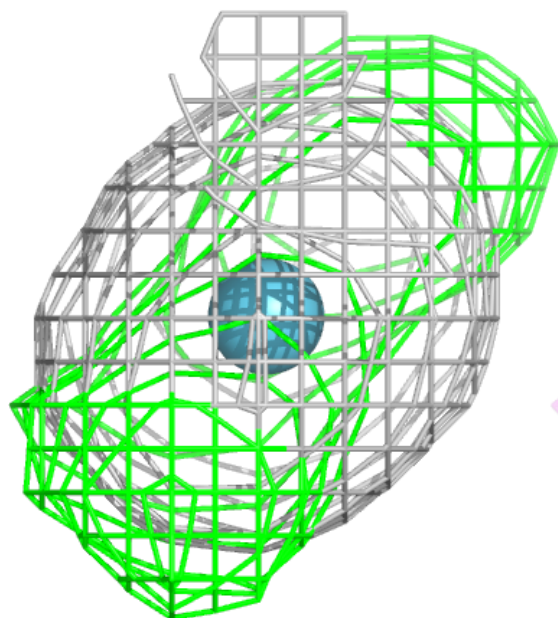
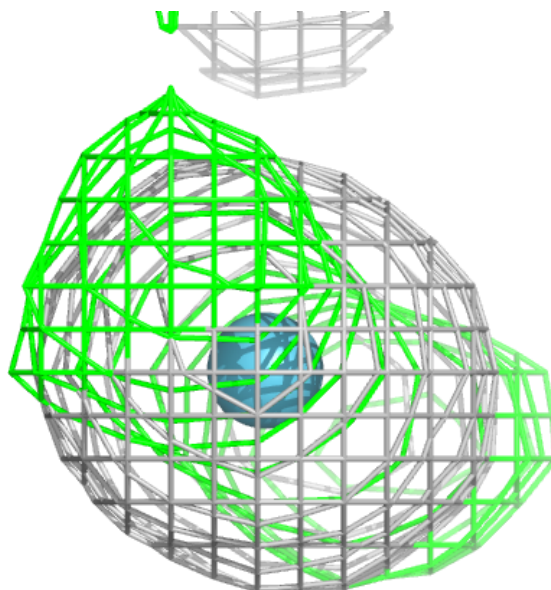
**Electron density around KR L 301:**

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



**Electron density around KR B 501:**

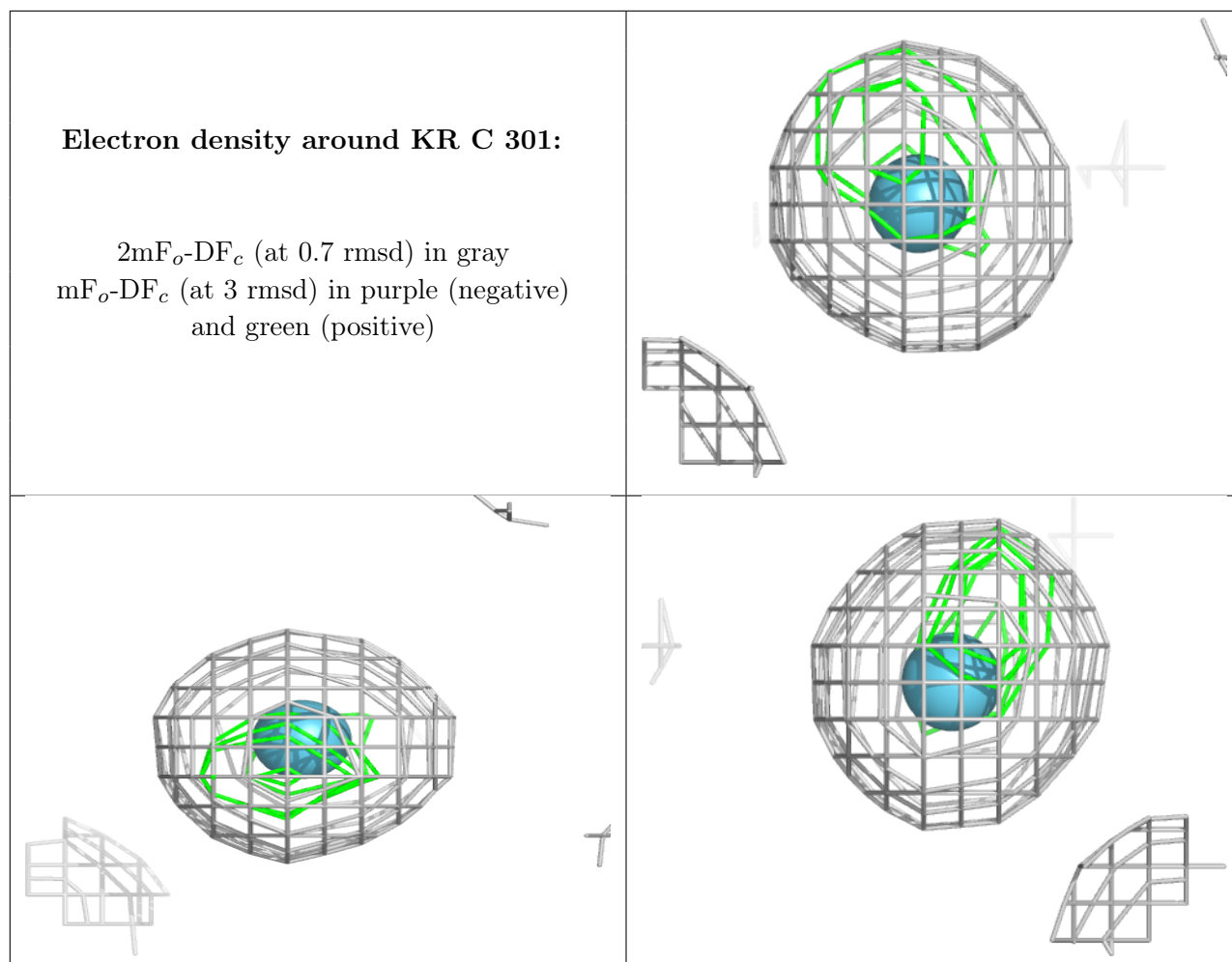
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





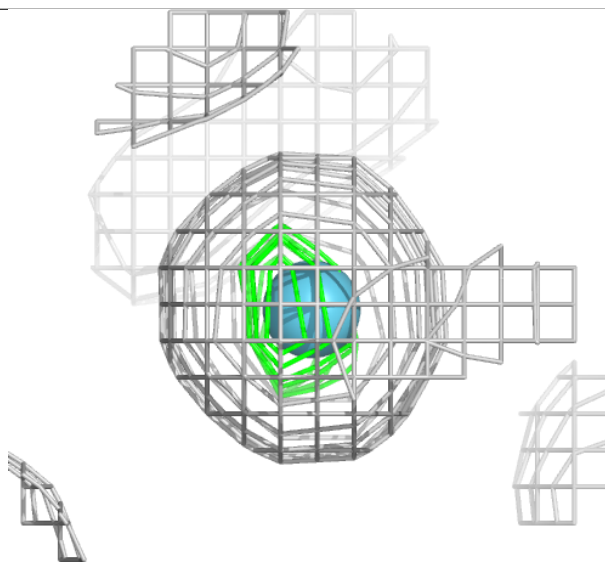
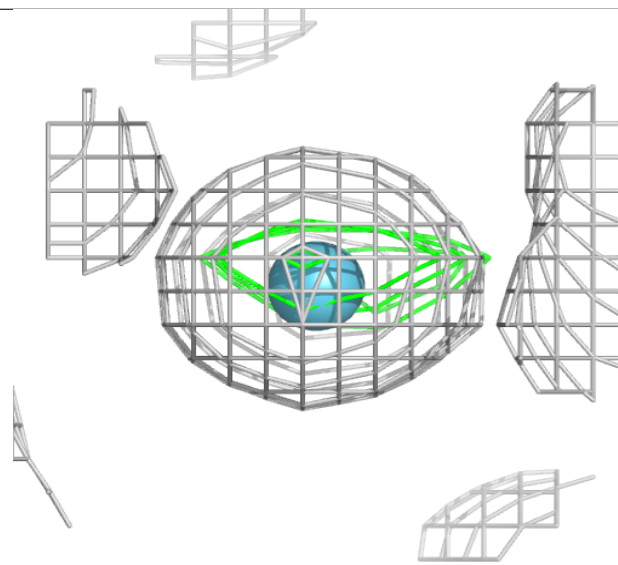
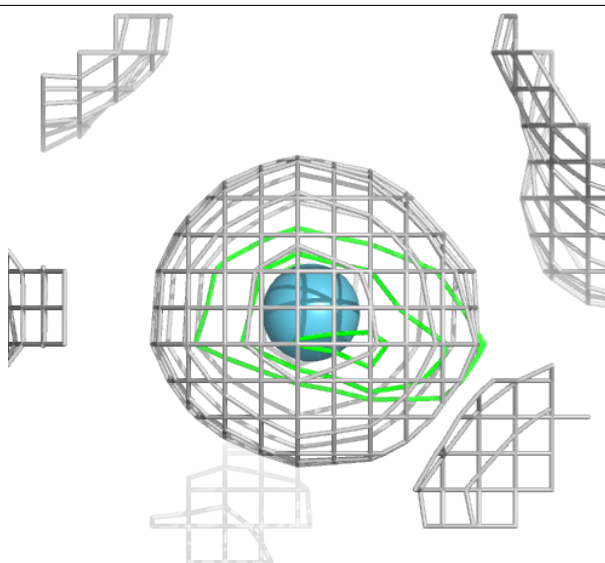
**Electron density around KR C 301:**

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



**Electron density around KR D 605:**

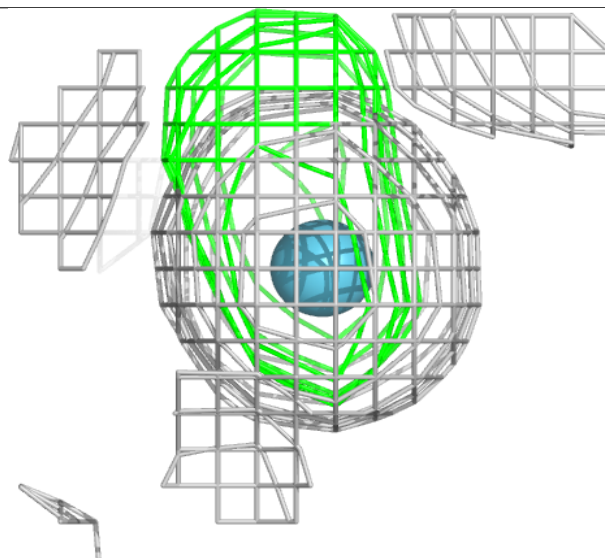
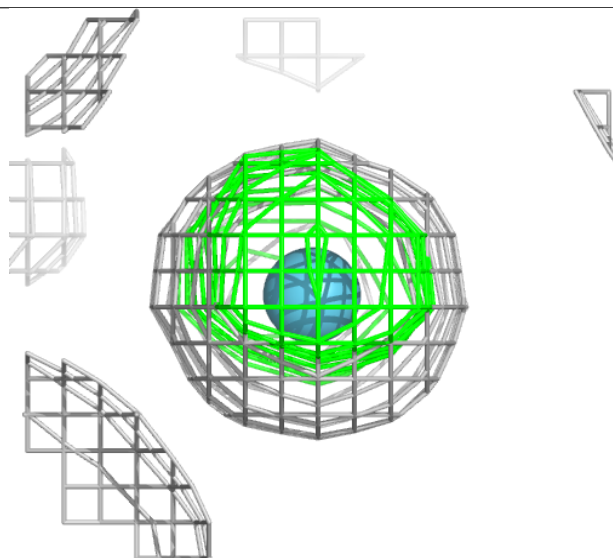
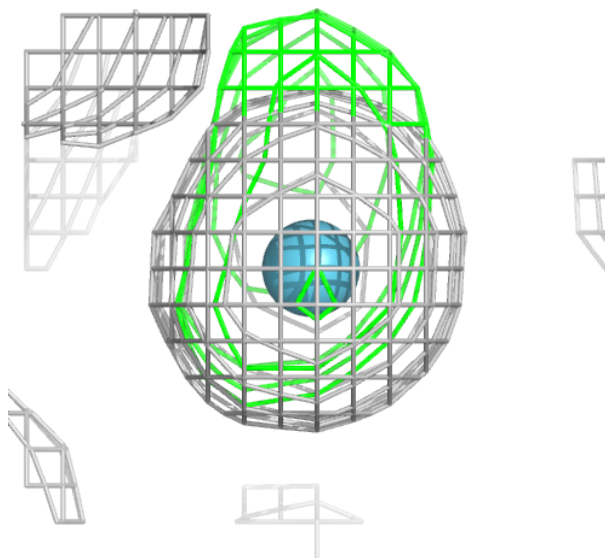
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





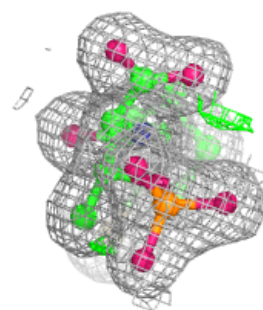
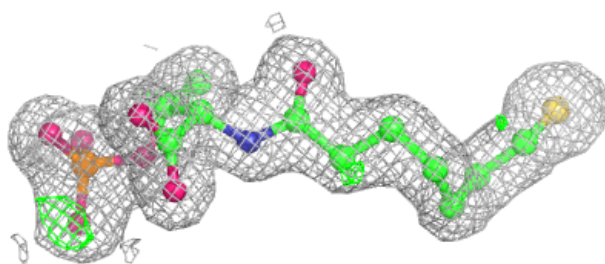
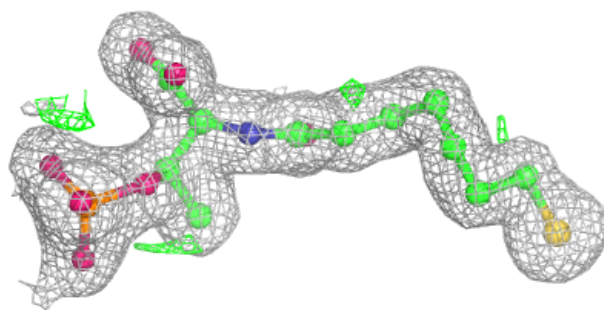
**Electron density around KR J 605:**

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

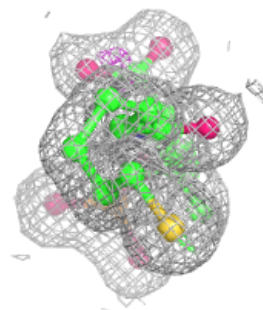
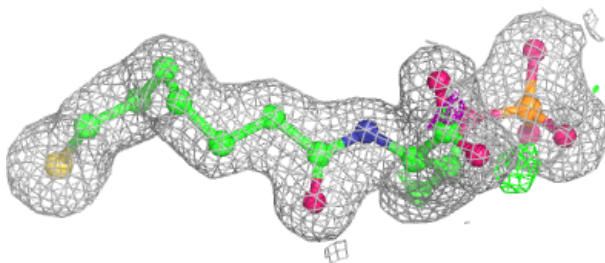
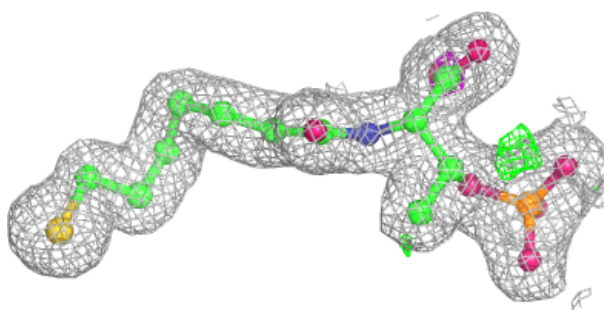


**Electron density around TP7 D 611:**

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

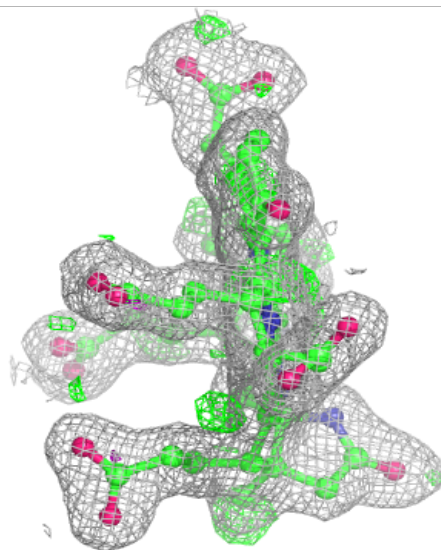
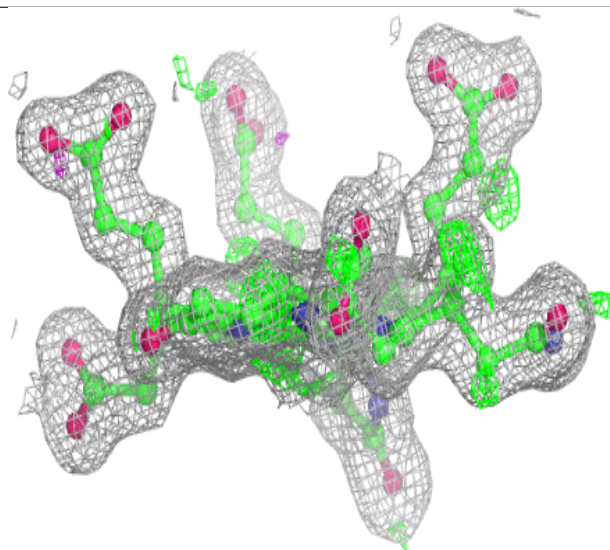
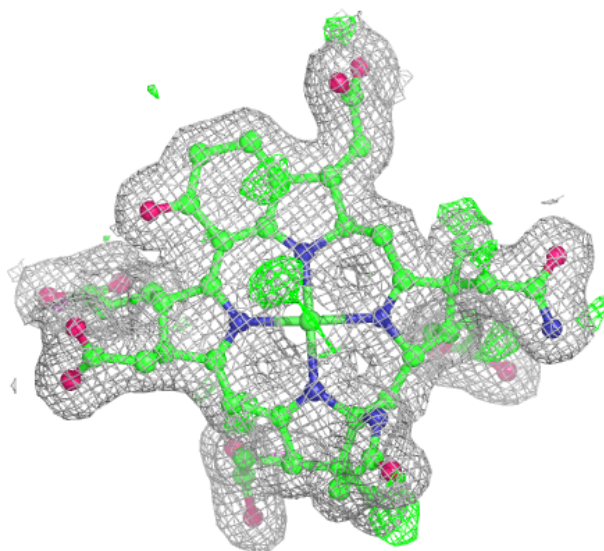
**Electron density around TP7 J 612:**

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



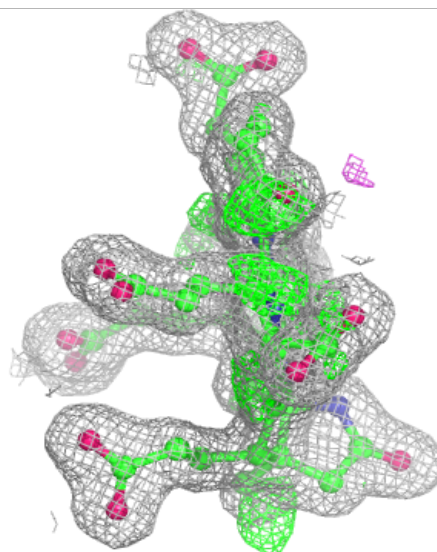
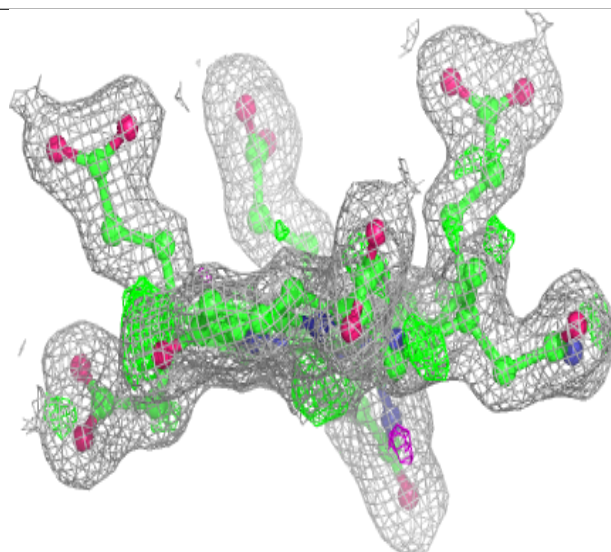
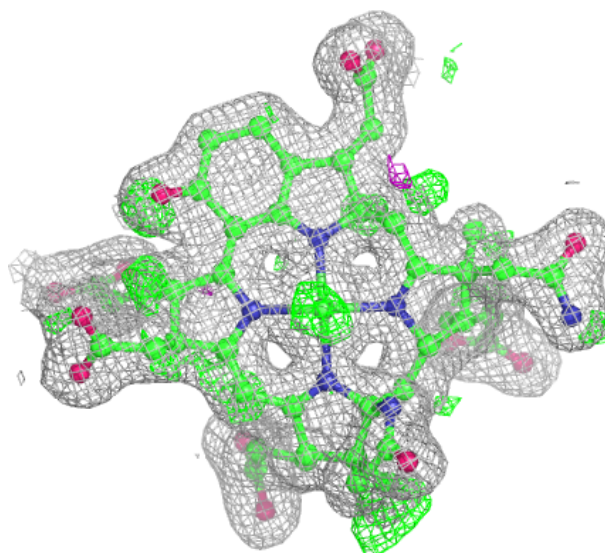
**Electron density around F43 D 613:**

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



**Electron density around F43 J 611:**

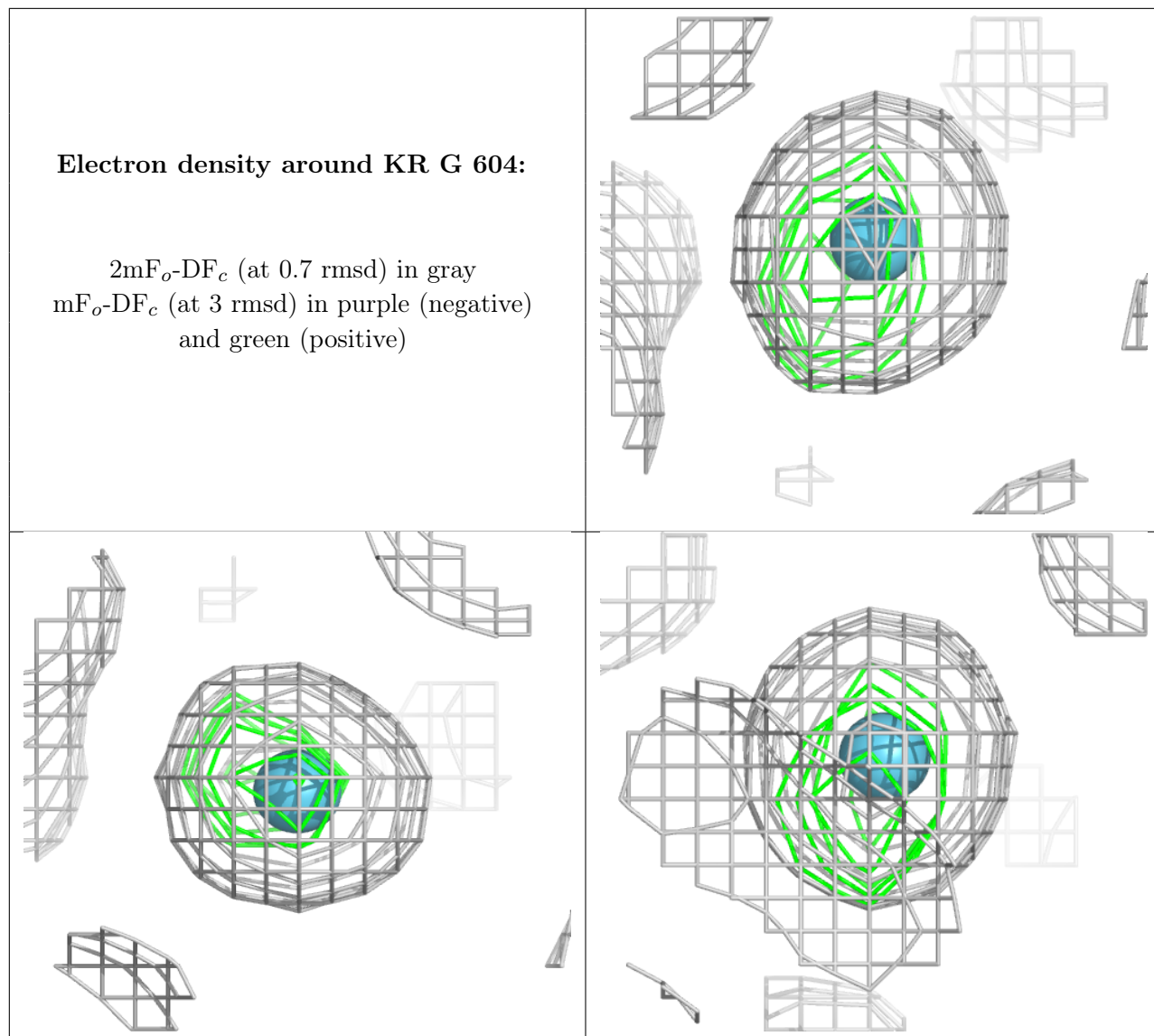
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





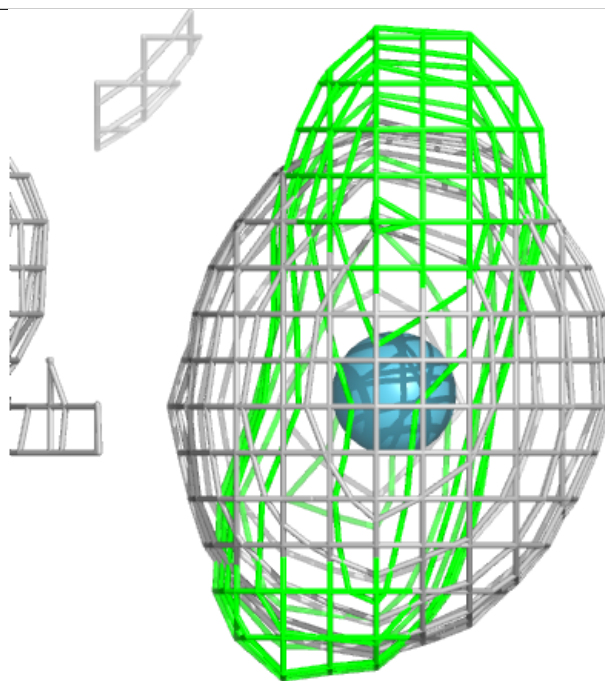
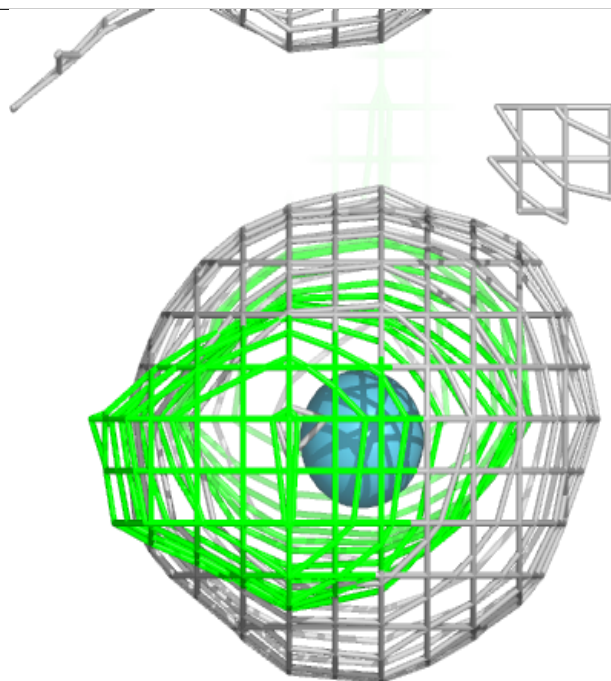
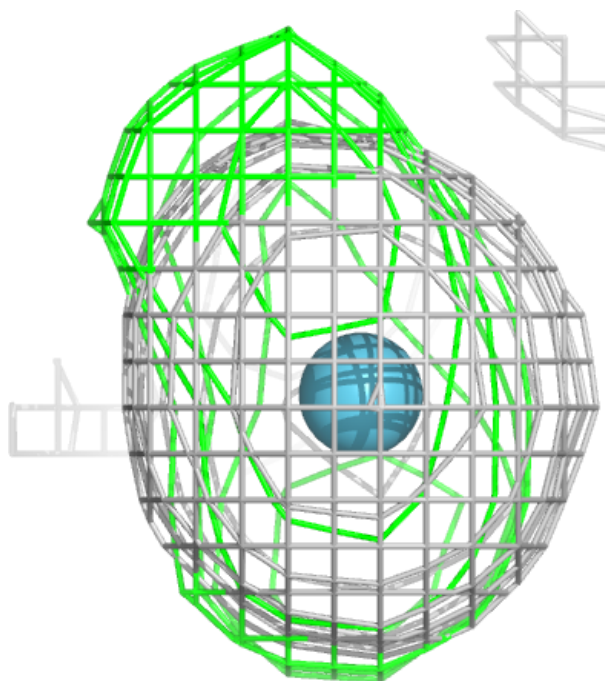
**Electron density around KR G 604:**

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



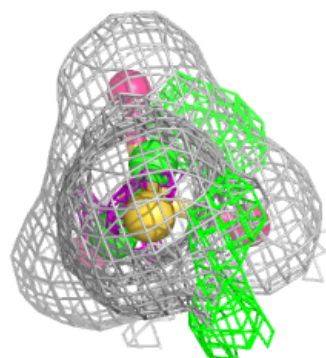
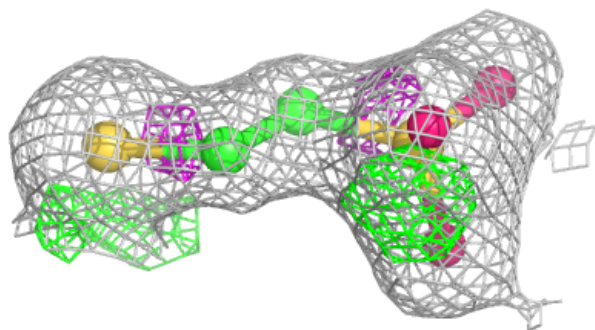
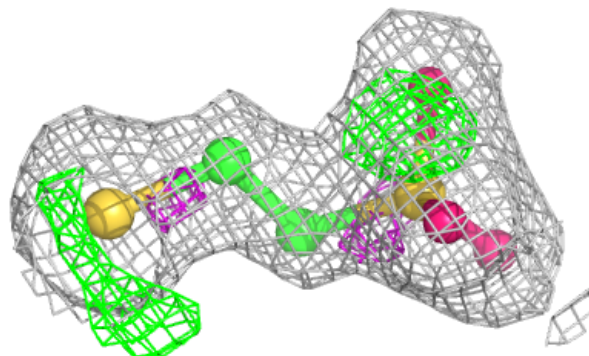
**Electron density around KR E 501:**

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



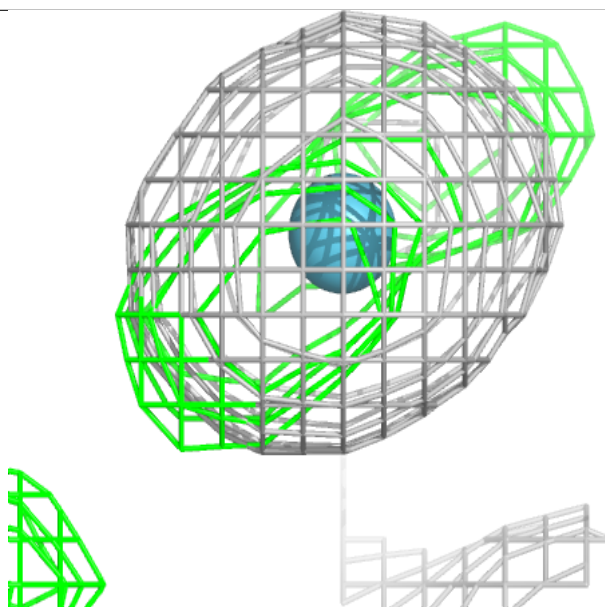
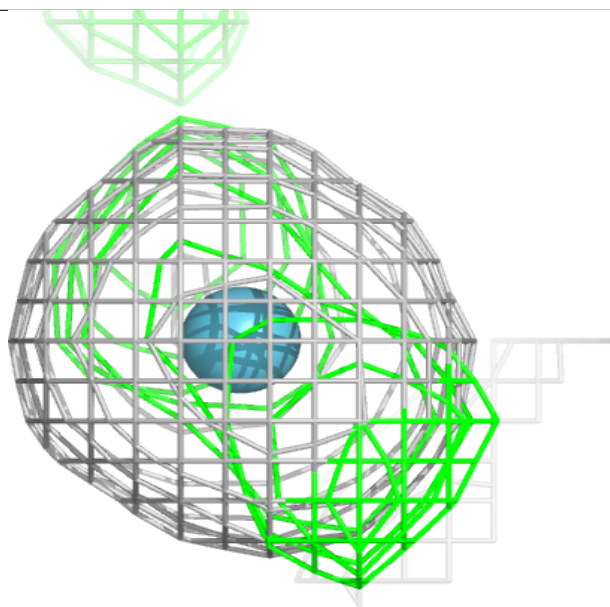
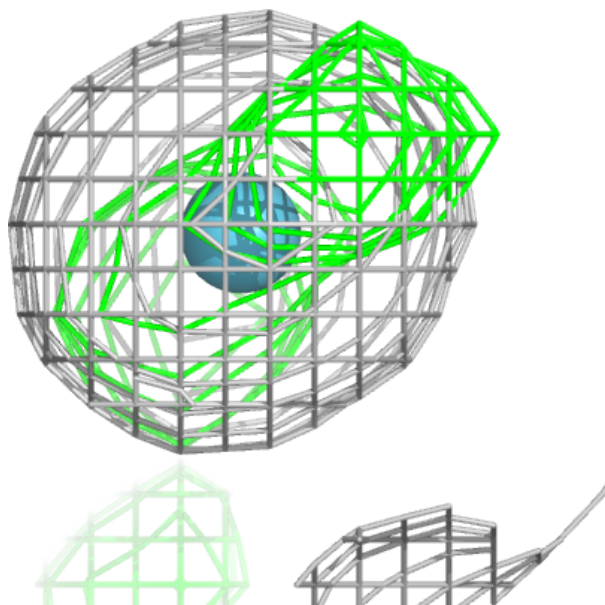
**Electron density around COM J 613:**

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



**Electron density around KR K 501:**

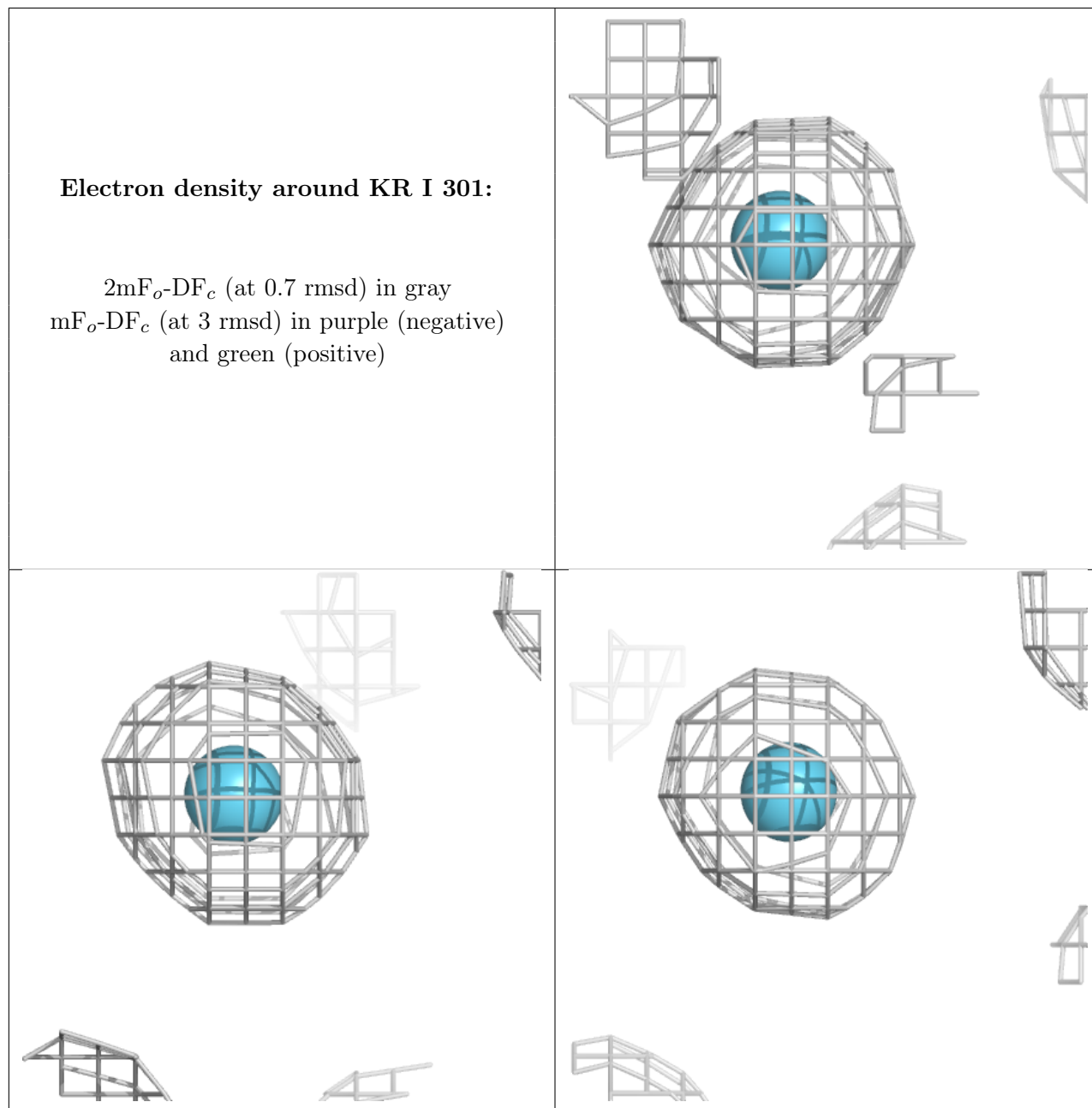
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





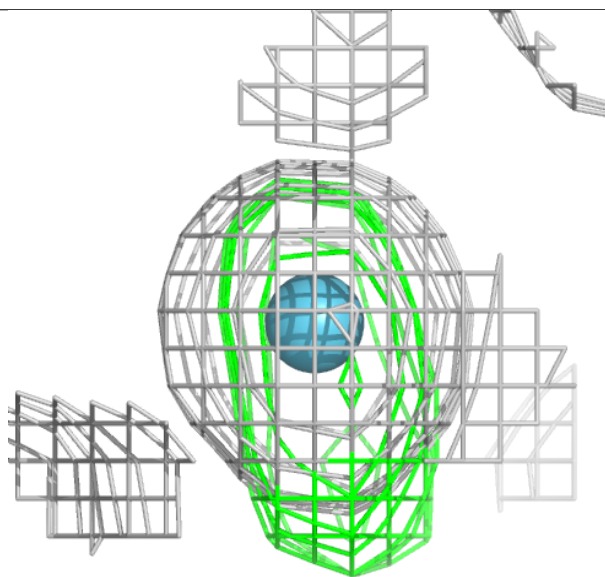
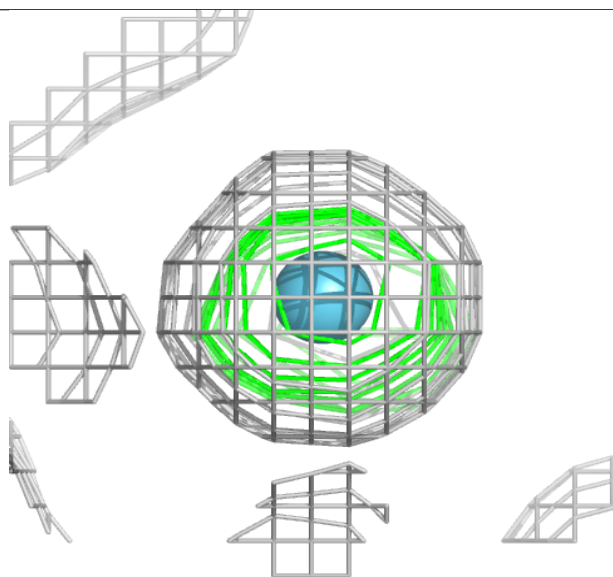
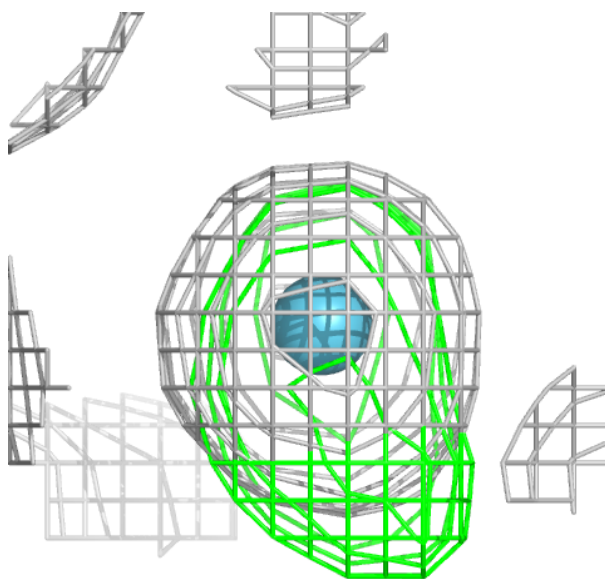
**Electron density around KR I 301:**

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



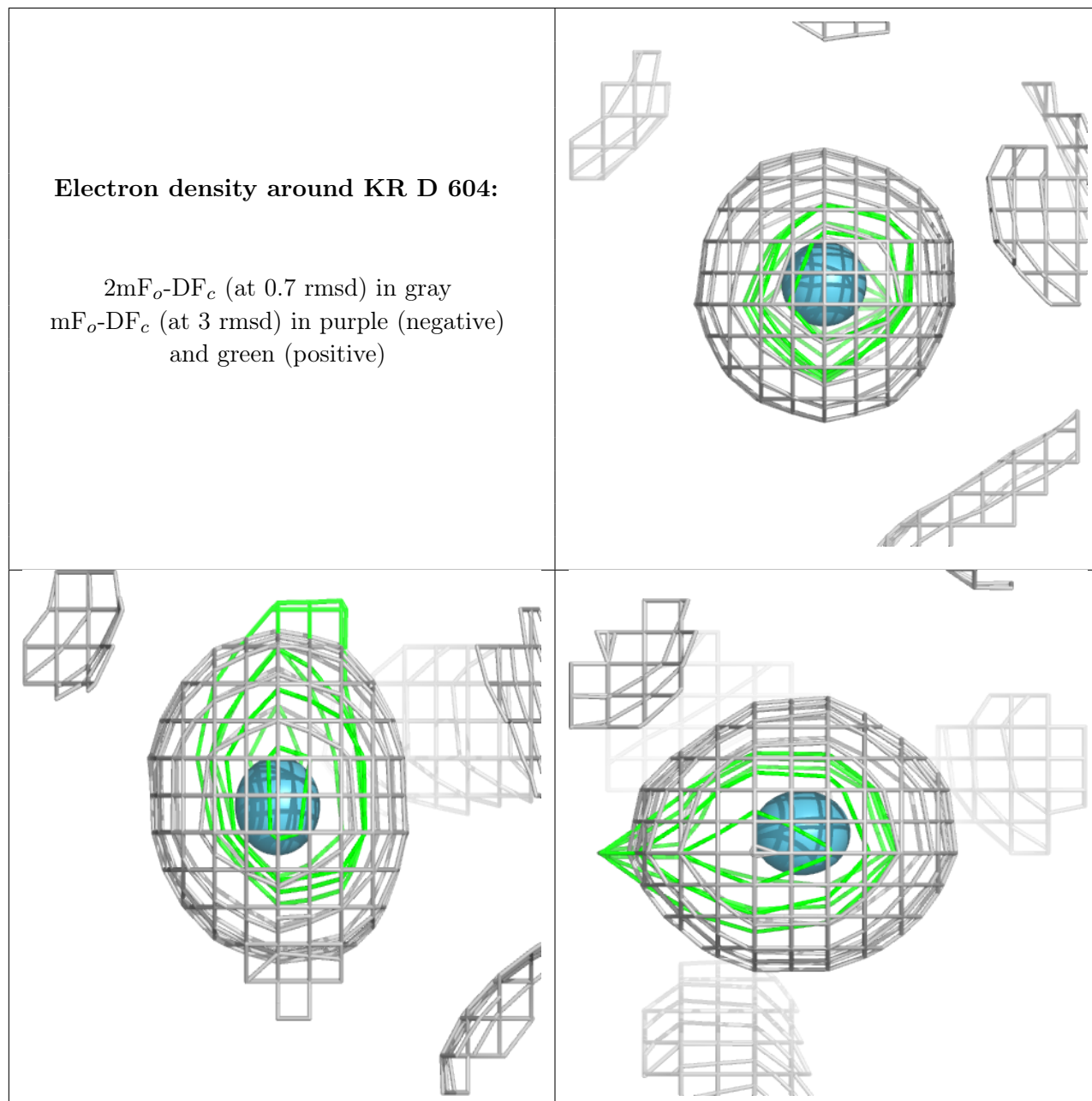
**Electron density around KR A 604:**

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



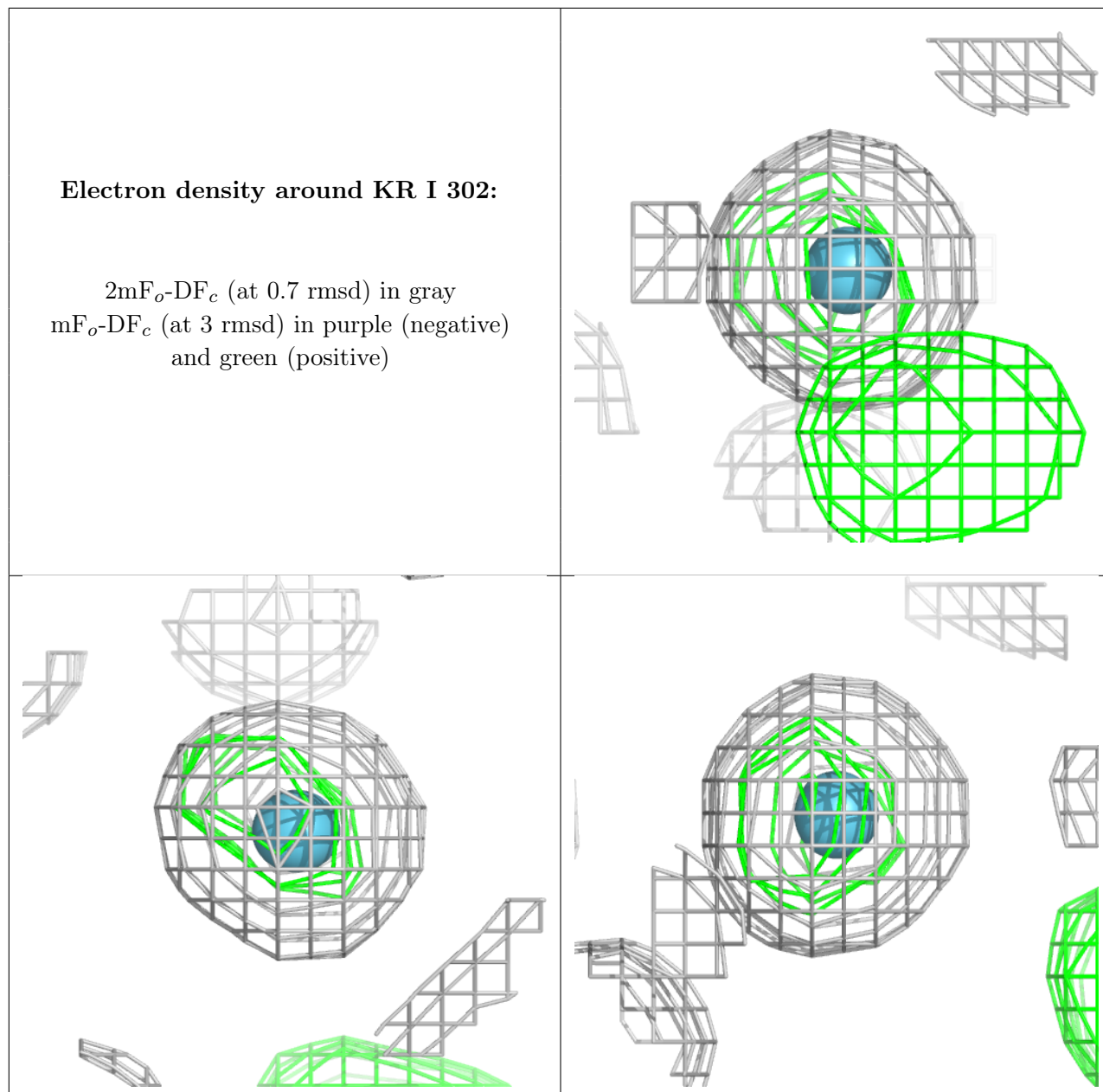
**Electron density around KR D 604:**

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



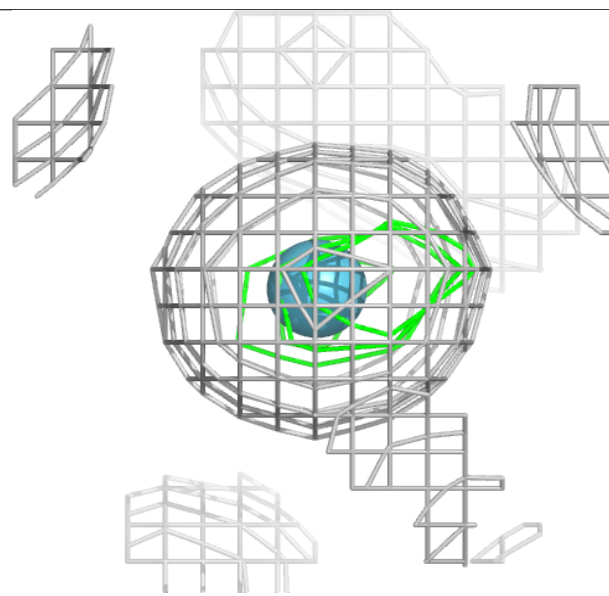
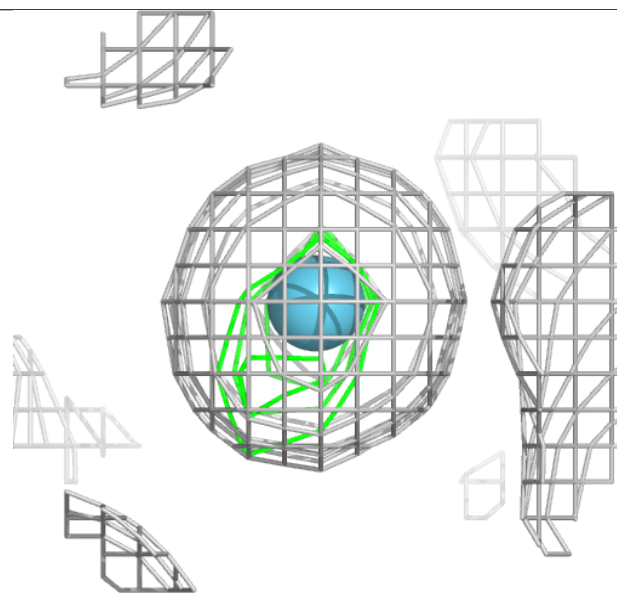
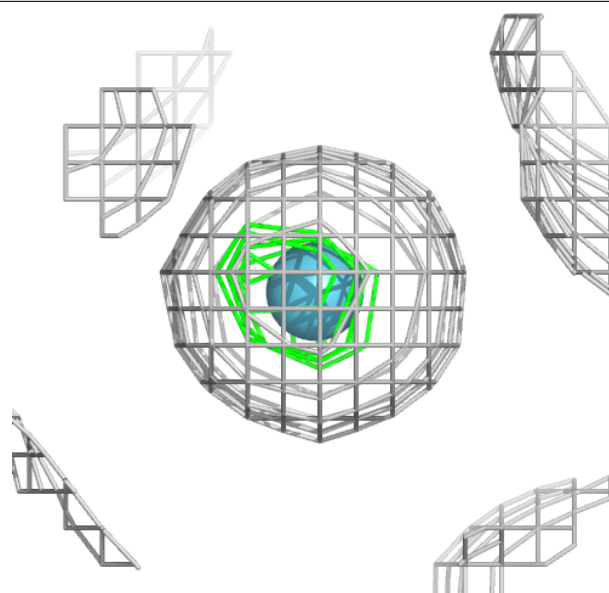
**Electron density around KR I 302:**

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



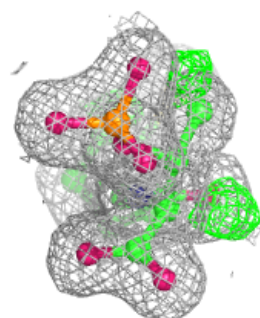
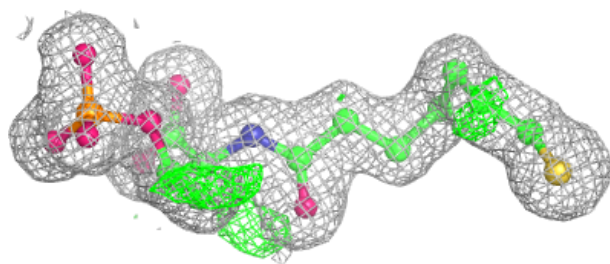
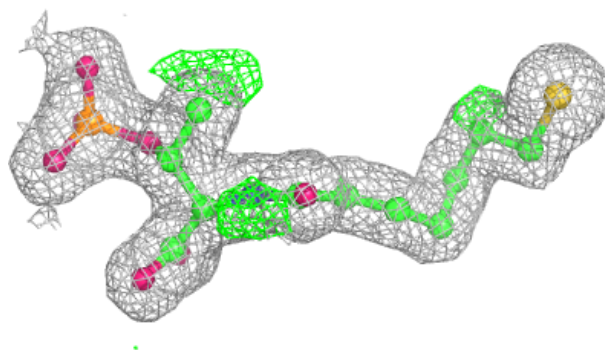
**Electron density around KR J 601:**

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



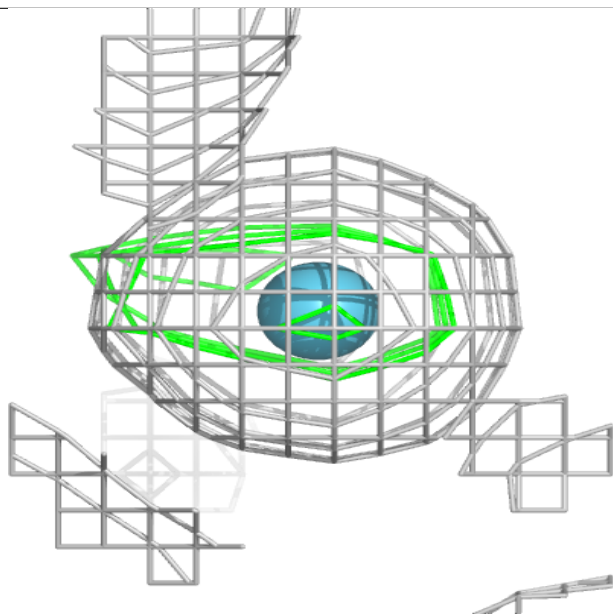
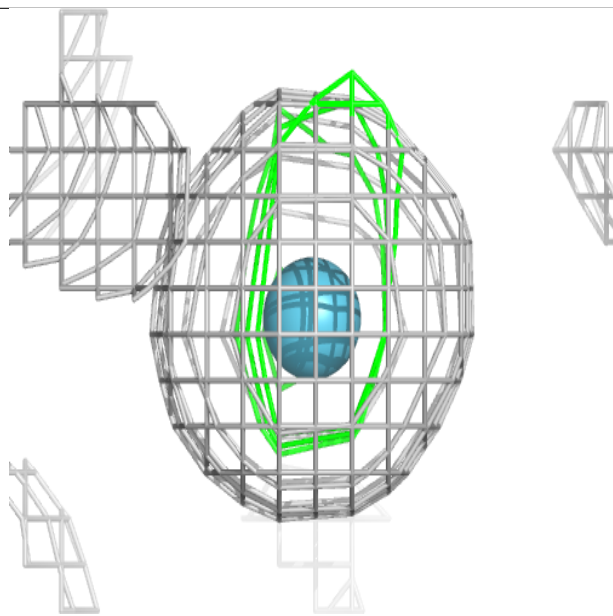
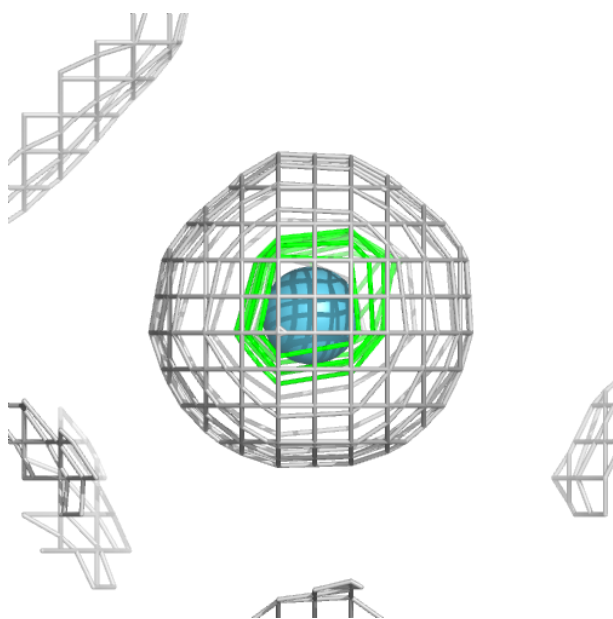
**Electron density around TP7 A 614:**

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



**Electron density around KR G 603:**

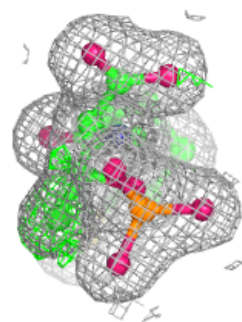
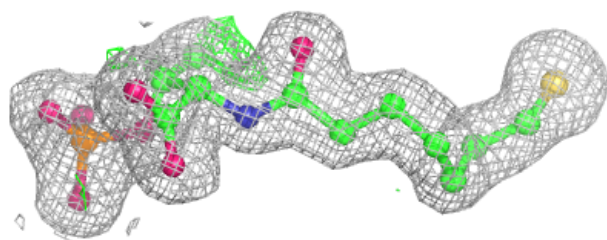
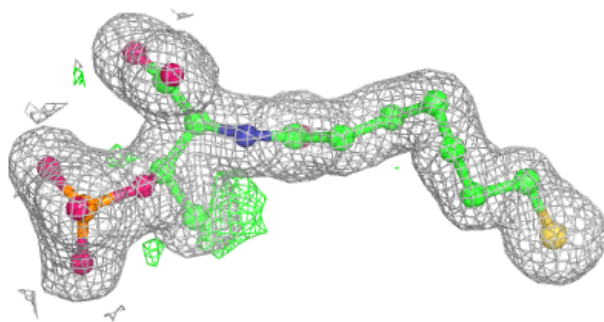
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around TP7 G 614:**

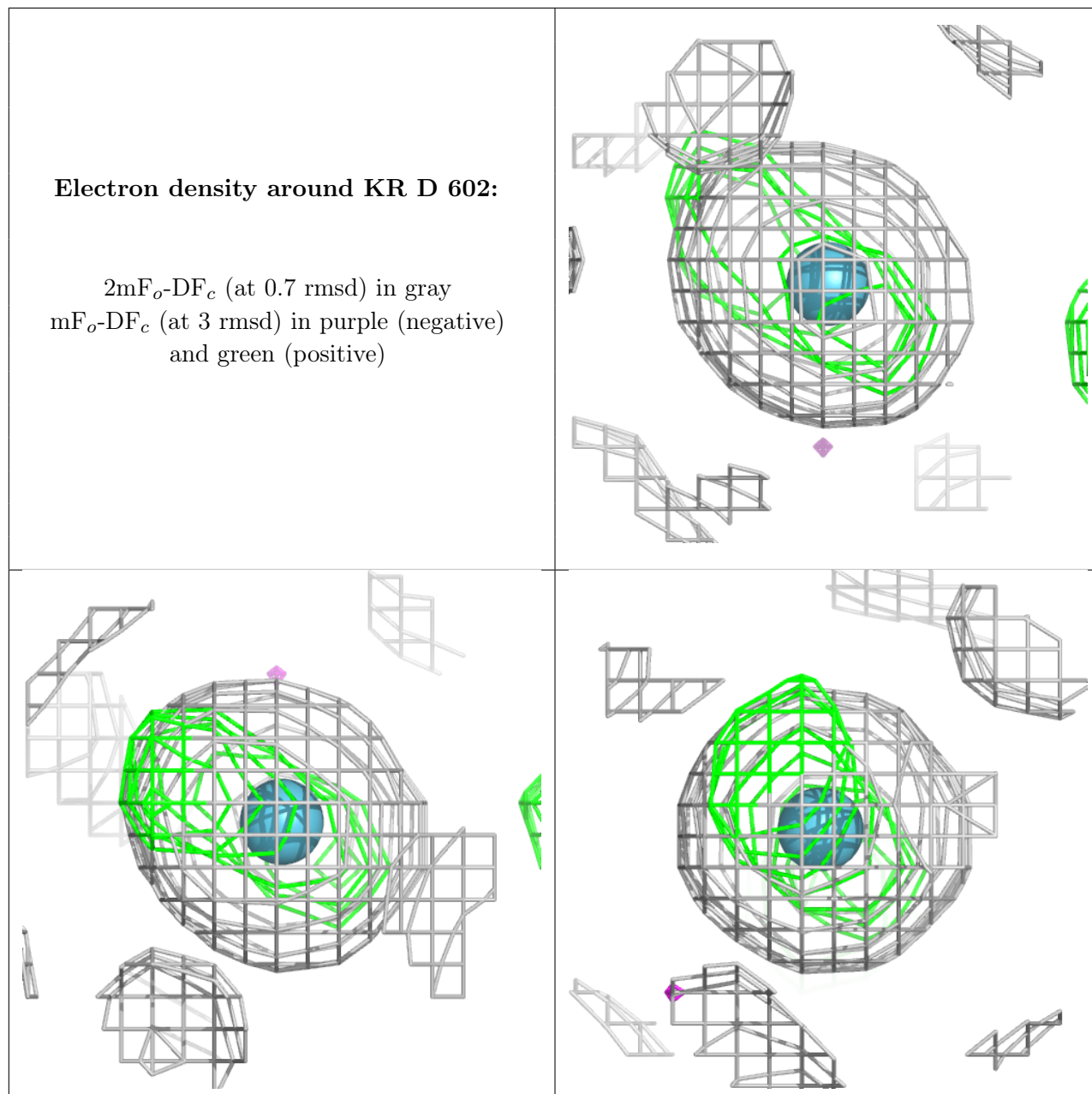
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





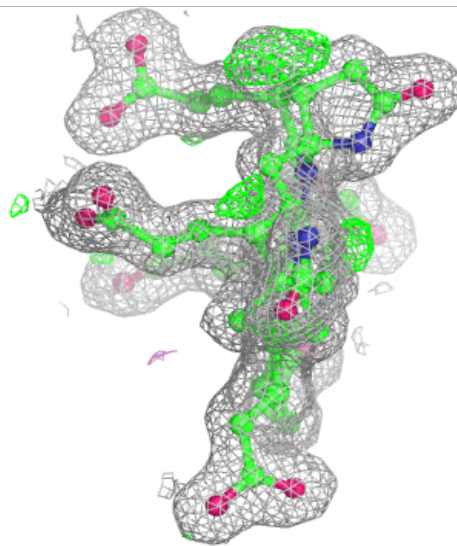
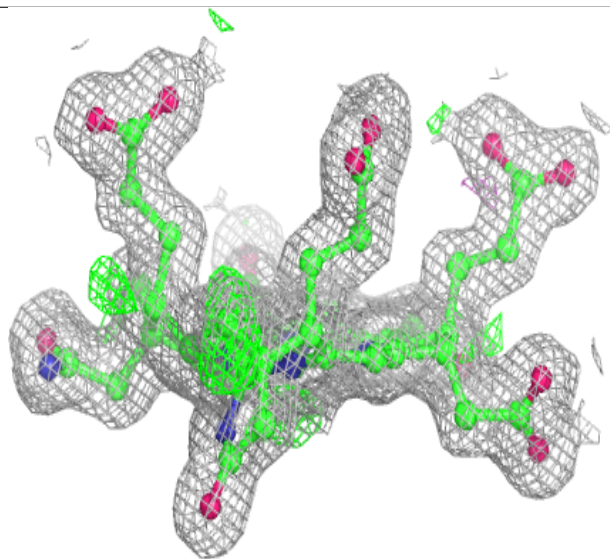
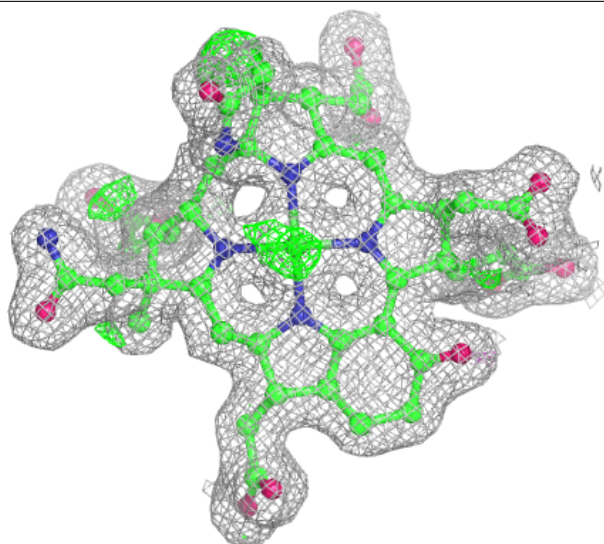
**Electron density around KR D 602:**

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



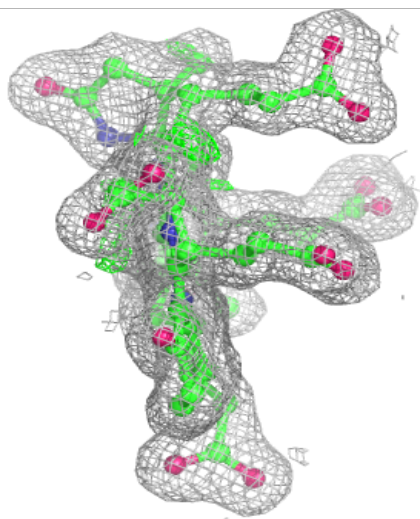
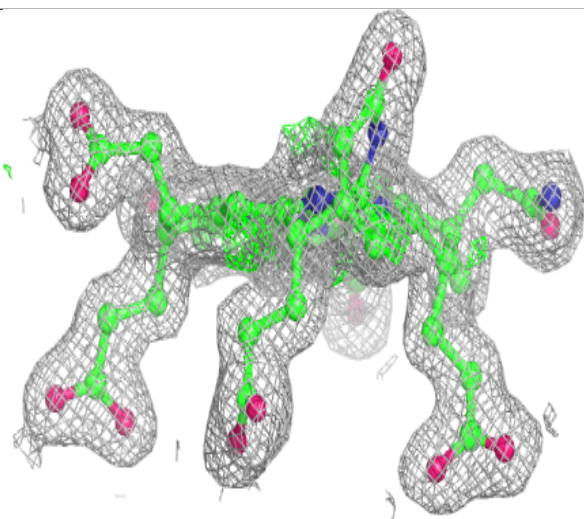
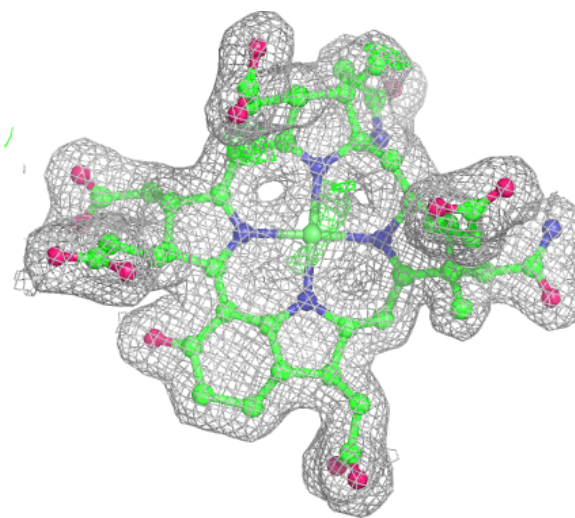
**Electron density around F43 A 615:**

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



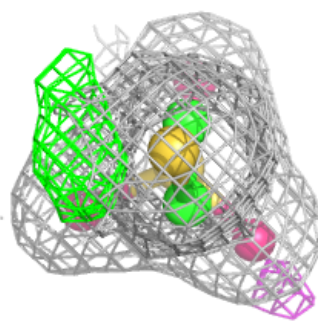
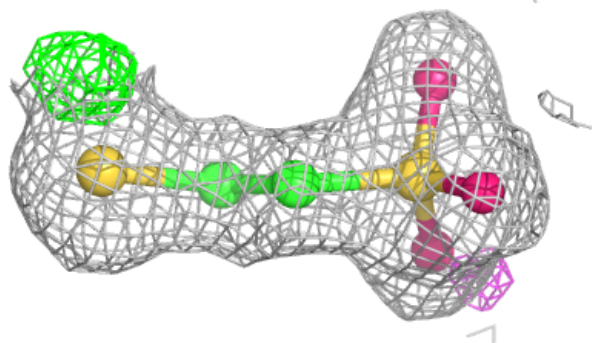
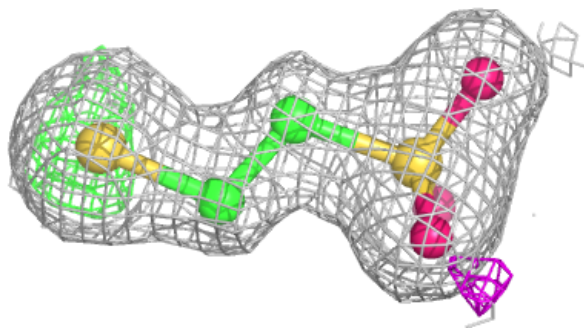
**Electron density around F43 G 619:**

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

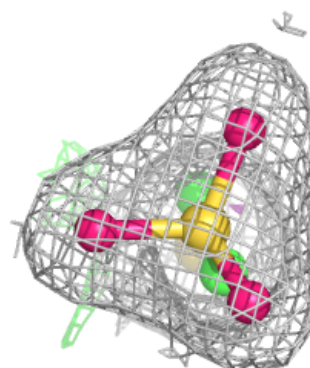
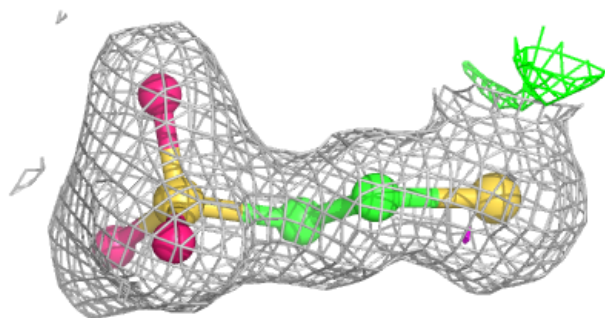
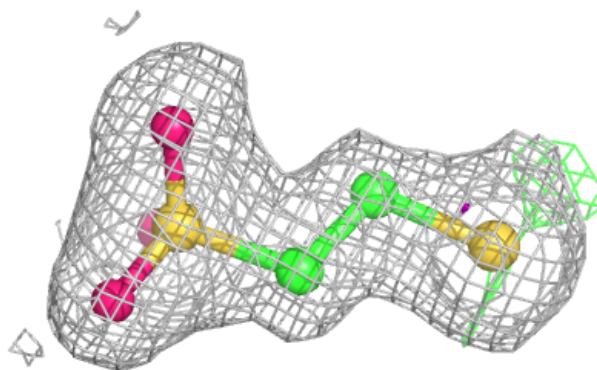


**Electron density around COM A 620:**

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

**Electron density around COM D 612:**

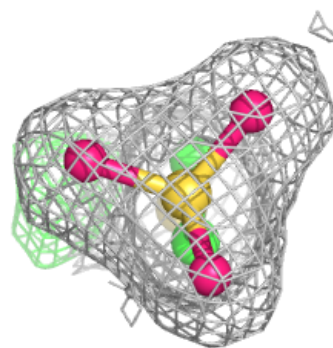
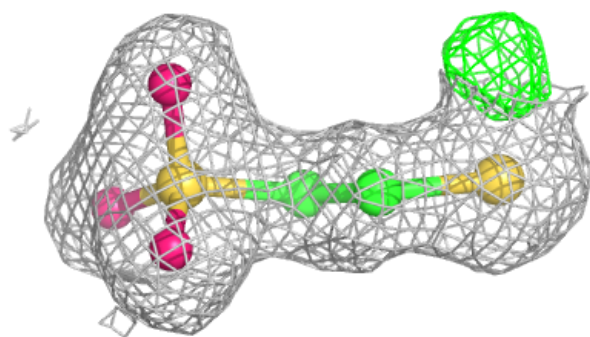
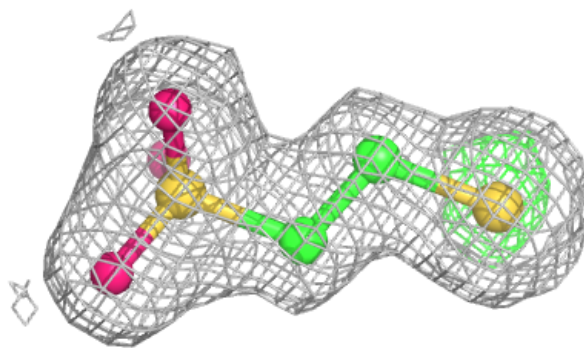
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





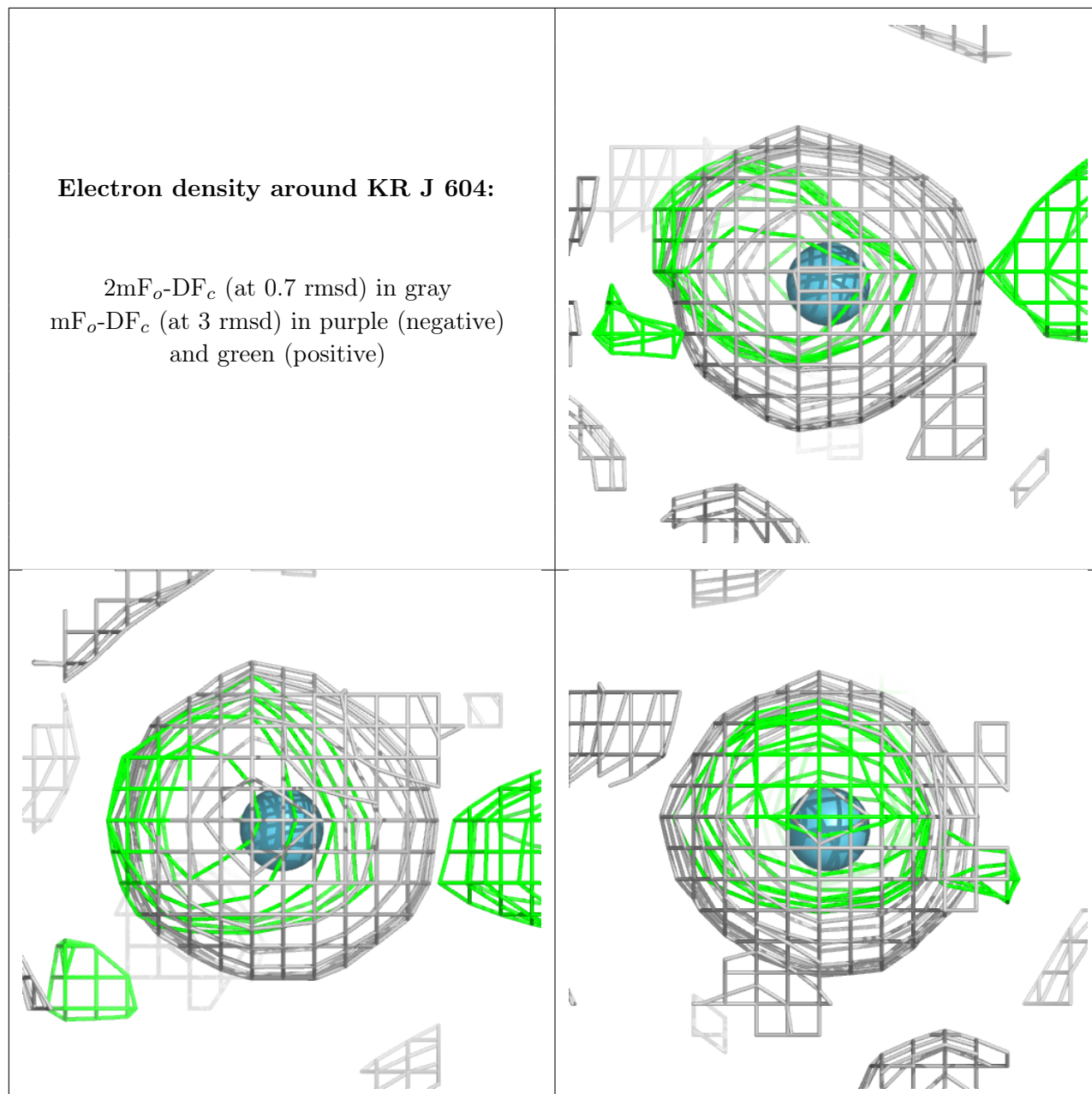
**Electron density around COM G 613:**

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



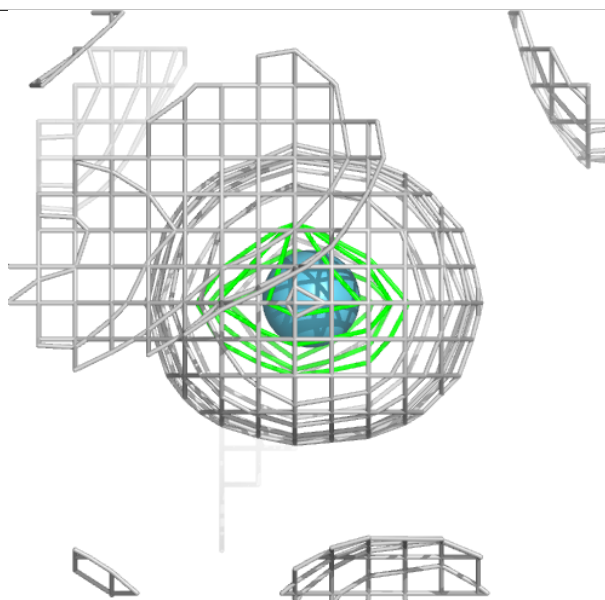
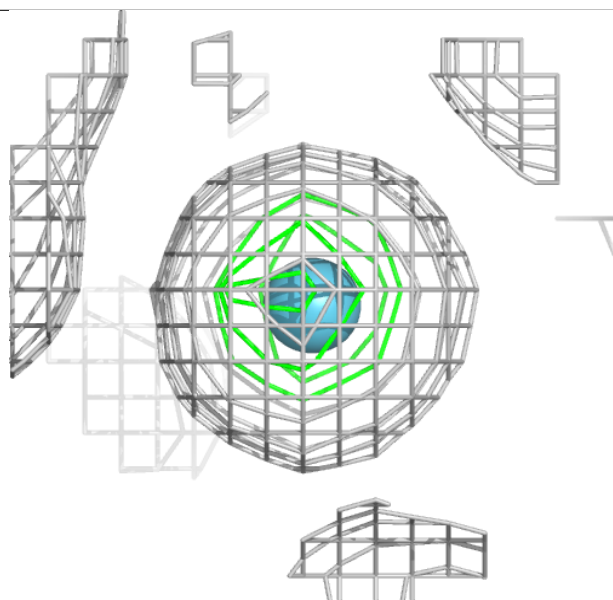
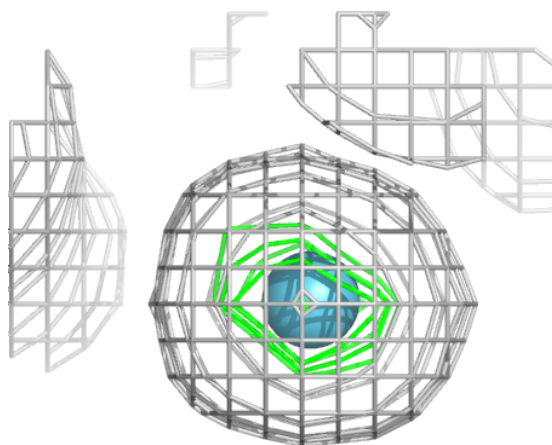
**Electron density around KR J 604:**

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



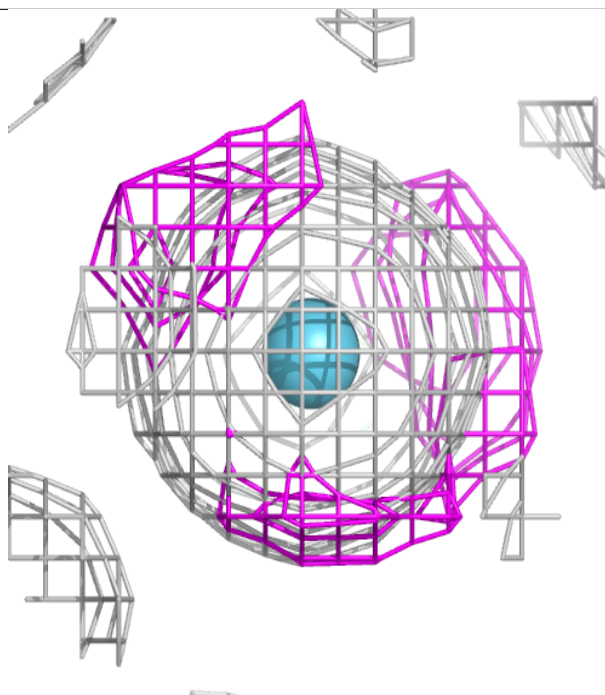
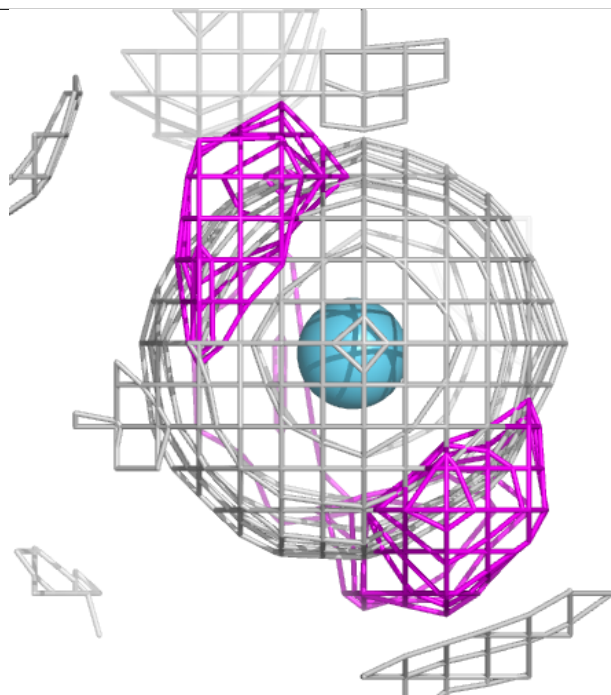
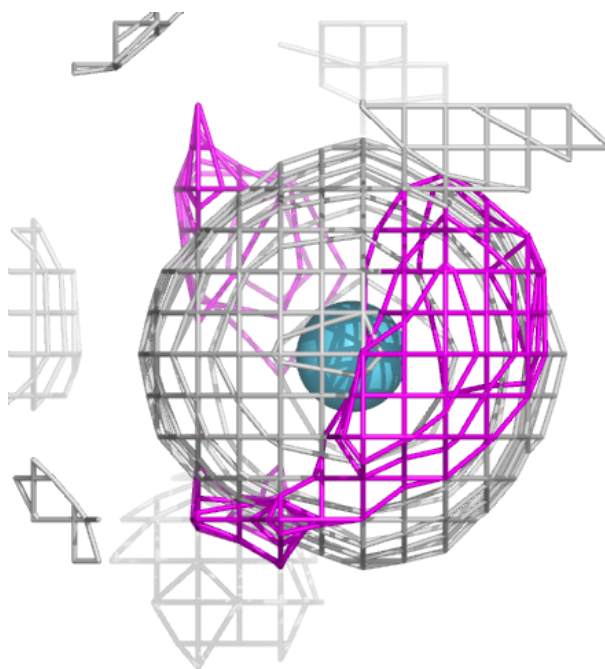
**Electron density around KR A 603:**

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



**Electron density around KR G 602:**

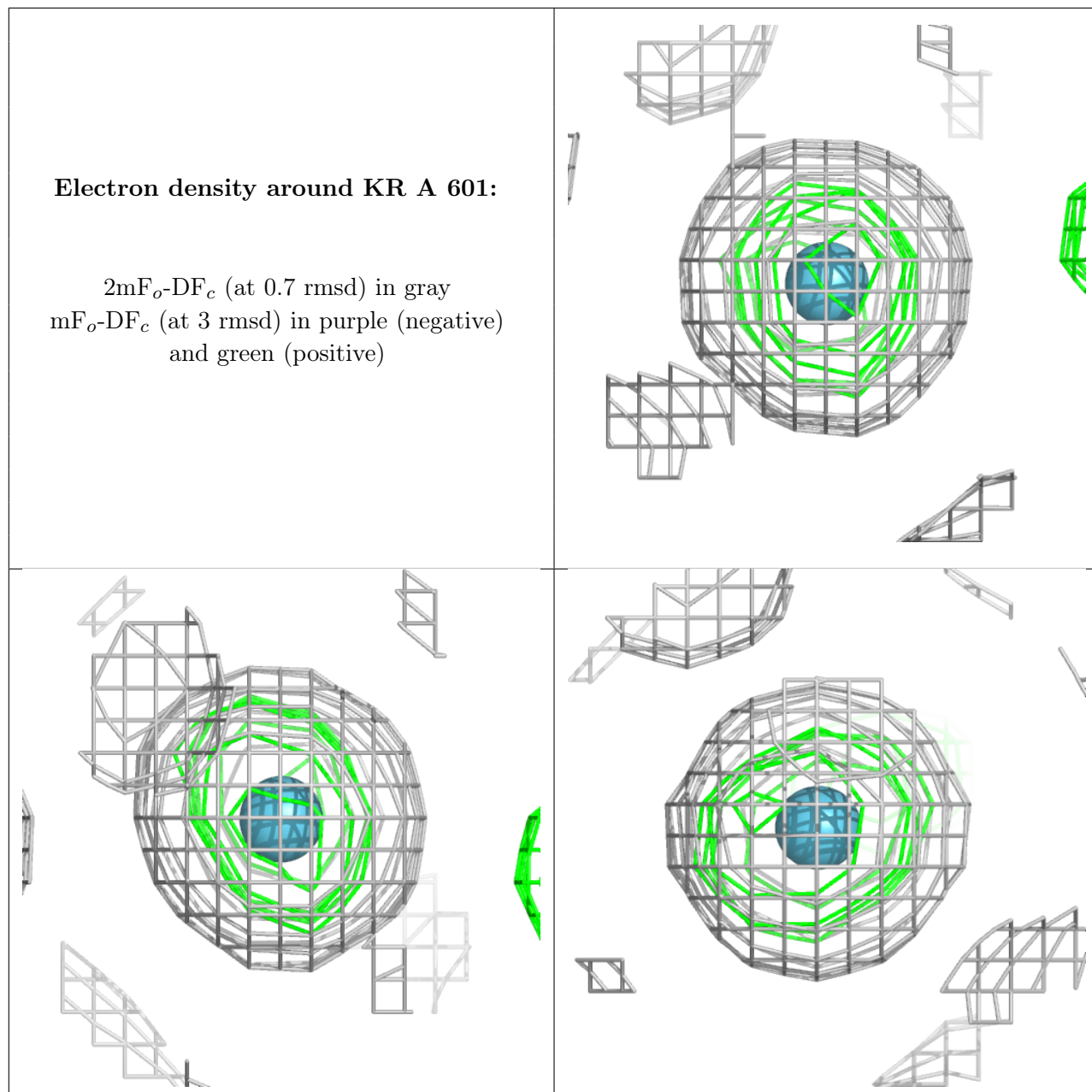
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around KR A 601:**

$2mF_o-DF_c$  (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.