



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:42 PM UTC

PDB ID : 7M2H / pdb_00007m2h
Title : Structural Snapshots of Intermediates in the Gating of a K⁺ Channel
Authors : Reddi, R.; Valiyaveetil, F.I.
Deposited on : 2021-03-16
Resolution : 2.64 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

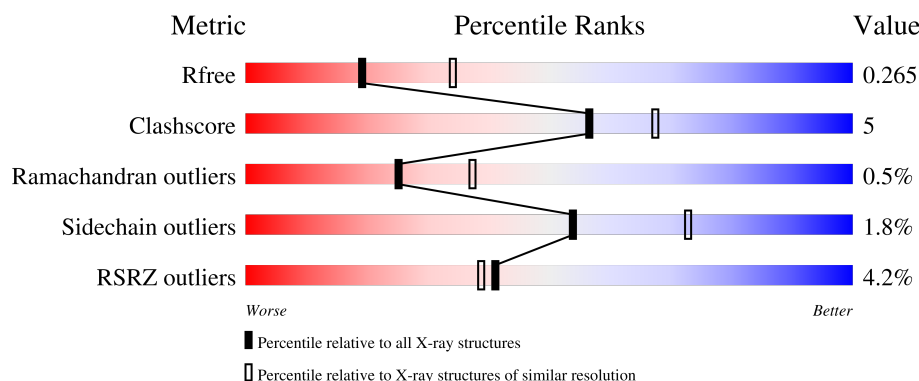
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	219	5% 86% 14%
1	D	219	5% 82% 16% .
2	B	212	2% 88% 12%
2	E	212	7% 89% 9% .
3	C	125	2% 74% 7% . 18%

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Mol	Chain	Length	Quality of chain
3	F	125	% 77%6%18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1615	1024	270	315	6			
1	D	217	Total	C	N	O	S	0	0	0
			1580	1004	260	310	6			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1642	1021	279	337	5			
2	E	209	Total	C	N	O	S	0	0	0
			1621	1009	275	332	5			

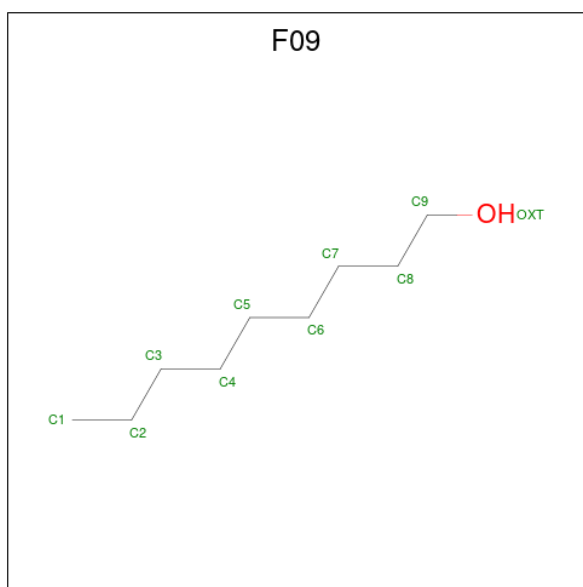
- Molecule 3 is a protein called pH-gated potassium channel KcsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			776	513	131	131	1			
3	F	103	Total	C	N	O	S	0	0	0
			776	513	131	131	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P0A334
C	2	ALA	-	expression tag	UNP P0A334
C	67	PHE	TRP	conflict	UNP P0A334
F	1	MET	-	initiating methionine	UNP P0A334
F	2	ALA	-	expression tag	UNP P0A334
F	67	PHE	TRP	conflict	UNP P0A334

- Molecule 4 is NONAN-1-OL (CCD ID: F09) (formula: C₉H₂₀O).

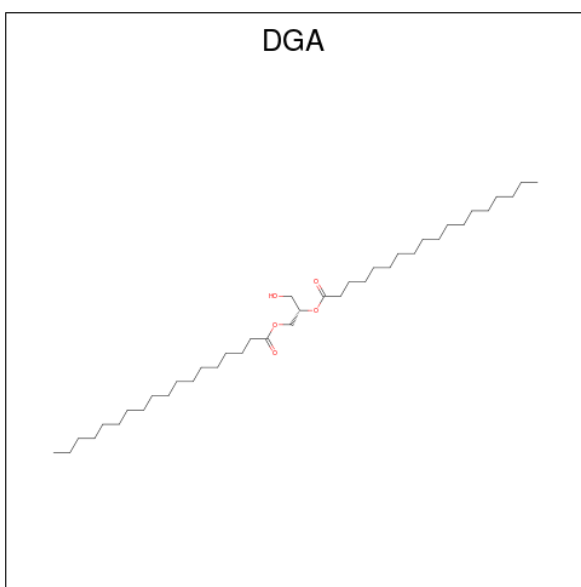


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	9	1		
4	D	1	Total	C	O	0	0
			10	9	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

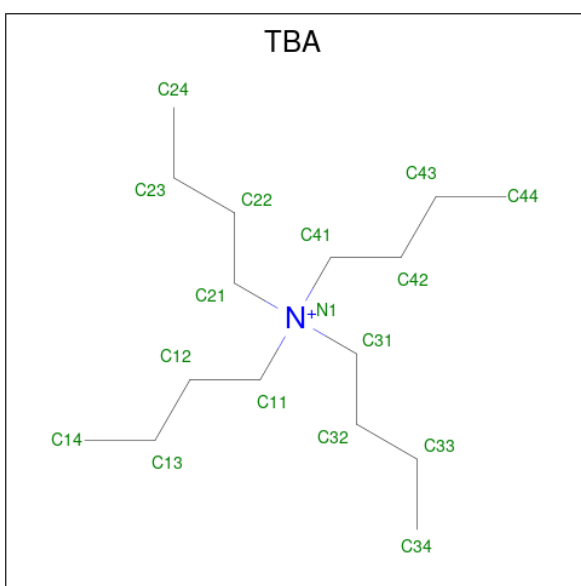
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total	K	0	0
			6	6		
5	F	6	Total	K	0	0
			6	6		

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			31	26	5		
6	F	1	Total	C	O	0	0
			31	26	5		

- Molecule 7 is TETRABUTYLAMMONIUM ION (CCD ID: TBA) (formula: $C_{16}H_{36}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	N	0	0
			17	16	1		
7	F	1	Total	C	N	0	0
			17	16	1		

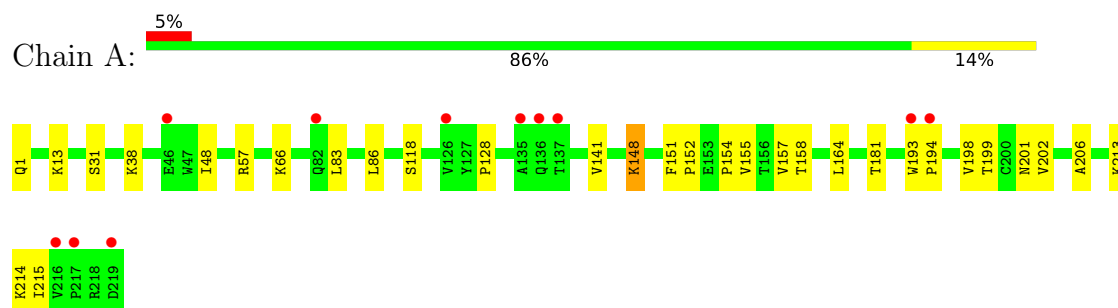
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total 24	O 24	0	0
8	B	28	Total 28	O 28	0	0
8	C	20	Total 20	O 20	0	0
8	D	6	Total 6	O 6	0	0
8	E	17	Total 17	O 17	0	0
8	F	32	Total 32	O 32	0	0

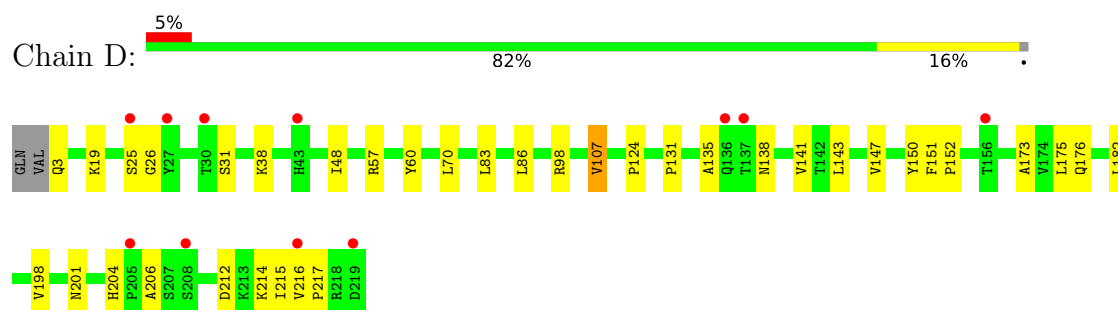
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

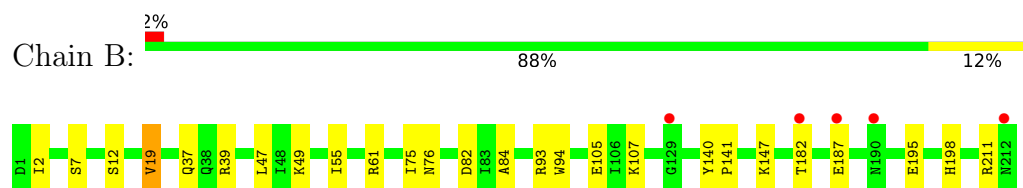
- Molecule 1: Fab heavy chain



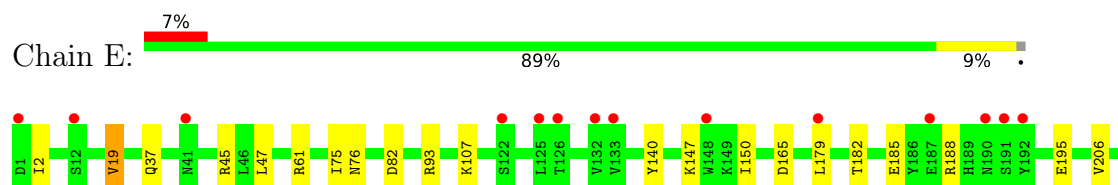
- Molecule 1: Fab heavy chain



- Molecule 2: Fab light chain



- Molecule 2: Fab light chain

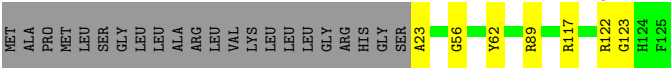
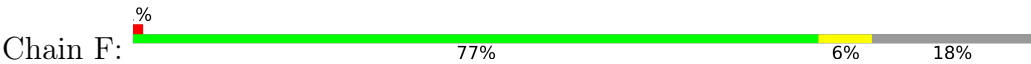




• Molecule 3: pH-gated potassium channel KcsA



• Molecule 3: pH-gated potassium channel KcsA



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	154.32Å 154.32Å 74.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.64 48.80 – 2.64	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.80-2.64) 91.4 (48.80-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.237 , 0.268 0.237 , 0.265	Depositor DCC
R_{free} test set	1999 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8265	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DGA, F09, K, TBA

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	0.35	0/1659	0.34	0/2275
1	D	0.11	0/1623	0.33	0/2227
2	B	0.36	1/1679 (0.1%)	0.33	0/2278
2	E	0.09	0/1658	0.30	0/2251
3	C	0.10	0/796	0.31	0/1092
3	F	0.09	0/796	0.27	0/1092
All	All	0.24	1/8211 (0.0%)	0.32	0/11215

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	TRP	C-O	-5.65	1.16	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1615	0	1549	20	0
1	D	1580	0	1502	21	0
2	B	1642	0	1565	15	0
2	E	1621	0	1551	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	776	0	791	8	0
3	F	776	0	791	5	0
4	A	10	0	20	1	0
4	D	10	0	20	1	0
5	C	6	0	0	0	0
5	F	6	0	0	0	0
6	C	31	0	44	0	0
6	F	31	0	44	2	0
7	C	17	0	36	0	0
7	F	17	0	36	0	0
8	A	24	0	0	0	0
8	B	28	0	0	3	0
8	C	20	0	0	2	0
8	D	6	0	0	1	0
8	E	17	0	0	0	0
8	F	32	0	0	1	0
All	All	8265	0	7949	73	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 5.

All (73) 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:1:GLN:HE22	1:D:217:PRO:HB3	1.37	0.89
1:A:1:GLN:HB2	1:D:131:PRO:HB2	1.68	0.75
2:B:198:HIS:NE2	8:B:301:HOH:O	2.18	0.75
2:B:141:PRO:O	8:B:301:HOH:O	2.09	0.71
1:D:83:LEU:HB3	1:D:86:LEU:HD21	1.75	0.66
2:B:2:ILE:HD11	2:B:93:ARG:HD2	1.77	0.66
1:A:157:VAL:HG22	1:A:202:VAL:HG22	1.78	0.66
1:D:38:LYS:HB2	1:D:48:ILE:HD11	1.79	0.65
1:A:199:THR:HG22	1:A:214:LYS:HA	1.76	0.65
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.78	0.65
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.80	0.63
3:C:120:GLU:O	3:C:122:ARG:N	2.31	0.61
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.81	0.61
1:D:173:ALA:HB2	1:D:182:LEU:HD23	1.84	0.59
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.85	0.59
1:D:214:LYS:NZ	1:D:215:ILE:O	2.32	0.58
2:B:147:LYS:HB3	2:B:195:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.40	0.54
1:A:158:THR:OG1	1:A:201:ASN:HB2	2.08	0.53
3:C:25:HIS:ND1	8:C:1001:HOH:O	2.33	0.52
1:D:201:ASN:ND2	1:D:212:ASP:OD1	2.31	0.52
2:E:37:GLN:OE1	2:E:45:ARG:NH2	2.43	0.50
2:E:182:THR:OG1	2:E:185:GLU:OE1	2.27	0.50
1:A:1:GLN:H3	1:D:135:ALA:HB3	1.76	0.50
2:E:61:ARG:NH1	2:E:82:ASP:OD1	2.46	0.49
1:A:152:PRO:HD2	1:A:206:ALA:CB	2.42	0.49
2:B:19:VAL:HG12	2:B:75:ILE:HB	1.93	0.49
2:E:185:GLU:HA	2:E:188:ARG:HG2	1.95	0.48
2:E:2:ILE:HD11	2:E:93:ARG:HD2	1.96	0.48
3:F:89:ARG:HH11	6:F:208:DGA:HA32	1.79	0.48
1:A:198:VAL:HG23	1:A:215:ILE:HB	1.96	0.47
3:C:108:ALA:O	3:C:112:THR:HG23	2.14	0.47
1:D:175:LEU:HG	1:D:176:GLN:N	2.29	0.47
1:A:57:ARG:HH21	4:A:301:F09:H81	1.79	0.47
1:D:31:SER:HB2	3:F:62:TYR:CE1	2.50	0.47
1:A:151:PHE:HA	1:A:152:PRO:HA	1.68	0.46
1:A:66:LYS:HE2	1:A:66:LYS:HB3	1.82	0.46
1:D:143:LEU:HD12	1:D:198:VAL:HG11	1.98	0.46
2:E:93:ARG:NH1	3:F:56:GLY:O	2.49	0.45
2:E:61:ARG:HG3	2:E:76:ASN:O	2.17	0.45
1:D:60:TYR:HH	1:D:70:LEU:H	1.61	0.45
1:A:128:PRO:HG3	1:A:213:LYS:HD2	1.98	0.45
1:D:26:GLY:O	8:D:401:HOH:O	2.21	0.45
2:B:39:ARG:HG2	2:B:84:ALA:HB2	2.00	0.44
2:E:19:VAL:HG12	2:E:75:ILE:HB	1.99	0.44
2:B:61:ARG:HG3	2:B:76:ASN:O	2.17	0.44
1:A:148:LYS:HB3	1:A:181:THR:HG23	1.99	0.44
3:F:89:ARG:HH11	6:F:208:DGA:CA3	2.31	0.44
1:A:1:GLN:N	1:D:135:ALA:HB3	2.32	0.43
2:B:49:LYS:HE3	8:B:303:HOH:O	2.17	0.43
2:B:93:ARG:NH1	3:C:56:GLY:O	2.51	0.43
3:C:120:GLU:C	3:C:122:ARG:N	2.75	0.43
2:E:147:LYS:HB3	2:E:195:GLU:HB2	2.00	0.43
2:B:107:LYS:HA	2:B:140:TYR:OH	2.19	0.42
1:D:3:GLN:HB3	1:D:25:SER:O	2.19	0.42
3:F:23:ALA:N	8:F:302:HOH:O	2.51	0.42
1:A:13:LYS:NZ	1:A:118:SER:O	2.51	0.42
1:D:124:PRO:HB3	1:D:150:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HB3	1:D:107:VAL:HG13	2.02	0.42
1:D:204:HIS:CE1	1:D:206:ALA:HB3	2.54	0.42
2:B:12:SER:OG	2:B:105:GLU:OE2	2.34	0.42
1:D:151:PHE:HA	1:D:152:PRO:HA	1.84	0.41
2:E:150:ILE:HD11	2:E:179:LEU:HD21	2.02	0.41
1:A:148:LYS:HA	1:A:181:THR:HA	2.02	0.41
1:A:193:TRP:CD1	1:A:194:PRO:HA	2.55	0.41
3:C:80:ASP:OD1	3:C:80:ASP:N	2.54	0.41
3:C:23:ALA:N	8:C:1004:HOH:O	2.54	0.41
1:D:57:ARG:CZ	4:D:301:F09:H82	2.51	0.41
2:E:107:LYS:HA	2:E:140:TYR:OH	2.21	0.41
1:A:31:SER:HB2	3:C:62:TYR:CE1	2.56	0.40
2:B:49:LYS:HG2	2:B:55:ILE:HD11	2.03	0.40
2:B:187:GLU:OE2	2:B:211:ARG:NH2	2.54	0.40
1:D:147:VAL:HB	1:D:182:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	25	37
1	D	215/219 (98%)	203 (94%)	11 (5%)	1 (0%)	25	37
2	B	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
2	E	207/212 (98%)	198 (96%)	9 (4%)	0	100	100
3	C	101/125 (81%)	97 (96%)	3 (3%)	1 (1%)	13	19
3	F	101/125 (81%)	99 (98%)	0	2 (2%)	6	8
All	All	1051/1112 (94%)	1002 (95%)	44 (4%)	5 (0%)	25	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	122	ARG
1	D	138	ASN
3	F	122	ARG
3	F	123	GLY
1	A	154	PRO

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	174/185 (94%)	170 (98%)	4 (2%)	45	65
1	D	168/185 (91%)	164 (98%)	4 (2%)	44	64
2	B	188/190 (99%)	185 (98%)	3 (2%)	58	75
2	E	187/190 (98%)	184 (98%)	3 (2%)	58	75
3	C	74/92 (80%)	73 (99%)	1 (1%)	62	78
3	F	74/92 (80%)	73 (99%)	1 (1%)	62	78
All	All	865/934 (93%)	849 (98%)	16 (2%)	54	73

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

Mol	Chain	Res	Type
1	A	141	VAL
1	A	148	LYS
1	A	155	VAL
1	A	164	LEU
2	B	7	SER
2	B	19	VAL
2	B	182	THR
3	C	35	LEU
1	D	19	LYS
1	D	107	VAL
1	D	141	VAL
1	D	216	VAL
2	E	19	VAL
2	E	165	ASP

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Mol	Chain	Res	Type
2	E	206	VAL
3	F	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	169	HIS
2	B	124	GLN
2	B	161	ASN
2	E	27	GLN
2	E	190	ASN
3	F	119	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	DGA	F	208	-	30,30,43	1.39	3 (10%)	32,32,45	1.25	2 (6%)
4	F09	A	301	-	9,9,9	0.31	0	8,8,8	0.82	0
7	TBA	F	201	-	16,16,16	0.97	0	18,18,18	0.68	0
4	F09	D	301	-	9,9,9	0.30	0	8,8,8	0.80	0
7	TBA	C	908	-	16,16,16	0.99	0	18,18,18	0.68	0
6	DGA	C	907	-	30,30,43	1.42	3 (10%)	32,32,45	1.24	2 (6%)

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	DGA	F	208	-	-	13/32/32/45	-
4	F09	A	301	-	-	1/7/7/7	-
7	TBA	F	201	-	-	1/20/20/20	-
4	F09	D	301	-	-	1/7/7/7	-
7	TBA	C	908	-	-	2/20/20/20	-
6	DGA	C	907	-	-	12/32/32/45	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	208	DGA	OG1-CA1	3.65	1.44	1.33
6	C	907	DGA	OG1-CA1	3.54	1.43	1.33
6	C	907	DGA	OG2-CB1	2.91	1.42	1.34
6	F	208	DGA	OG2-CG2	-2.88	1.39	1.46
6	F	208	DGA	OG2-CB1	2.88	1.42	1.34
6	C	907	DGA	OG2-CG2	-2.76	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	907	DGA	OG2-CB1-CB2	4.03	120.20	111.48
6	F	208	DGA	OG2-CB1-CB2	3.94	120.00	111.48
6	F	208	DGA	OG1-CA1-CA2	2.54	119.59	111.83
6	C	907	DGA	OG1-CA1-CA2	2.49	119.42	111.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	907	DGA	OB1-CB1-OG2-CG2
6	C	907	DGA	CG1-CG2-CG3-OXT
6	C	907	DGA	OG2-CG2-CG3-OXT
6	F	208	DGA	CA2-CA1-OG1-CG1
6	F	208	DGA	OA1-CA1-OG1-CG1
6	F	208	DGA	OB1-CB1-OG2-CG2
6	C	907	DGA	CB2-CB1-OG2-CG2
6	F	208	DGA	CB2-CB1-OG2-CG2
6	C	907	DGA	CB3-CB4-CB5-CB6
6	F	208	DGA	CA1-CA2-CA3-CA4
6	C	907	DGA	CA1-CA2-CA3-CA4
7	C	908	TBA	N1-C11-C12-C13
7	C	908	TBA	N1-C31-C32-C33
7	F	201	TBA	N1-C31-C32-C33
4	D	301	F09	C6-C7-C8-C9
6	F	208	DGA	CB7-CB8-CB9-CAB
6	C	907	DGA	CB6-CB7-CB8-CB9
6	F	208	DGA	CA3-CA4-CA5-CA6
6	C	907	DGA	CB4-CB5-CB6-CB7
6	F	208	DGA	CB5-CB6-CB7-CB8
6	F	208	DGA	CA6-CA7-CA8-CA9
6	C	907	DGA	OG1-CG1-CG2-OG2
6	F	208	DGA	OG1-CG1-CG2-OG2
6	C	907	DGA	OG1-CG1-CG2-CG3
6	F	208	DGA	CB6-CB7-CB8-CB9
6	C	907	DGA	CA3-CA4-CA5-CA6
6	F	208	DGA	OG1-CG1-CG2-CG3
6	F	208	DGA	CBB-CAB-CB9-CB8
4	A	301	F09	C1-C2-C3-C4
6	C	907	DGA	CB5-CB6-CB7-CB8

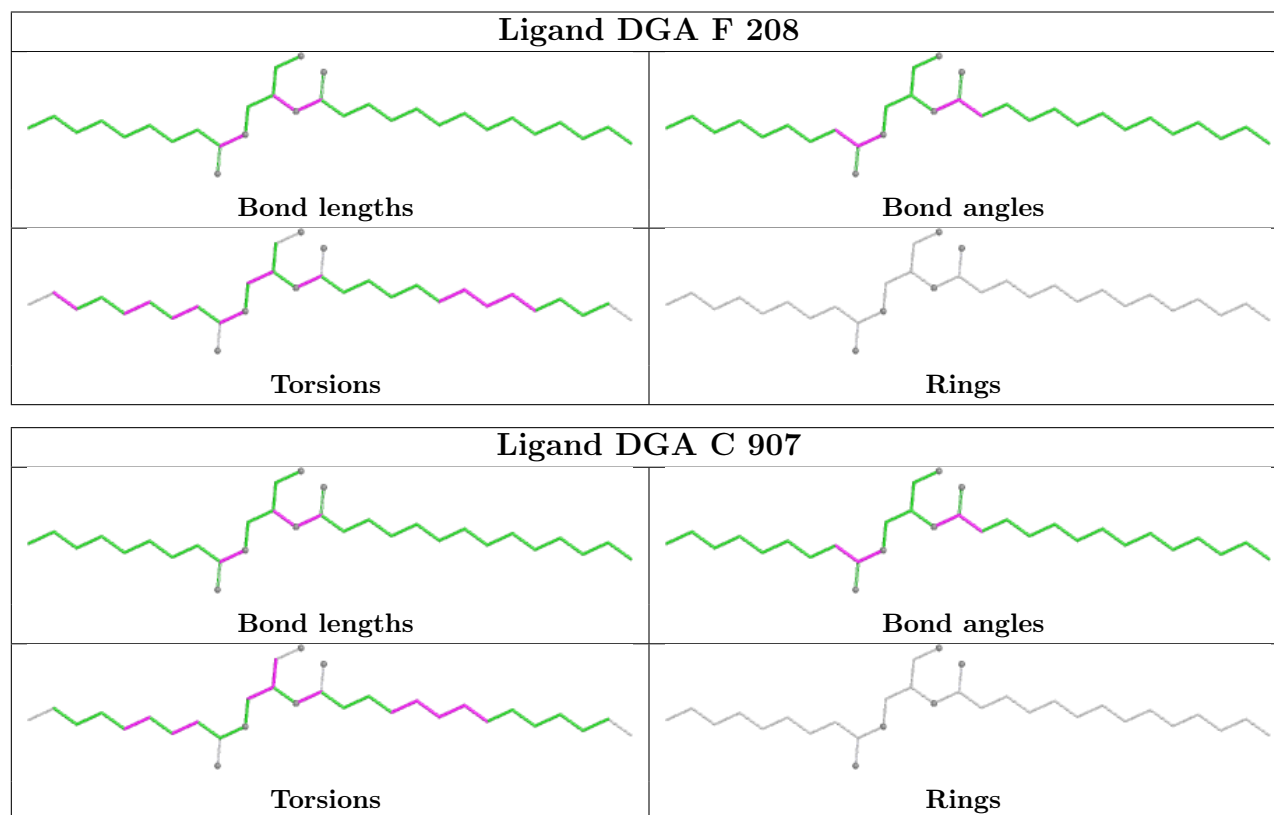
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	208	DGA	2	0
4	A	301	F09	1	0
4	D	301	F09	1	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.



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/219 (100%)	0.25	11 (5%) 35 34	18, 44, 70, 85	0
1	D	217/219 (99%)	0.25	11 (5%) 34 33	20, 42, 60, 81	0
2	B	212/212 (100%)	0.10	5 (2%) 59 58	12, 43, 77, 90	0
2	E	209/212 (98%)	0.26	15 (7%) 23 22	17, 41, 70, 87	0
3	C	103/125 (82%)	-0.28	2 (1%) 66 65	11, 19, 29, 35	0
3	F	103/125 (82%)	-0.36	1 (0%) 79 78	15, 21, 32, 40	0
All	All	1063/1112 (95%)	0.11	45 (4%) 41 39	11, 37, 68, 90	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	5.1
2	E	191	SER	4.6
1	D	27	TYR	3.8
2	E	148	TRP	3.6
1	A	219	ASP	3.6
1	A	217	PRO	3.5
1	A	82	GLN	3.5
1	A	194	PRO	3.3
2	E	125	LEU	3.2
2	E	209	PHE	3.1
2	E	126	THR	3.0
1	A	46	GLU	2.9
2	E	122	SER	2.9
1	D	219	ASP	2.9
1	D	30	THR	2.8
3	C	121	ARG	2.8
1	A	135	ALA	2.8
2	B	187	GLU	2.8
2	E	132	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	41	ASN	2.7
2	E	133	VAL	2.7
1	D	156	THR	2.7
2	B	212	ASN	2.6
2	E	12	SER	2.6
1	D	136	GLN	2.6
2	E	190	ASN	2.5
3	F	122	ARG	2.5
1	D	43	HIS	2.5
1	D	137	THR	2.5
3	C	122	ARG	2.5
1	A	193	TRP	2.4
1	D	208	SER	2.4
1	D	216	VAL	2.4
2	E	1	ASP	2.4
2	E	192	TYR	2.3
2	E	179	LEU	2.2
2	E	187	GLU	2.2
2	B	190	ASN	2.2
1	A	216	VAL	2.1
2	B	129	GLY	2.1
1	D	205	PRO	2.1
1	A	137	THR	2.1
1	D	25	SER	2.1
2	B	182	THR	2.0
1	A	126	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

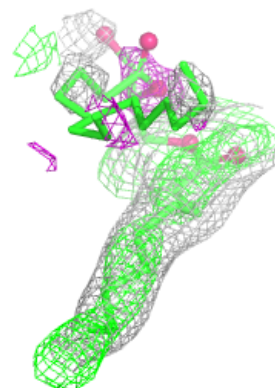
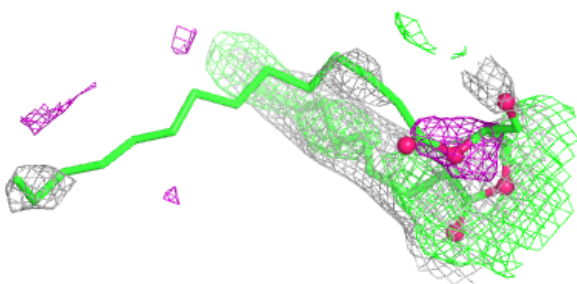
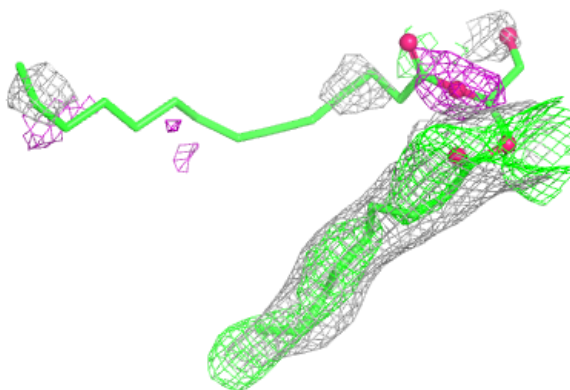
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DGA	F	208	31/44	0.65	0.38	66,68,72,75	0
6	DGA	C	907	31/44	0.72	0.34	66,68,72,75	0
5	K	F	205	1/1	0.72	0.18	30,30,30,30	1
4	F09	D	301	10/10	0.80	0.14	20,20,20,20	0
4	F09	A	301	10/10	0.83	0.14	20,20,20,20	0
5	K	C	901	1/1	0.84	0.07	30,30,30,30	1
5	K	F	206	1/1	0.84	0.09	30,30,30,30	1
5	K	C	904	1/1	0.86	0.07	30,30,30,30	1
5	K	C	906	1/1	0.88	0.11	30,30,30,30	1
5	K	F	204	1/1	0.93	0.03	30,30,30,30	1
5	K	F	207	1/1	0.93	0.09	30,30,30,30	1
5	K	F	202	1/1	0.94	0.04	30,30,30,30	1
5	K	F	203	1/1	0.94	0.11	30,30,30,30	1
5	K	C	903	1/1	0.96	0.03	30,30,30,30	1
7	TBA	C	908	17/17	0.96	0.12	20,20,20,20	17
7	TBA	F	201	17/17	0.97	0.08	20,20,20,20	17
5	K	C	905	1/1	0.98	0.08	30,30,30,30	1
5	K	C	902	1/1	0.99	0.07	30,30,30,30	1

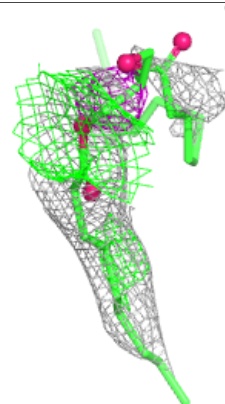
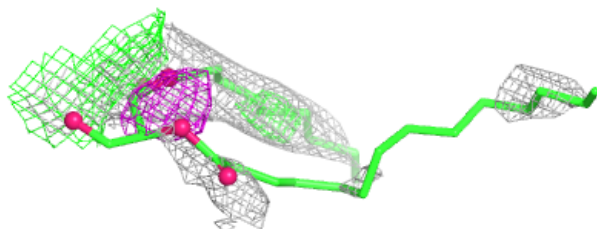
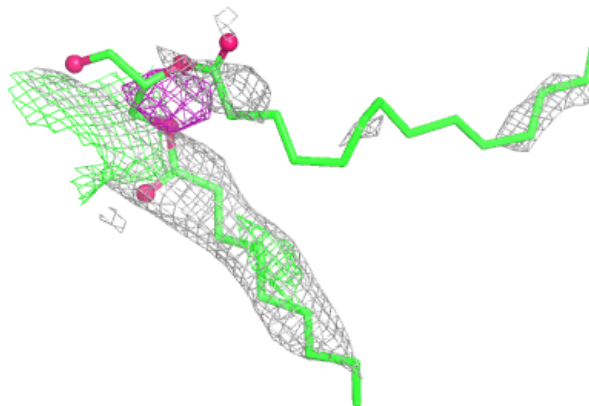
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGA F 208:

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

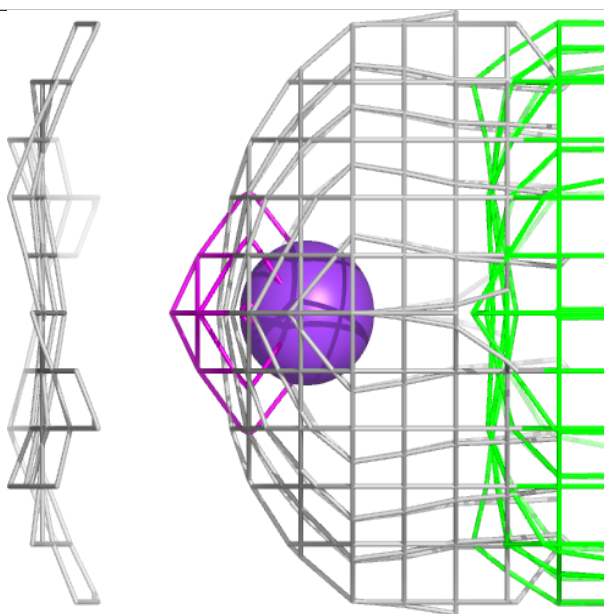
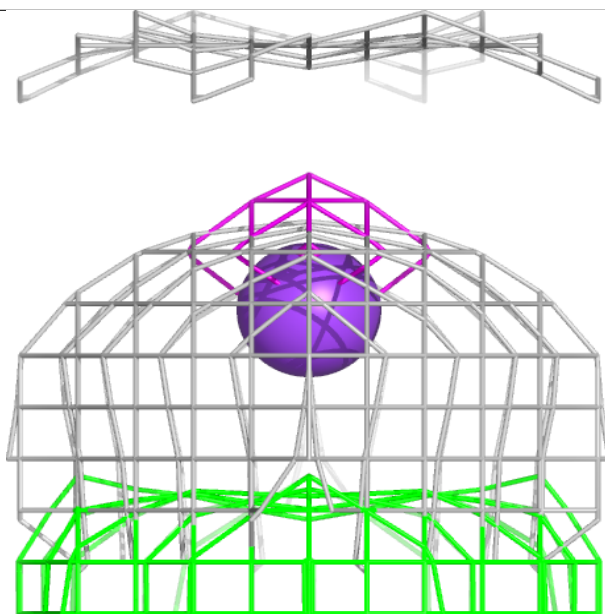
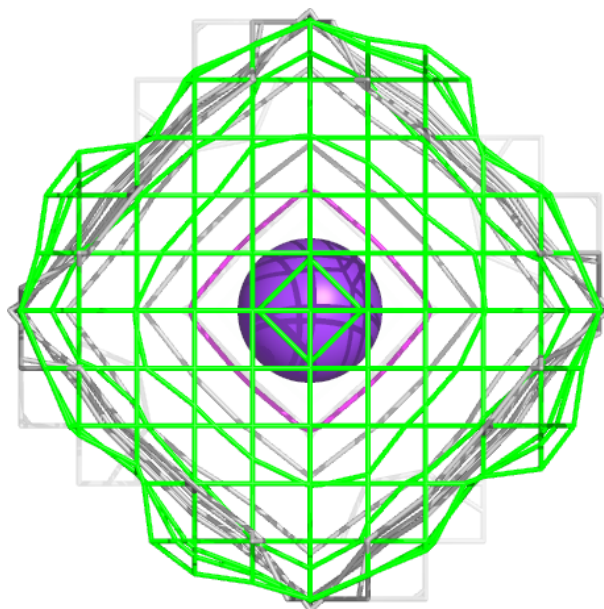
**Electron density around DGA C 907:**

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



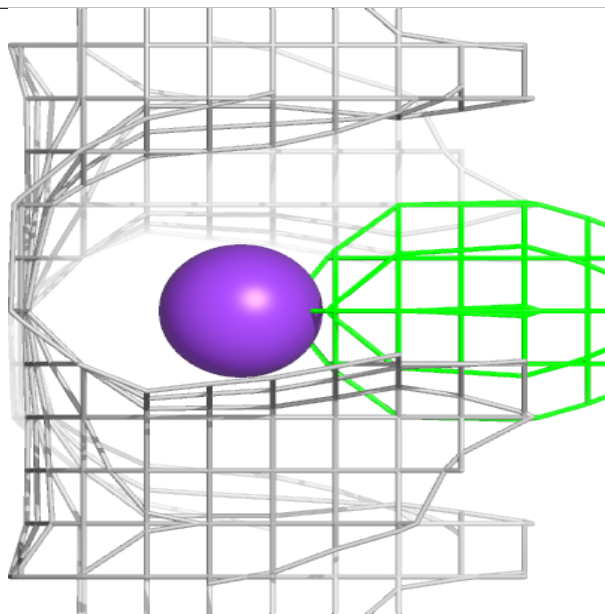
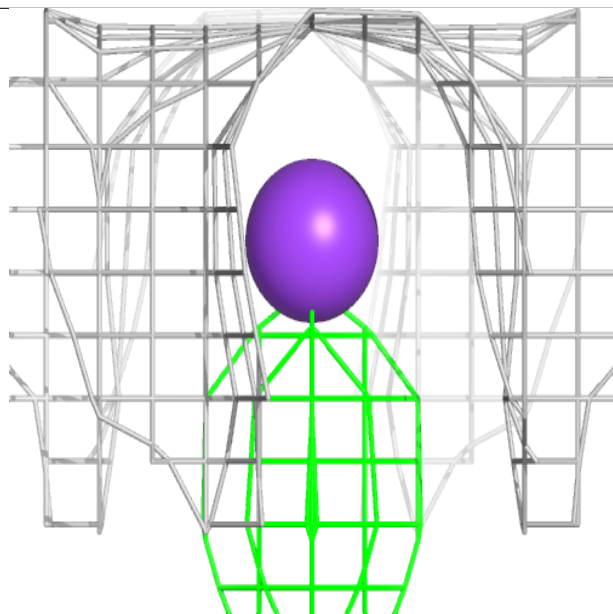
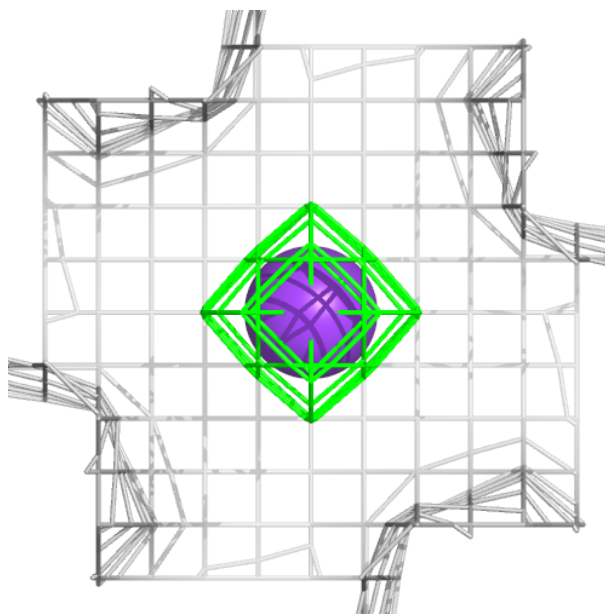
Electron density around K F 205:

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



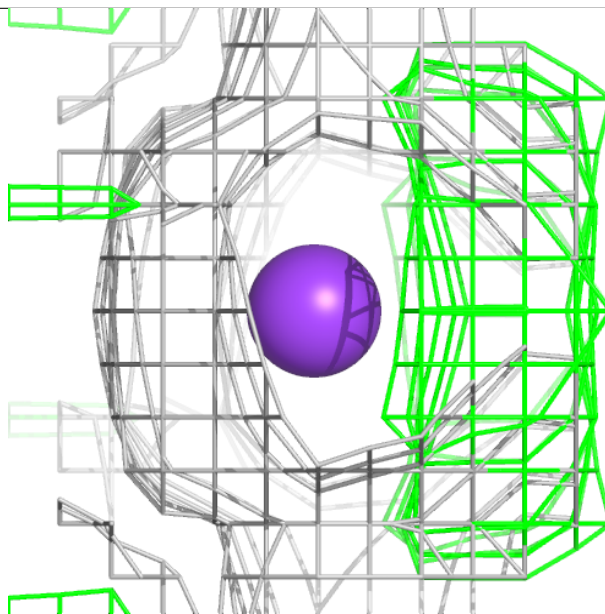
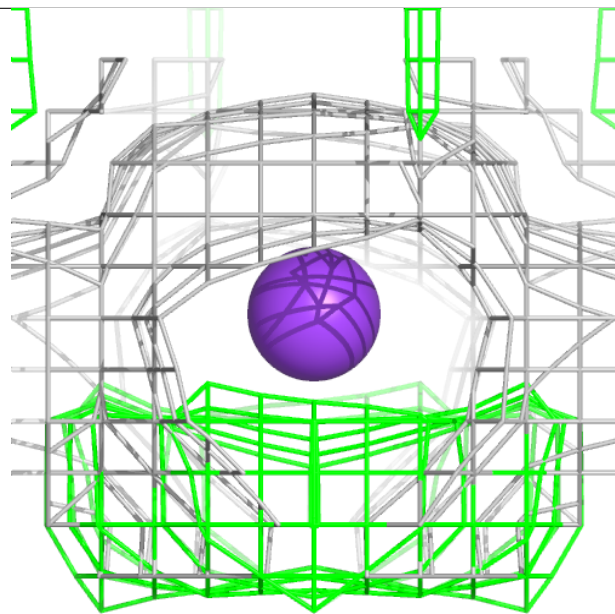
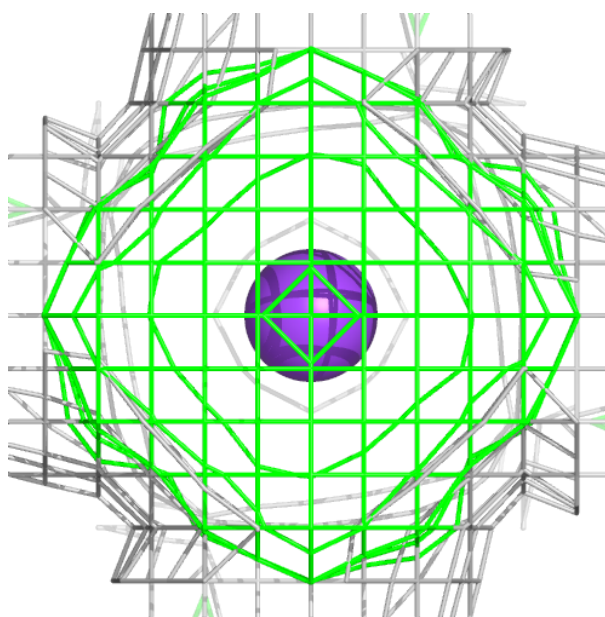
Electron density around K C 901:

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



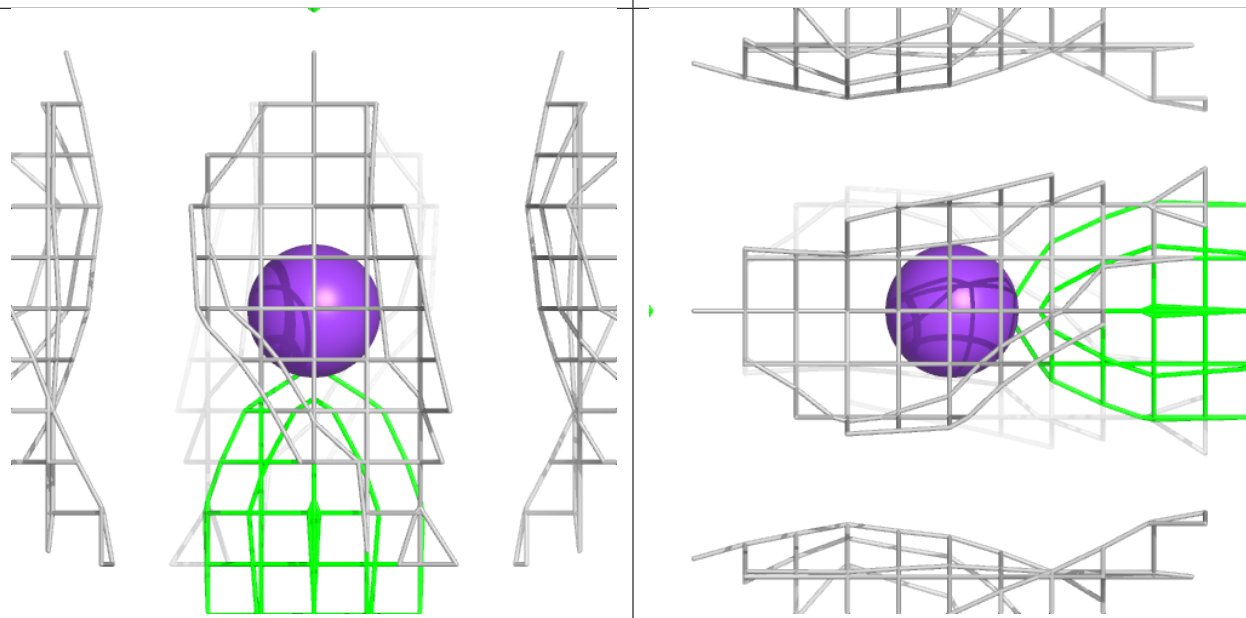
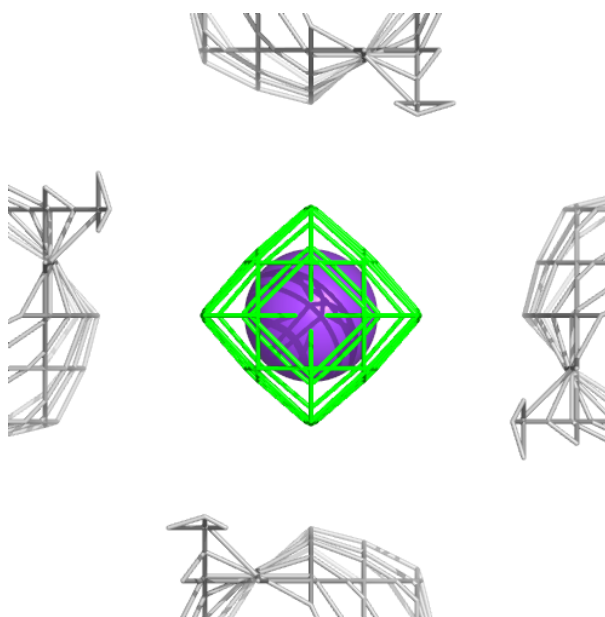
Electron density around K F 206:

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and green (positive)



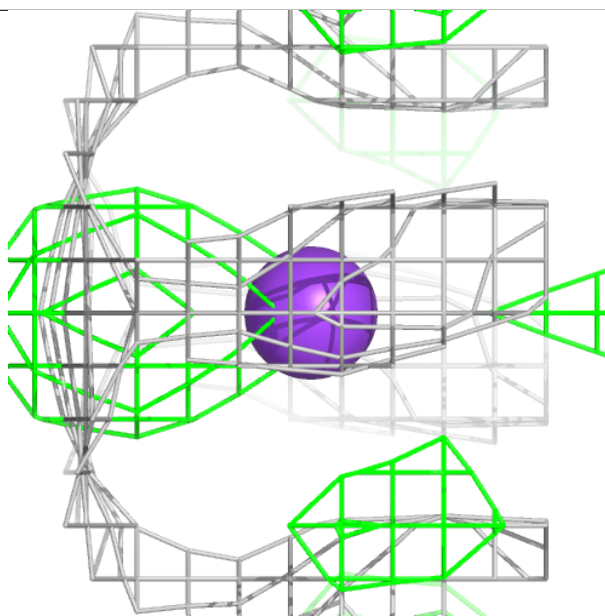
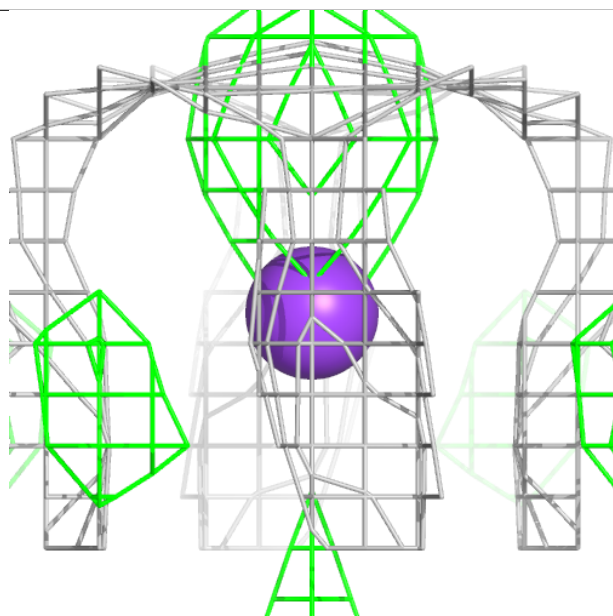
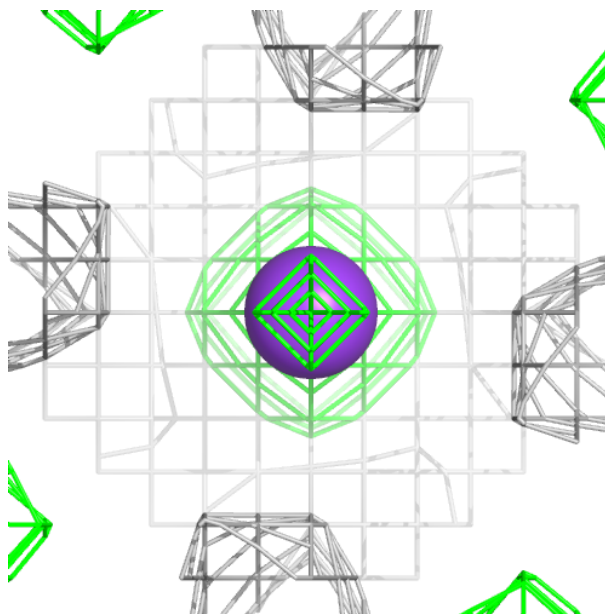
Electron density around K C 904:

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and green (positive)



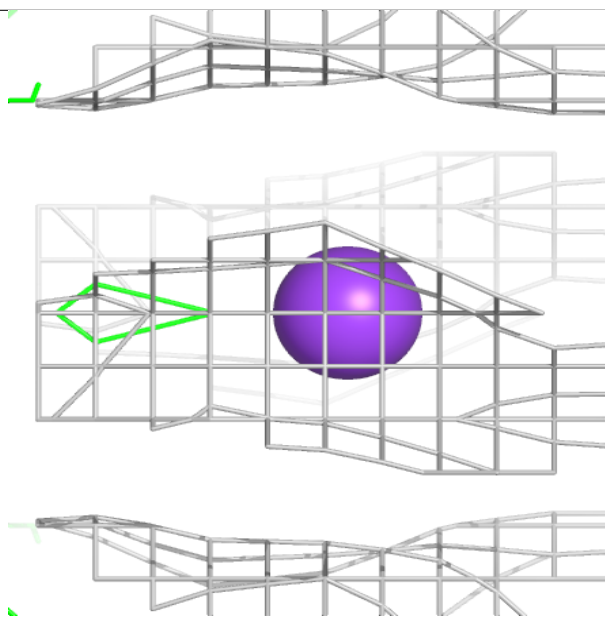
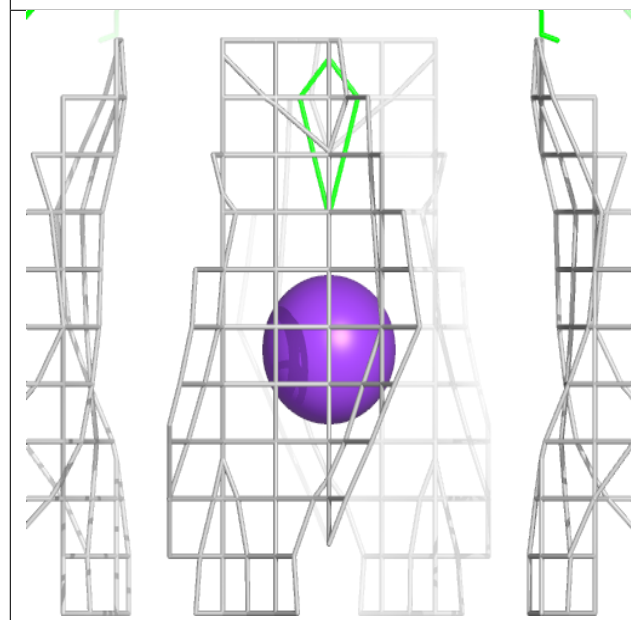
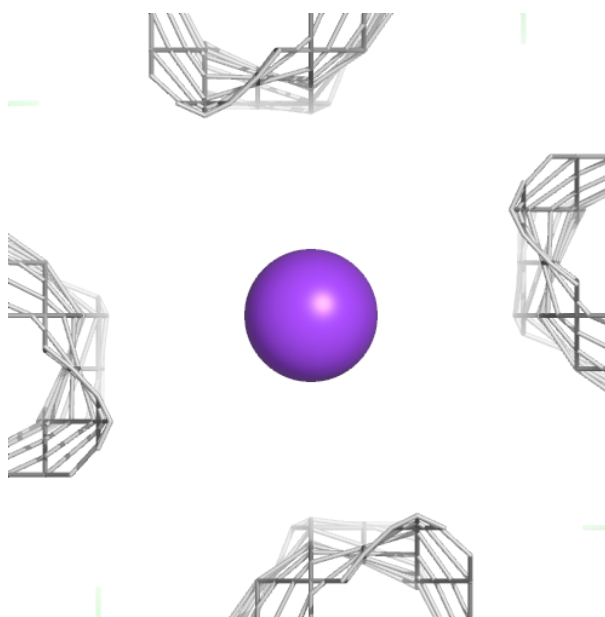
Electron density around K C 906:

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and green (positive)



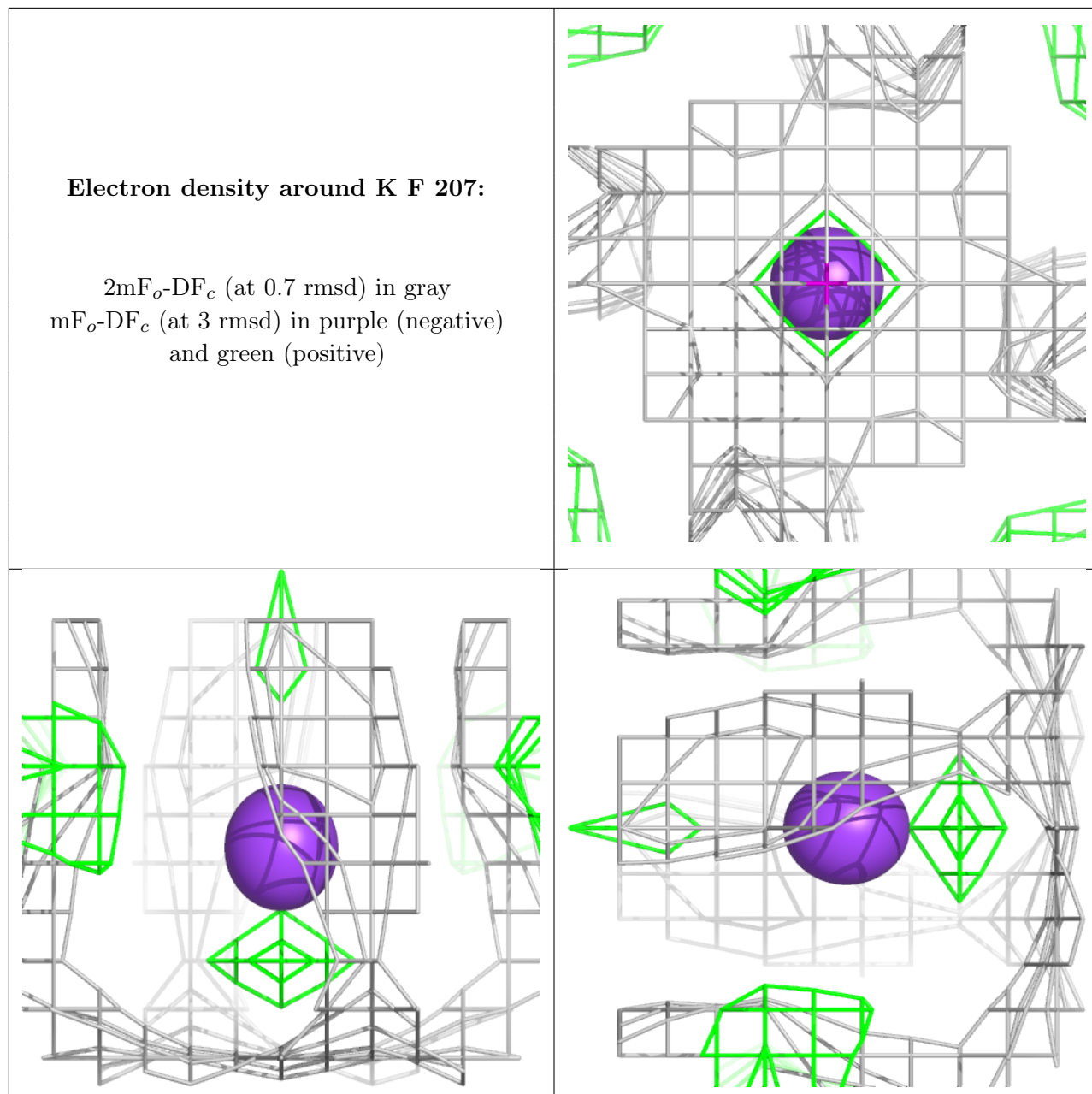
Electron density around K F 204:

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and green (positive)



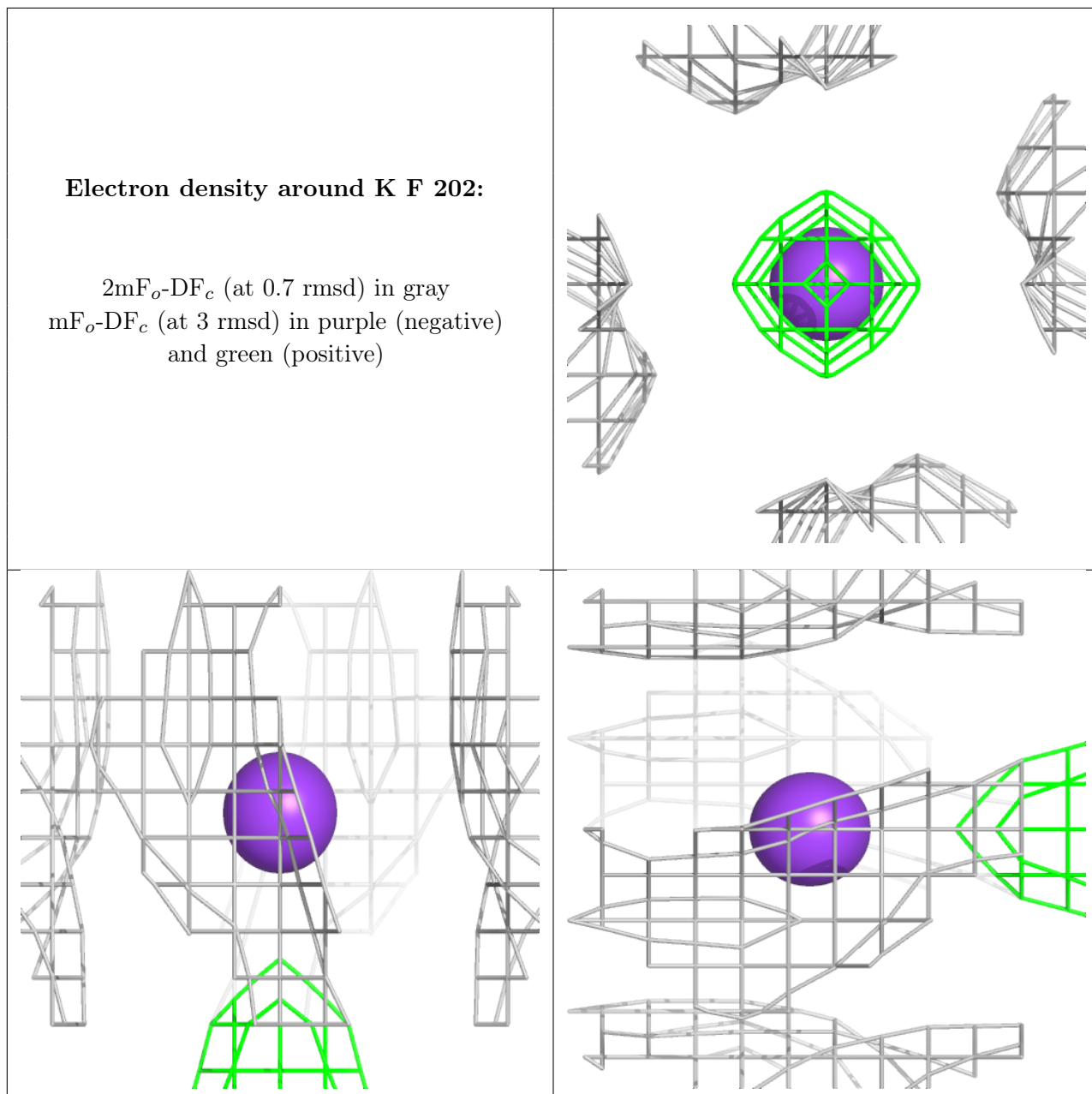
Electron density around K F 207:

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



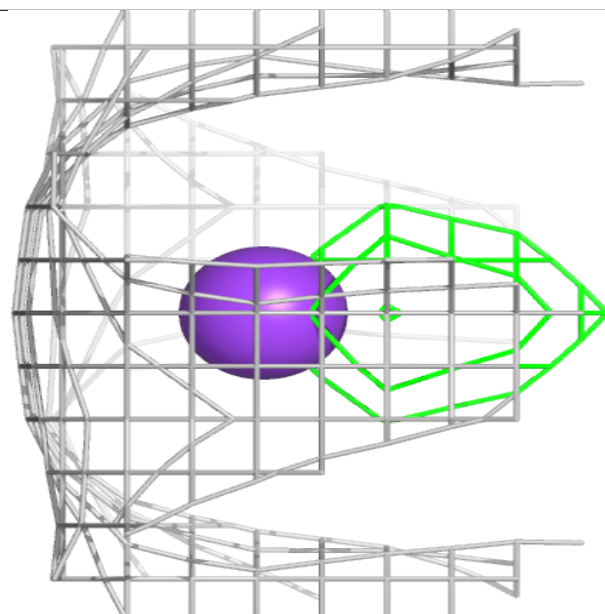
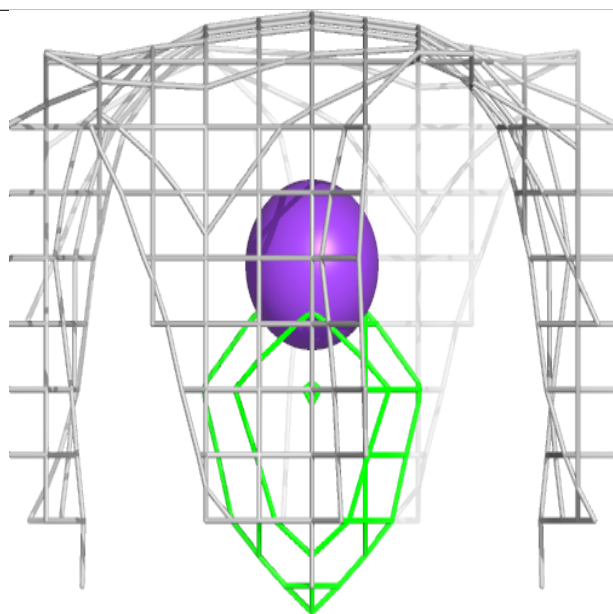
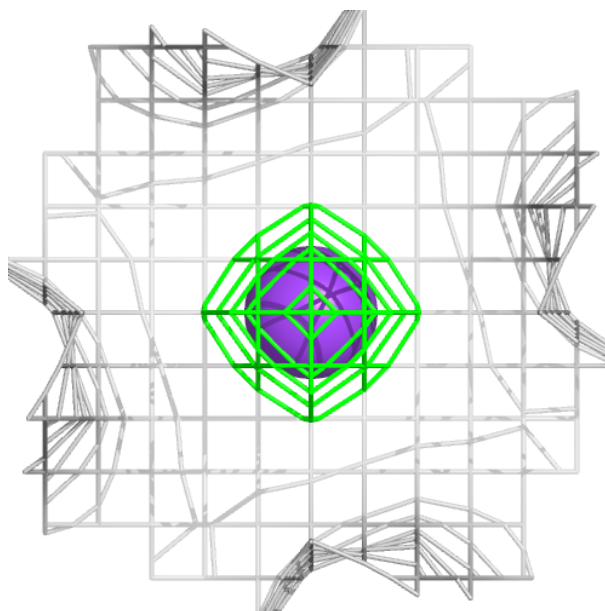
Electron density around K F 202:

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and green (positive)



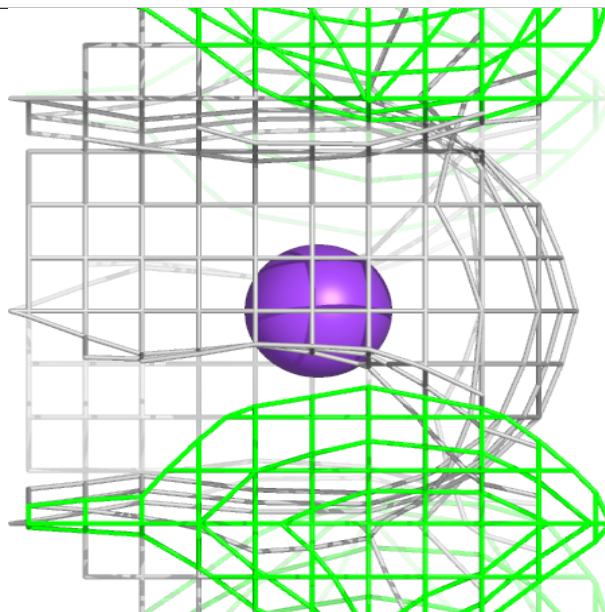
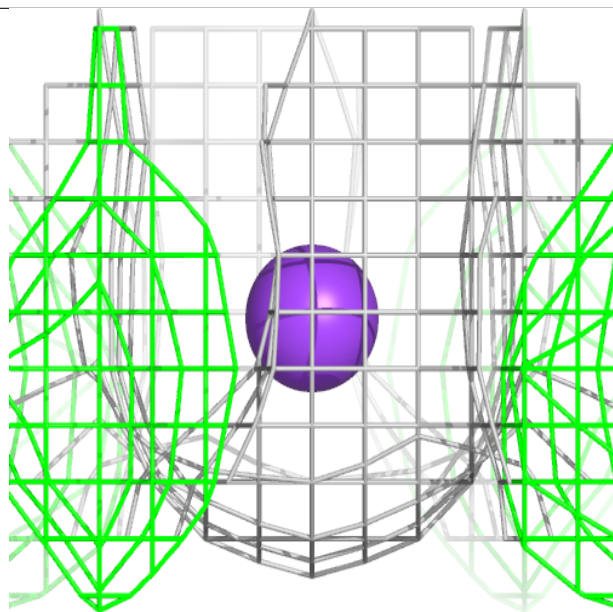
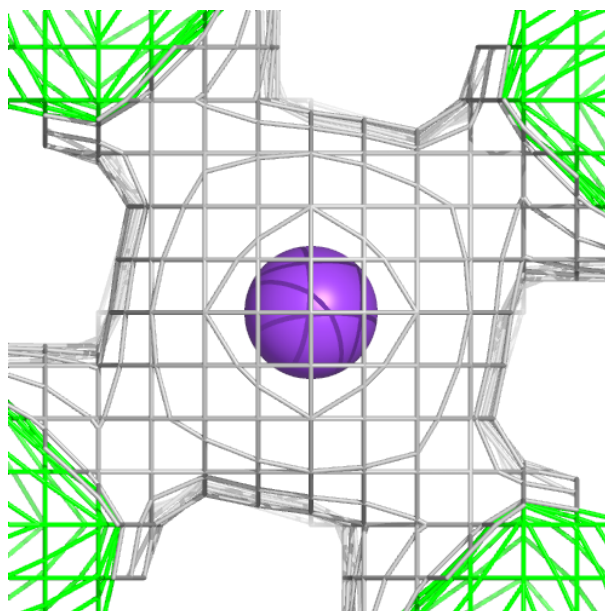
Electron density around K F 203:

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and green (positive)



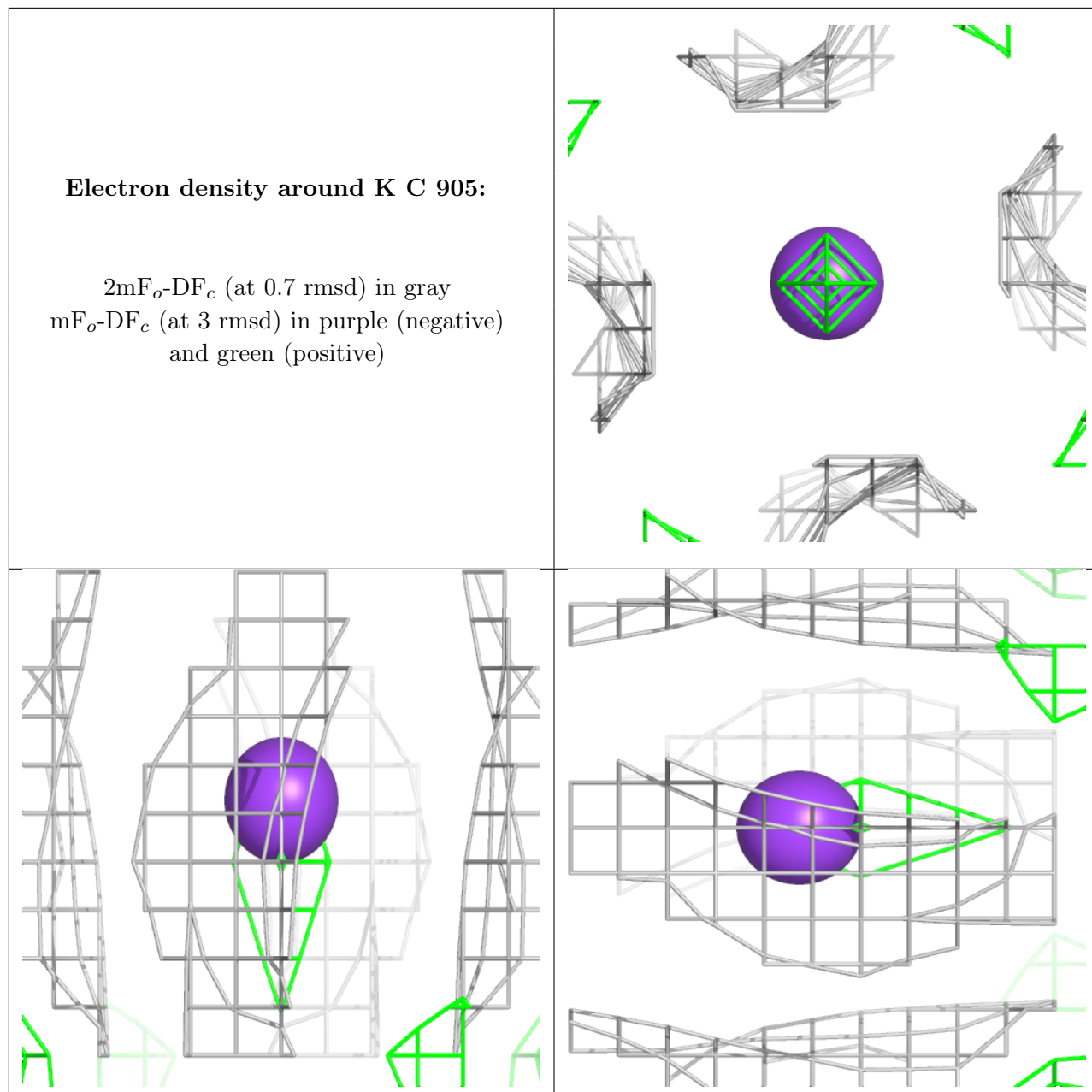
Electron density around K C 903:

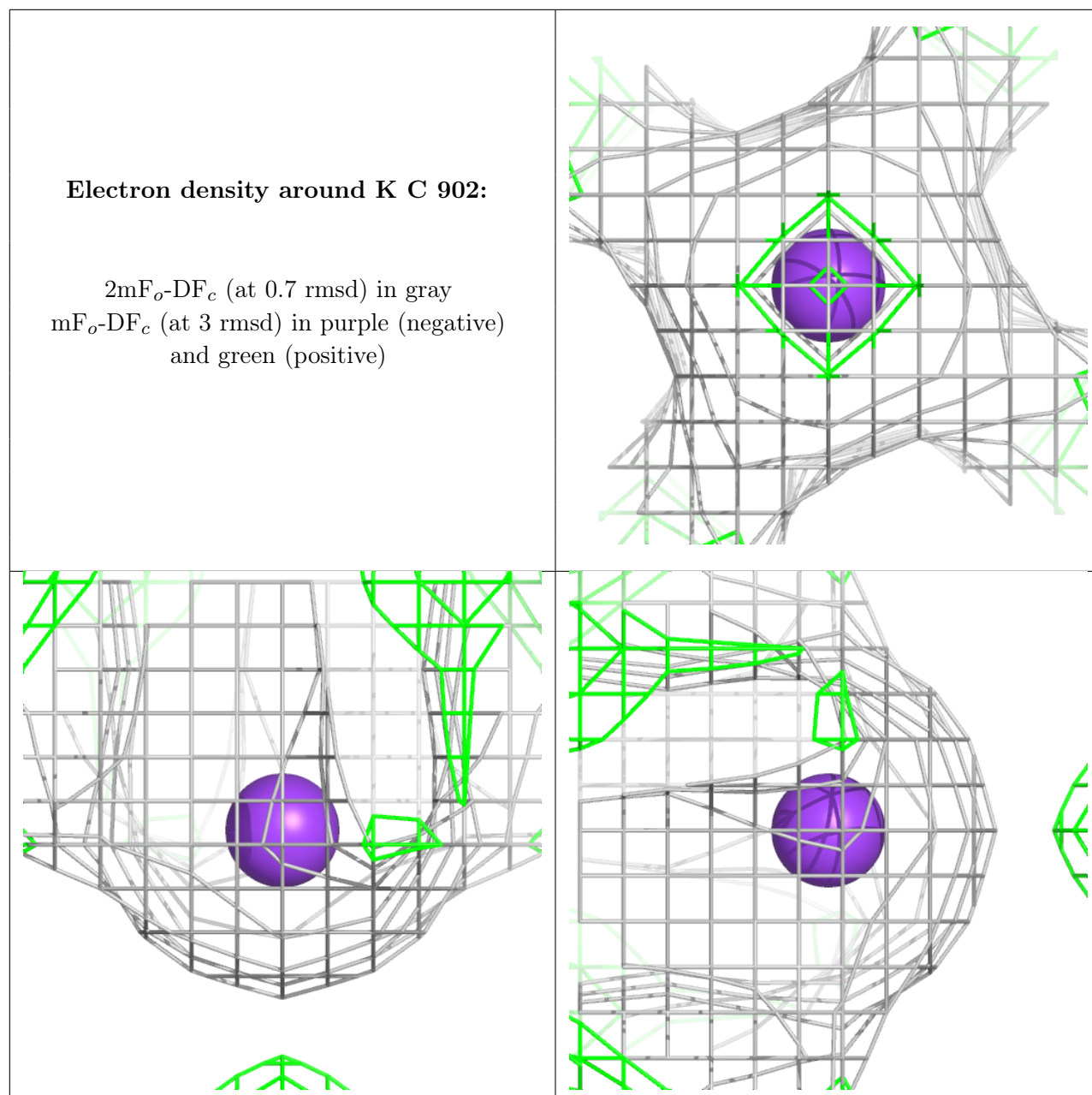
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K C 905:

$2mF_o-DF_c$ (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.