Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 08:33 PM EDT

PDB ID	:	5BKL
Title	:	Crystallographic structure of the cubic crystal form of STMV (77.9 degree rotation) grown from NaCl
Authors	:	McPherson, A.
Deposited on	:	2021-03-20
Resolution	:	2.94 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:

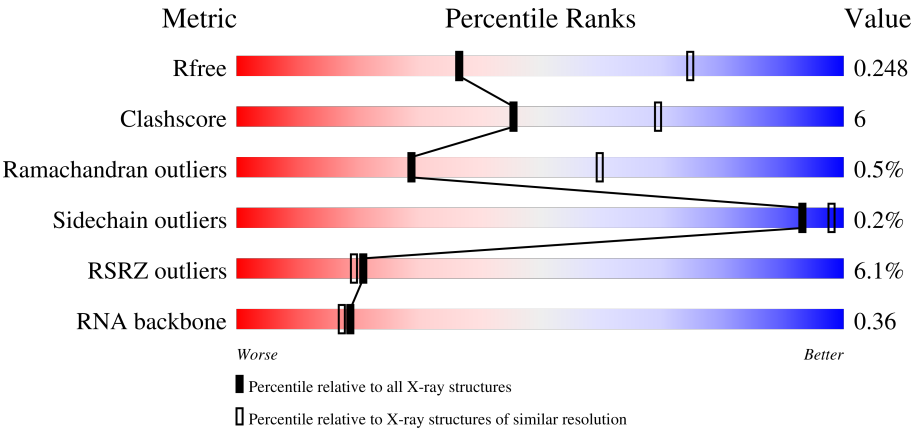
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)
RNA backbone	3102	1060 (3.20-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	3% 82% 8% • 9%
1	B	159	% 79% 11% • 10%
1	C	159	82% 6% • 11%
1	D	159	3% 83% 8% 9%

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Mol	Chain	Length	Quality of chain
1	E	159	2% 84% 6% 9%
1	F	159	3% 82% 8% 9%
1	G	159	3% 81% 11% 8%
1	GG	159	90% 9%
1	H	159	2% 82% 9% 9%
1	HH	159	3% 83% 8% 9%
1	I	159	2% 87% 9%
1	II	159	81% 9% 10%
1	J	159	4% 82% 11% 8%
1	JJ	159	81% 10% 9%
1	K	159	4% 85% 6% 9%
1	KK	159	83% 8% 9%
1	L	159	9% 86% 9%
1	M	159	5% 80% 10% 9%
1	N	159	3% 79% 11% 9%
1	O	159	9% 86% 8% 6%
2	P	12	50% 33% 17% 8% 42%
2	S	12	33% 33% 17% 8% 42%
2	T	12	25% 8% 8% 58%
2	UU	12	25% 25% 33% 42%
2	V	12	50% 33% 25% 8% 33%
2	X	12	67% 58% 8% 33%
2	bb	12	67% 42% 50% 8%
3	TT	11	45% 9% 9% 27% 9% 45%
3	Y	11	64% 36% 18% 18% 9% 18%

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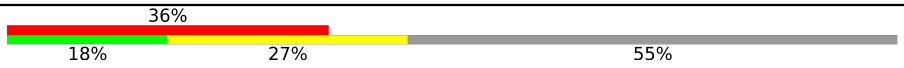
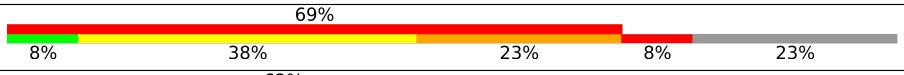
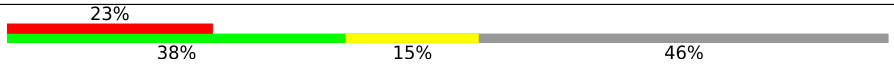
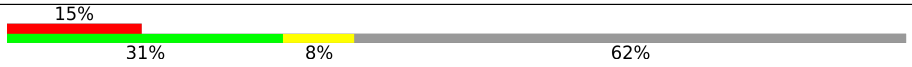
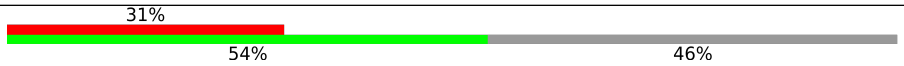
Mol	Chain	Length	Quality of chain
3	a	11	
4	WW	13	
4	e	13	
4	h	13	
4	i	13	
4	kk	13	
4	ll	13	
4	n	13	
4	qq	13	
5	m	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	B	301	-	-	-	X
6	CL	B	302	-	-	-	X
6	CL	B	303	-	-	X	-
6	CL	B	304	-	-	X	-
6	CL	C	204	-	-	-	X
6	CL	C	206	-	-	X	-
6	CL	F	201	-	-	X	X
6	CL	G	301	-	-	X	-
6	CL	H	201	-	-	X	-
6	CL	H	202	-	-	X	-
6	CL	HH	402	-	-	-	X
6	CL	JJ	301	-	-	-	X
6	CL	JJ	302	-	-	X	-
6	CL	KK	201	-	-	X	-
7	MG	E	201	-	-	-	X
7	MG	F	203	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 50583 atoms, of which 23747 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 Coat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	S	2	13	0
			2292	721	1147	204	213	7			
1	B	143	Total	C	H	N	O	S	0	12	0
			2212	703	1097	197	208	7			
1	C	142	Total	C	H	N	O	S	2	21	0
			2223	701	1110	198	208	6			
1	D	144	Total	C	H	N	O	S	1	21	0
			2259	711	1132	199	210	7			
1	E	144	Total	C	H	N	O	S	0	19	0
			2241	712	1109	200	213	7			
1	F	144	Total	C	H	N	O	S	0	17	0
			2298	723	1152	202	214	7			
1	G	146	Total	C	H	N	O	S	2	15	0
			2268	720	1124	202	215	7			
1	H	145	Total	C	H	N	O	S	1	14	0
			2248	711	1117	200	213	7			
1	I	144	Total	C	H	N	O	S	0	13	0
			2259	711	1130	200	211	7			
1	J	147	Total	C	H	N	O	S	0	15	0
			2302	732	1138	205	220	7			
1	K	145	Total	C	H	N	O	S	1	16	0
			2356	739	1181	211	219	6			
1	L	157	Total	C	H	N	O	S	14	15	0
			2465	800	1194	227	236	8			
1	M	144	Total	C	H	N	O	S	0	13	0
			2366	740	1194	207	218	7			
1	N	144	Total	C	H	N	O	S	1	13	0
			2329	730	1172	201	217	9			
1	O	150	Total	C	H	N	O	S	0	23	0
			2296	735	1123	209	222	7			
1	GG	145	Total	C	H	N	O	S	1	19	0
			2254	711	1123	200	213	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HH	145	Total	C	H	N	O	S	0	15	0
			2295	724	1145	204	215	7			
1	II	143	Total	C	H	N	O	S	0	16	0
			2238	710	1112	198	210	8			
1	JJ	144	Total	C	H	N	O	S	0	16	0
			2230	703	1112	199	210	6			
1	KK	144	Total	C	H	N	O	S	0	10	0
			2210	707	1087	199	210	7			

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	7	Total	C	H	N	O	P	0	7	0
			220	70	66	35	42	7			
2	S	7	Total	C	H	N	O	P	0	6	0
			209	70	55	35	42	7			
2	T	5	Total	C	H	N	O	P	0	5	0
			156	50	46	25	30	5			
2	V	8	Total	C	H	N	O	P	0	6	0
			233	80	57	40	48	8			
2	X	8	Total	C	H	N	O	P	0	8	0
			264	80	88	40	48	8			
2	UU	7	Total	C	H	N	O	P	0	7	0
			215	70	61	35	42	7			
2	bb	11	Total	C	H	N	O	P	0	8	0
			314	110	72	55	66	11			

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Y	9	Total	C	H	N	O	P	0	6	0
			258	90	60	45	54	9			
3	a	5	Total	C	H	N	O	P	0	5	0
			165	50	55	25	30	5			
3	TT	6	Total	C	H	N	O	P	0	4	0
			171	60	39	30	36	6			

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	e	11	Total	C	H	N	O	P	0	10	0
			300	99	80	22	88	11			
4	h	7	Total	C	H	N	O	P	0	7	0
			198	63	58	14	56	7			
4	i	5	Total	C	H	N	O	P	0	5	0
			140	45	40	10	40	5			
4	n	7	Total	C	H	N	O	P	0	7	0
			198	63	58	14	56	7			
4	WW	10	Total	C	H	N	O	P	0	2	0
			211	90	11	20	80	10			
4	kk	6	Total	C	H	N	O	P	0	5	0
			160	54	40	12	48	6			
4	ll	5	Total	C	H	N	O	P	0	5	0
			140	45	40	10	40	5			
4	qq	6	Total	C	H	N	O	P	0	4	0
			152	54	32	12	48	6			

- Molecule 5 is a RNA chain called RNA (5'-R(UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	m	9	Total	C	H	N	O	P	0	9	0
			270	81	90	18	72	9			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cl	0	0
			4	4		
6	C	6	Total	Cl	0	0
			6	6		
6	D	2	Total	Cl	0	0
			2	2		
6	F	2	Total	Cl	0	0
			2	2		
6	G	2	Total	Cl	0	0
			2	2		
6	H	2	Total	Cl	0	0
			2	2		
6	K	2	Total	Cl	0	0
			2	2		
6	L	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	1	Total Cl 1 1	0	0
6	GG	1	Total Cl 1 1	0	0
6	HH	2	Total Cl 2 2	0	0
6	II	3	Total Cl 3 3	0	0
6	JJ	5	Total Cl 5 5	0	0
6	KK	5	Total Cl 5 5	0	0
6	TT	1	Total Cl 1 1	0	0
6	ll	1	Total Cl 1 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	2	Total Mg 2 2	0	0
7	F	2	Total Mg 2 2	0	0
7	G	1	Total Mg 1 1	0	0
7	I	1	Total Mg 1 1	0	0
7	K	1	Total Mg 1 1	0	0
7	GG	1	Total Mg 1 1	0	0
7	HH	2	Total Mg 2 2	0	0
7	JJ	2	Total Mg 2 2	0	0
7	KK	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	25	Total O 25 25	0	0
8	B	32	Total O 32 32	0	0
8	C	41	Total O 41 41	0	0
8	D	53	Total O 53 53	0	0
8	E	19	Total O 19 19	0	0
8	F	24	Total O 24 24	0	0
8	G	37	Total O 37 37	0	0
8	H	23	Total O 23 23	0	0
8	I	24	Total O 24 24	0	0
8	J	21	Total O 21 21	0	0
8	K	24	Total O 24 24	0	0
8	L	16	Total O 16 16	0	0
8	M	16	Total O 16 16	0	0
8	N	14	Total O 14 14	0	0
8	O	49	Total O 49 49	0	0
8	P	4	Total O 4 4	0	0
8	S	14	Total O 14 14	0	0
8	T	4	Total O 4 4	0	0
8	V	19	Total O 19 19	0	0
8	X	3	Total O 3 3	0	0
8	Y	10	Total O 10 10	0	0
8	a	8	Total O 8 8	0	0

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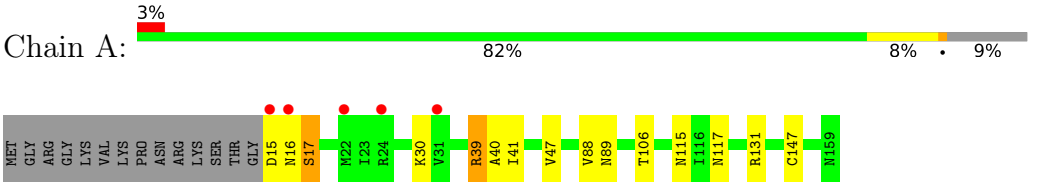
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	e	40	Total O 40 40	0	0
8	h	9	Total O 9 9	0	0
8	i	5	Total O 5 5	0	0
8	m	7	Total O 7 7	0	0
8	n	8	Total O 8 8	0	0
8	GG	38	Total O 38 38	0	0
8	HH	60	Total O 60 60	0	0
8	II	60	Total O 60 60	0	0
8	JJ	54	Total O 54 54	0	0
8	KK	54	Total O 54 54	0	0
8	TT	9	Total O 9 9	0	0
8	UU	14	Total O 14 14	0	0
8	WW	10	Total O 10 10	0	0
8	bb	42	Total O 42 42	0	0
8	kk	7	Total O 7 7	0	0
8	ll	9	Total O 9 9	0	0
8	qq	9	Total O 9 9	0	0

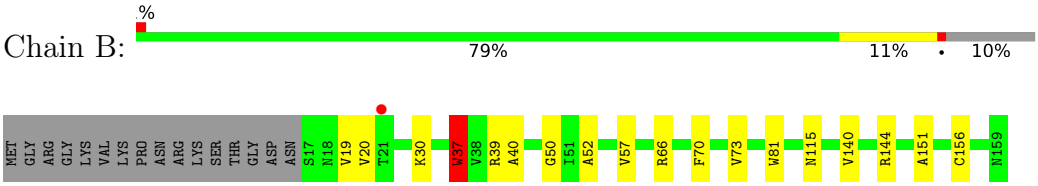
3 Residue-property plots (i)

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.

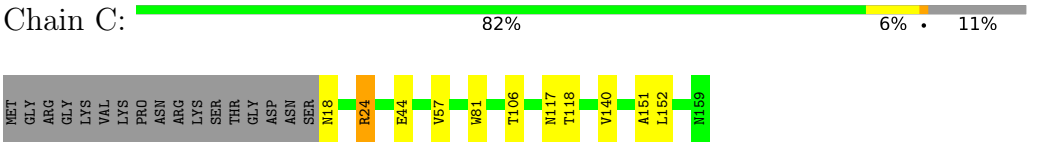
• Molecule 1: Coat protein



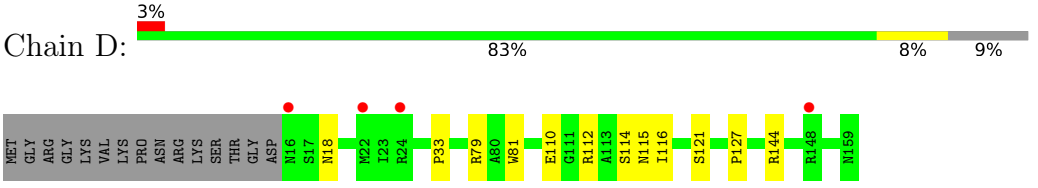
• Molecule 1: Coat protein



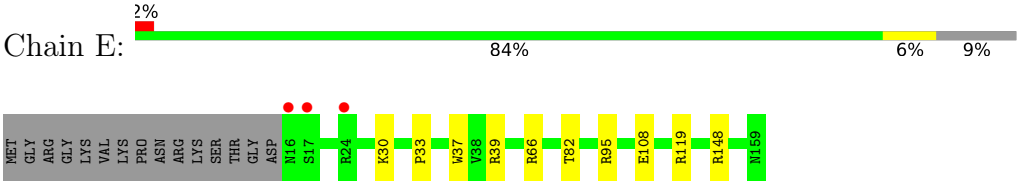
• Molecule 1: Coat protein



• Molecule 1: Coat protein

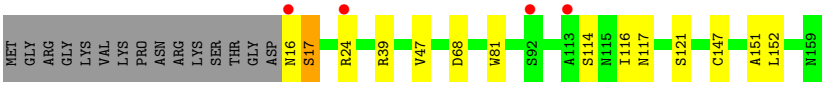


• Molecule 1: Coat protein



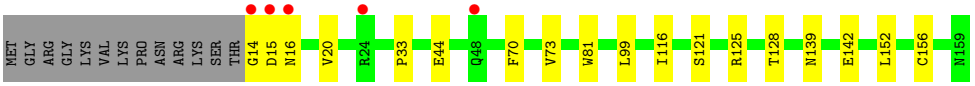
• Molecule 1: Coat protein

Chain F:



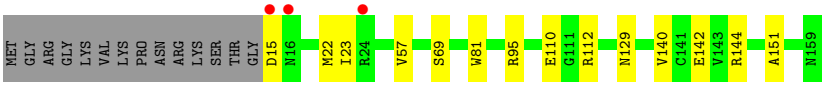
• Molecule 1: Coat protein

Chain G:



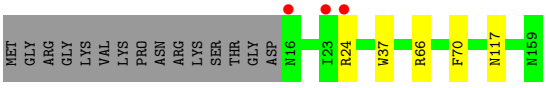
• Molecule 1: Coat protein

Chain H:



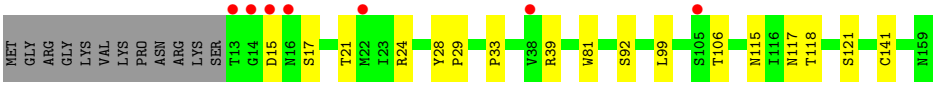
• Molecule 1: Coat protein

Chain I:



• Molecule 1: Coat protein

Chain J:

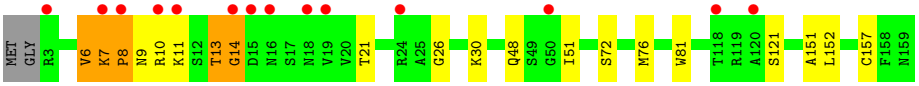


• Molecule 1: Coat protein

Chain K:

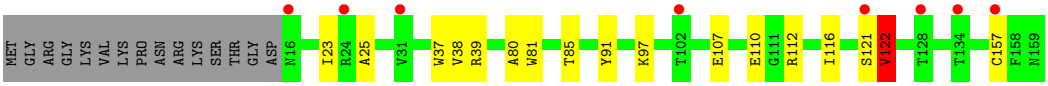
• Molecule 1: Coat protein

Chain L:



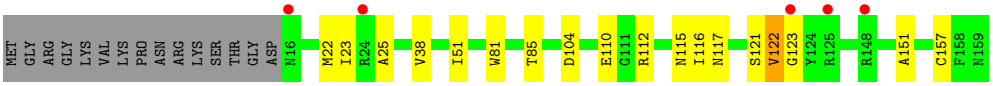
• Molecule 1: Coat protein

Chain M:



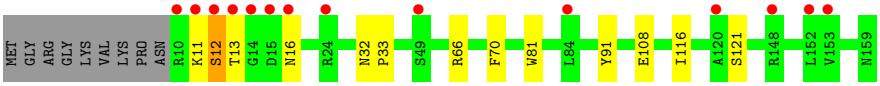
• Molecule 1: Coat protein

Chain N:



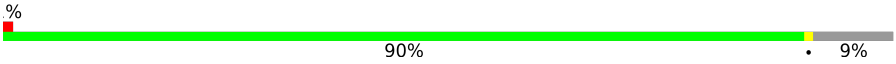
• Molecule 1: Coat protein

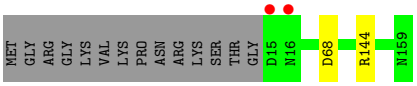
Chain O:



• Molecule 1: Coat protein

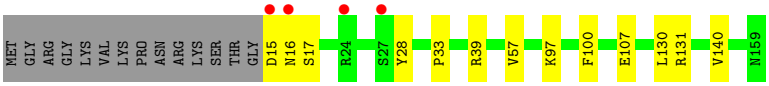
Chain GG:





• Molecule 1: Coat protein

Chain HH:

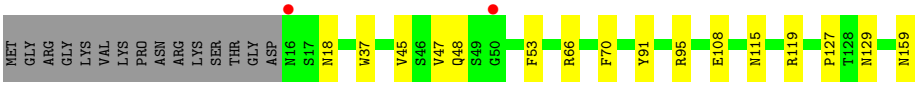


• Molecule 1: Coat protein

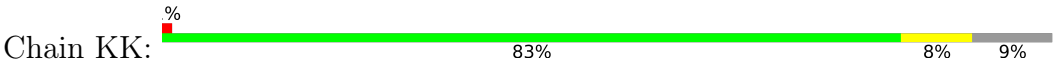
Chain II:

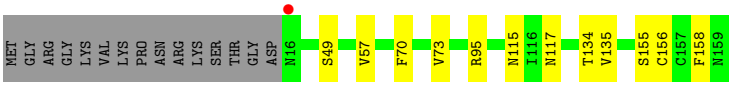
• Molecule 1: Coat protein

Chain JJ:

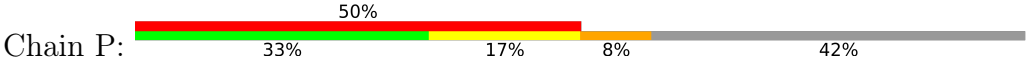


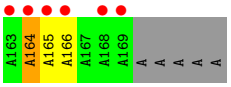
• Molecule 1: Coat protein



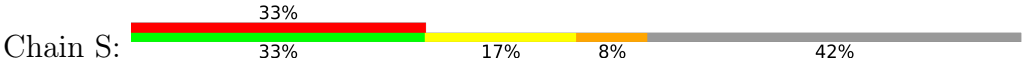


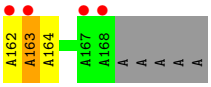
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')





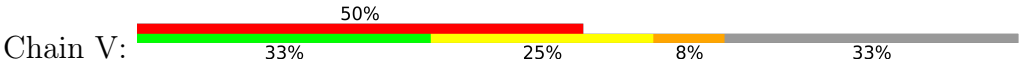
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

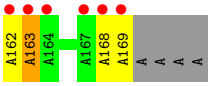




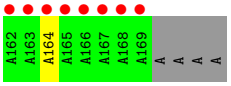
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



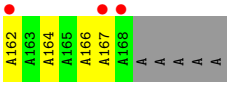


• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



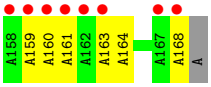
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain UU:



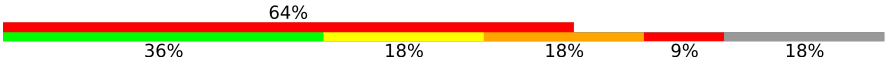
• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

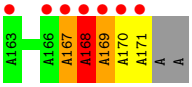
Chain bb:



• Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

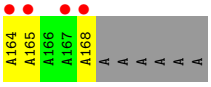
Chain Y:





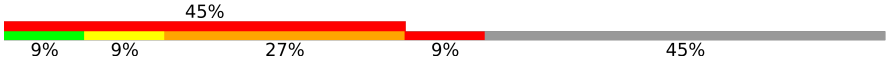
• Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

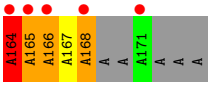
Chain a:



• Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

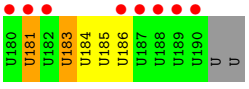
Chain TT:





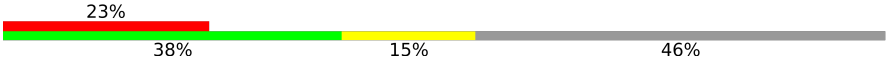
• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

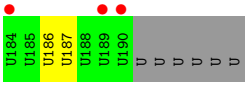
Chain e:



• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain h:



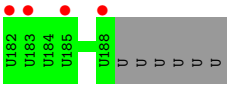


• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain i:

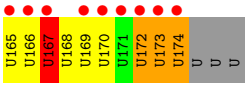
• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain n:



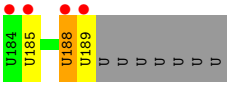
• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain WW:



• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain kk:

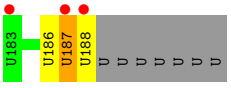


• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain ll:

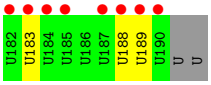
• Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain qq:



• Molecule 5: RNA (5'-R(UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain m:


U182
U183
U184
U185
U186
U187
U188
U189
U190
U
U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	234.65Å 234.65Å 234.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.22 – 2.94 78.22 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.4 (78.22-2.94) 80.9 (78.22-2.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.217 , 0.256 0.211 , 0.248	Depositor DCC
R_{free} test set	3717 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	50583	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/1193	0.55	0/1623
1	B	0.28	0/1154	0.55	0/1571
1	C	0.29	0/1153	0.56	0/1571
1	D	0.29	0/1192	0.54	0/1624
1	E	0.29	0/1186	0.56	0/1614
1	F	0.28	0/1222	0.54	0/1665
1	G	0.28	0/1205	0.54	0/1641
1	GG	0.29	0/1174	0.57	0/1599
1	H	0.28	0/1179	0.54	0/1606
1	HH	0.29	0/1205	0.55	0/1641
1	I	0.28	0/1167	0.53	0/1589
1	II	0.30	0/1198	0.55	0/1630
1	J	0.28	0/1223	0.53	0/1664
1	JJ	0.29	0/1142	0.56	0/1556
1	K	0.28	0/1263	0.55	0/1720
1	KK	0.30	0/1150	0.55	0/1566
1	L	0.29	0/1358	0.57	0/1844
1	M	0.27	0/1248	0.56	0/1697
1	N	0.27	0/1241	0.54	0/1689
1	O	0.27	0/1203	0.55	0/1636
2	P	0.33	0/174	0.85	0/269
2	S	0.20	0/174	0.65	0/269
2	T	0.27	0/124	0.77	0/191
2	UU	0.26	0/174	0.85	0/269
2	V	0.22	0/199	0.73	0/308
2	X	0.20	0/199	0.73	0/308
2	bb	0.38	0/274	0.85	0/425
3	TT	1.18	1/148 (0.7%)	1.62	2/226 (0.9%)
3	Y	0.34	0/224	1.39	4/347 (1.2%)
3	a	0.61	0/124	1.56	2/191 (1.0%)
4	WW	0.50	0/219	1.66	8/336 (2.4%)
4	e	0.28	0/241	1.05	1/370 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	h	0.18	0/153	0.82	0/234
4	i	0.25	0/109	0.88	0/166
4	kk	0.39	0/131	1.32	3/200 (1.5%)
4	ll	0.25	0/109	0.87	0/166
4	n	0.16	0/153	0.84	0/234
4	qq	0.40	0/131	1.31	1/200 (0.5%)
5	m	0.15	0/197	0.78	0/302
All	All	0.30	1/27313 (0.0%)	0.64	21/37757 (0.1%)

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	C	0	1
1	E	0	1
1	GG	0	1
1	K	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	TT	164[A]	A	C4'-C3'	6.50	1.60	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	WW	166[A]	U	OP1-P-O3'	-11.84	79.15	105.20
3	Y	167[A]	A	OP1-P-O3'	-11.39	80.15	105.20
3	Y	167[A]	A	OP2-P-O3'	-9.74	83.77	105.20
3	a	164[A]	A	O4'-C1'-N9	9.48	115.78	108.20
3	Y	168[A]	A	O4'-C1'-N9	9.26	115.61	108.20
4	WW	166[A]	U	OP2-P-O3'	-9.10	85.19	105.20
3	TT	164[A]	A	O4'-C1'-N9	-7.82	101.95	108.20
4	WW	167[A]	U	O5'-P-OP2	7.75	120.01	110.70
4	e	181[A]	U	OP1-P-OP2	-7.60	108.20	119.60
3	Y	168[A]	A	OP1-P-OP2	7.43	130.74	119.60
4	kk	188[A]	U	O4'-C1'-N1	7.12	113.90	108.20
4	WW	167[A]	U	O5'-C5'-C4'	6.85	124.72	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	WW	167[A]	U	P-O5'-C5'	6.58	131.43	120.90
4	WW	166[A]	U	C2-N1-C1'	6.56	125.57	117.70
4	kk	188[A]	U	C6-N1-C1'	5.93	129.51	121.20
3	TT	166[A]	A	C8-N9-C4	5.53	108.01	105.80
4	kk	188[A]	U	C2-N1-C1'	-5.51	111.09	117.70
4	WW	167[A]	U	N1-C1'-C2'	-5.37	106.09	112.00
3	a	164[A]	A	C8-N9-C1'	5.28	137.21	127.70
4	WW	166[A]	U	C6-N1-C2	-5.25	117.85	121.00
4	qq	187[A]	U	C5-C4-O4	-5.01	122.89	125.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39[A]	ARG	Sidechain
1	A	39[B]	ARG	Sidechain
1	C	24	ARG	Sidechain
1	E	148	ARG	Sidechain
1	GG	144	ARG	Sidechain
1	K	148[A]	ARG	Sidechain
1	K	148[B]	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1145	1147	1113	13	1
1	B	1115	1097	1093	14	0
1	C	1113	1110	1048	10	0
1	D	1127	1132	1066	13	0
1	E	1132	1109	1071	8	0
1	F	1146	1152	1085	11	0
1	G	1144	1124	1095	19	0
1	GG	1131	1123	1057	1	0
1	H	1131	1117	1078	12	1
1	HH	1150	1145	1113	13	0
1	I	1129	1130	1096	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	II	1126	1112	1085	15	0
1	J	1164	1138	1130	15	0
1	JJ	1118	1112	1078	13	0
1	K	1175	1181	1125	13	0
1	KK	1123	1087	1105	10	0
1	L	1271	1194	1264	18	2
1	M	1172	1194	1177	9	1
1	N	1157	1172	1135	11	1
1	O	1173	1123	1118	15	0
2	P	154	66	78	4	0
2	S	154	55	78	3	1
2	T	110	46	56	5	0
2	UU	154	61	78	3	0
2	V	176	57	89	3	0
2	X	176	88	89	0	1
2	bb	242	72	122	0	1
3	TT	132	39	68	5	0
3	Y	198	60	100	5	0
3	a	110	55	56	0	0
4	WW	200	11	95	10	0
4	e	220	80	111	0	1
4	h	140	58	71	0	0
4	i	100	40	51	0	0
4	kk	120	40	61	0	0
4	ll	100	40	51	0	1
4	n	140	58	71	0	0
4	qq	120	32	61	0	0
5	m	180	90	91	0	0
6	B	4	0	0	4	0
6	C	6	0	0	3	0
6	D	2	0	0	2	0
6	F	2	0	0	3	0
6	G	2	0	0	2	0
6	GG	1	0	0	0	0
6	H	2	0	0	8	0
6	HH	2	0	0	1	0
6	II	3	0	0	3	0
6	JJ	5	0	0	4	0
6	K	2	0	0	1	0
6	KK	5	0	0	5	0
6	L	1	0	0	1	0
6	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	TT	1	0	0	0	1
6	ll	1	0	0	0	0
7	E	2	0	0	0	0
7	F	2	0	0	0	0
7	G	1	0	0	0	0
7	GG	1	0	0	0	0
7	HH	2	0	0	0	0
7	I	1	0	0	0	0
7	JJ	2	0	0	0	0
7	K	1	0	0	0	0
7	KK	1	0	0	0	0
8	A	25	0	0	0	0
8	B	32	0	0	1	1
8	C	41	0	0	1	0
8	D	53	0	0	1	0
8	E	19	0	0	1	0
8	F	24	0	0	1	0
8	G	37	0	0	1	0
8	GG	38	0	0	1	0
8	H	23	0	0	1	0
8	HH	60	0	0	0	0
8	I	24	0	0	0	1
8	II	60	0	0	4	1
8	J	21	0	0	1	0
8	JJ	54	0	0	3	1
8	K	24	0	0	0	0
8	KK	54	0	0	0	1
8	L	16	0	0	1	0
8	M	16	0	0	0	0
8	N	14	0	0	0	1
8	O	49	0	0	1	0
8	P	4	0	0	0	0
8	S	14	0	0	1	0
8	T	4	0	0	0	0
8	TT	9	0	0	1	0
8	UU	14	0	0	0	0
8	V	19	0	0	1	0
8	WW	10	0	0	0	0
8	X	3	0	0	0	0
8	Y	10	0	0	0	0
8	a	8	0	0	0	0
8	bb	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	e	40	0	0	0	0
8	h	9	0	0	0	0
8	i	5	0	0	0	0
8	kk	7	0	0	0	0
8	ll	9	0	0	0	0
8	m	7	0	0	0	0
8	n	8	0	0	0	0
8	qq	9	0	0	0	0
All	All	26836	23747	23609	232	9

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 6.

All (232) 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)
8:GG:306:HOH:O	6:KK:201:CL:CL	2.01	1.14
8:II:309:HOH:O	6:KK:201:CL:CL	2.02	1.11
6:F:202:CL:CL	8:F:308:HOH:O	2.04	1.09
1:K:79[B]:ARG:NH2	3:Y:169:A:OP1	1.86	1.09
6:B:304:CL:CL	8:E:306:HOH:O	2.09	1.05
1:B:39:ARG:NH2	6:B:303:CL:CL	2.33	0.98
6:B:304:CL:CL	8:C:323:HOH:O	2.19	0.97
1:L:6:VAL:HG13	1:L:7:LYS:H	1.27	0.96
1:C:18:ASN:N	6:C:203:CL:CL	2.41	0.90
1:A:39[B]:ARG:NH2	1:O:32:ASN:O	2.06	0.88
1:G:14:GLY:N	2:UU:162[A]:A:HO2'	1.72	0.86
2:S:163[A]:A:O2'	8:S:201:HOH:O	1.94	0.83
1:L:6:VAL:O	1:L:7:LYS:HG2	1.78	0.83
1:L:6:VAL:HG13	1:L:7:LYS:N	1.94	0.81
1:A:16:ASN:OD1	1:A:17:SER:N	2.14	0.81
4:WW:167[A]:U:H2'	4:WW:168:U:O5'	1.81	0.81
8:II:319:HOH:O	6:KK:201:CL:CL	2.37	0.79
4:WW:173:U:O2'	4:WW:174:U:O5'	2.01	0.79
1:G:20:VAL:O	8:G:401:HOH:O	2.02	0.76
1:JJ:119:ARG:O	8:JJ:401:HOH:O	2.04	0.76
1:O:108:GLU:O	8:O:201:HOH:O	2.03	0.75
6:G:301:CL:CL	1:HH:28:TYR:OH	2.41	0.74
1:L:152:LEU:O	8:L:601:HOH:O	2.05	0.74
1:K:148[B]:ARG:HG2	1:K:148[B]:ARG:HH11	1.53	0.73
1:G:14:GLY:N	2:UU:162[A]:A:O2'	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ASN:ND2	6:HH:402:CL:CL	2.59	0.72
1:L:11:LYS:HB2	1:L:21:THR:HG21	1.73	0.71
4:WW:167[A]:U:C2'	4:WW:168:U:O5'	2.39	0.70
1:H:69:SER:OG	8:H:301:HOH:O	2.09	0.70
1:J:21:THR:HG22	2:P:165[A]:A:H5"	1.74	0.69
1:J:17:SER:HA	2:P:164[A]:A:H4'	1.76	0.68
1:II:39:ARG:NH2	6:II:201:CL:CL	2.64	0.67
1:N:38:VAL:HG22	1:N:157[B]:CYS:SG	2.36	0.66
4:WW:172:U:OP2	4:WW:172:U:H2'	1.96	0.65
2:UU:166[A]:A:H2'	2:UU:167[A]:A:O4'	1.96	0.65
1:L:6:VAL:O	1:L:7:LYS:CG	2.45	0.64
1:II:82:THR:HG21	1:II:92[B]:SER:OG	1.97	0.64
1:H:129:ASN:ND2	1:HH:131:ARG:O	2.26	0.64
1:M:121:SER:O	1:M:122:VAL:HG12	1.97	0.64
1:JJ:159:ASN:OXT	8:JJ:402:HOH:O	2.15	0.63
1:J:28:TYR:OH	6:K:302:CL:CL	2.48	0.62
2:V:168[A]:A:N3	8:V:201:HOH:O	2.31	0.62
1:A:39[B]:ARG:HG2	1:A:41:ILE:HD11	1.82	0.61
1:B:40:ALA:O	6:B:303:CL:CL	2.56	0.61
1:J:92:SER:OG	8:J:201:HOH:O	2.16	0.60
1:N:121:SER:O	1:N:122:VAL:HG12	2.02	0.60
1:O:11:LYS:HE3	2:T:168[A]:A:N1	2.16	0.60
1:H:95:ARG:HD3	6:H:202:CL:CL	2.38	0.60
1:L:6:VAL:CG1	1:L:7:LYS:N	2.66	0.58
1:KK:95:ARG:HD3	6:KK:203:CL:CL	2.41	0.57
1:A:39[B]:ARG:NH2	1:A:40:ALA:O	2.38	0.57
2:T:164[A]:A:H5'	1:HH:16:ASN:HB3	1.86	0.57
1:D:79:ARG:NE	6:D:202:CL:CL	2.72	0.56
6:H:202:CL:CL	1:HH:33:PRO:CD	2.90	0.56
1:D:127:PRO:HB3	1:II:17:SER:O	2.06	0.56
1:D:110:GLU:OE1	8:D:301:HOH:O	2.17	0.56
1:H:144:ARG:NE	6:H:201:CL:CL	2.74	0.56
1:J:99:LEU:HG	1:J:141:CYS:HA	1.88	0.56
2:S:162:A:H1'	2:S:163[A]:A:C8	2.41	0.55
1:D:18:ASN:HA	1:II:129:ASN:HD21	1.73	0.54
1:O:11:LYS:HE3	2:T:168[A]:A:H61	1.73	0.54
1:G:14:GLY:HA2	1:G:15:ASP:OD1	2.09	0.53
4:WW:173:U:HO2'	4:WW:174:U:H6	1.57	0.52
1:JJ:91:TYR:N	6:JJ:303:CL:CL	2.79	0.51
1:K:79[B]:ARG:NH2	3:Y:169:A:P	2.81	0.51
1:KK:57:VAL:HG21	1:KK:134:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:II:17:SER:N	8:II:303:HOH:O	2.42	0.51
1:K:106:THR:OG1	1:O:66:ARG:NH2	2.39	0.51
1:A:106:THR:OG1	1:E:66:ARG:NH2	2.35	0.51
1:E:30:LYS:NZ	1:G:121:SER:O	2.41	0.49
1:K:155:SER:OG	3:Y:168[A]:A:OP1	2.30	0.49
1:JJ:95:ARG:HD3	6:JJ:302:CL:CL	2.49	0.49
1:II:81:TRP:CD1	1:II:121:SER:HB3	2.48	0.49
1:A:39[B]:ARG:HG2	1:A:41:ILE:CD1	2.42	0.49
1:JJ:47:VAL:HG12	1:JJ:48:GLN:N	2.28	0.49
1:E:95:ARG:HD3	1:E:108[B]:GLU:CD	2.33	0.49
1:B:57:VAL:HG22	1:B:140:VAL:HG22	1.95	0.49
1:E:82:THR:O	1:E:119:ARG:NH1	2.46	0.49
2:V:162:A:H2'	2:V:163:A:C8	2.47	0.48
1:H:110:GLU:OE1	6:H:202:CL:CL	2.67	0.48
1:II:82:THR:HG21	1:II:92[B]:SER:HG	1.77	0.48
6:II:202:CL:CL	8:II:306:HOH:O	2.57	0.48
1:B:19:VAL:HG22	1:B:20:VAL:H	1.78	0.48
1:E:95:ARG:HD3	1:E:108[B]:GLU:CG	2.44	0.48
1:M:23:ILE:O	1:M:25:ALA:N	2.45	0.48
1:KK:70:PHE:CD1	1:KK:158:PHE:HB3	2.49	0.48
1:HH:100:PHE:CD2	1:HH:130[B]:LEU:HD21	2.49	0.48
1:B:81:TRP:O	1:B:151:ALA:N	2.43	0.48
1:F:116:ILE:HD11	1:J:117:ASN:OD1	2.14	0.48
1:B:37:TRP:HH2	1:B:66:ARG:HD2	1.79	0.47
1:G:128:THR:HG23	1:HH:15:ASP:CB	2.44	0.47
1:II:37:TRP:HH2	1:II:66:ARG:HD2	1.79	0.47
1:D:33:PRO:CD	6:JJ:302:CL:CL	2.99	0.47
1:C:117:ASN:OD1	1:D:116:ILE:HD11	2.14	0.47
1:G:44:GLU:OE2	1:H:112:ARG:NH2	2.39	0.47
1:K:79[B]:ARG:HH22	3:Y:169:A:P	2.36	0.47
1:C:44:GLU:OE2	1:D:112:ARG:NH2	2.46	0.47
1:G:14:GLY:HA2	1:G:15:ASP:HA	1.57	0.46
1:JJ:47:VAL:HG12	1:JJ:48:GLN:H	1.80	0.46
1:KK:73:VAL:HG22	1:KK:156:CYS:HB2	1.97	0.46
1:JJ:18[A]:ASN:O	8:JJ:404:HOH:O	2.21	0.46
2:P:165[A]:A:C2	2:P:166[A]:A:C5	3.03	0.46
1:H:81:TRP:O	1:H:151:ALA:N	2.47	0.46
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.51	0.46
1:F:152:LEU:O	6:F:201:CL:CL	2.70	0.46
1:N:85:THR:HG22	1:O:116:ILE:HG21	1.98	0.46
1:L:48:GLN:HB2	1:L:51:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:II:117:ASN:O	1:JJ:115:ASN:HA	2.15	0.45
1:C:44:GLU:OE2	1:D:112:ARG:NH1	2.47	0.45
1:G:99:LEU:HD11	1:G:142:GLU:HG3	1.97	0.45
1:L:81:TRP:O	1:L:151:ALA:N	2.41	0.45
2:V:162:A:O2'	2:V:163:A:O5'	2.28	0.45
1:KK:73:VAL:CG2	1:KK:156:CYS:HB2	2.46	0.45
1:E:95:ARG:HD3	1:E:108[B]:GLU:HG2	1.99	0.45
1:O:13:THR:O	1:O:13:THR:OG1	2.30	0.45
1:O:16:ASN:O	1:O:16:ASN:ND2	2.50	0.45
1:KK:115:ASN:OD1	1:KK:117:ASN:N	2.47	0.45
3:TT:164[A]:A:C8	3:TT:164[A]:A:H5"	2.52	0.45
1:G:125:ARG:NH2	4:WW:170:U:H5"	2.32	0.45
2:S:162:A:H1'	2:S:163[A]:A:N7	2.32	0.45
1:B:37:TRP:CE2	1:B:39:ARG:HD3	2.52	0.45
1:C:152:LEU:O	6:C:206:CL:CL	2.72	0.45
1:A:117:ASN:O	1:B:115:ASN:HA	2.17	0.44
1:G:99:LEU:HD13	1:G:139[B]:ASN:ND2	2.32	0.44
1:K:148[B]:ARG:HG2	1:K:148[B]:ARG:NH1	2.28	0.44
4:WW:173:U:O2	4:WW:173:U:O4'	2.35	0.44
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.53	0.44
1:F:68:ASP:OD1	1:F:68:ASP:N	2.51	0.44
1:L:81:TRP:CD1	1:L:121:SER:HB3	2.53	0.44
1:M:110:GLU:OE2	1:M:112:ARG:NE	2.50	0.44
1:I:66:ARG:NH2	1:J:106:THR:OG1	2.36	0.44
1:M:97:LYS:HA	1:M:107:GLU:O	2.17	0.44
1:J:33:PRO:O	1:K:65:PHE:HA	2.18	0.44
1:M:37:TRP:CE2	1:M:39:ARG:HD3	2.53	0.44
1:HH:100:PHE:CE2	1:HH:130[B]:LEU:HD21	2.53	0.44
1:KK:49:SER:N	6:KK:205:CL:CL	2.88	0.44
1:O:91:TYR:CE2	1:O:116:ILE:HG23	2.53	0.44
1:HH:97:LYS:HA	1:HH:107:GLU:O	2.18	0.44
1:C:81:TRP:O	1:C:151:ALA:N	2.50	0.43
1:A:115:ASN:OD1	1:A:117:ASN:N	2.50	0.43
1:N:122:VAL:HG22	1:N:123:GLY:H	1.83	0.43
3:TT:165:A:H5'	8:TT:301:HOH:O	2.18	0.43
3:TT:167[A]:A:C2	3:TT:168[A]:A:H1'	2.52	0.43
1:A:39[A]:ARG:NH2	1:O:33:PRO:O	2.51	0.43
1:KK:70:PHE:CG	1:KK:158:PHE:HB3	2.53	0.43
6:H:202:CL:CL	1:HH:33:PRO:HD2	2.55	0.43
1:I:37:TRP:HH2	1:I:66:ARG:HD2	1.83	0.43
4:WW:167[A]:U:P	4:WW:167[A]:U:H3'	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:TT:165:A:C8	3:TT:165:A:OP2	2.71	0.43
1:KK:57:VAL:HB	1:KK:135:VAL:O	2.18	0.43
1:L:7:LYS:HA	1:L:7:LYS:HD3	1.86	0.43
1:HH:57:VAL:HG22	1:HH:140:VAL:CG2	2.48	0.43
1:F:151:ALA:HB1	6:F:201:CL:CL	2.56	0.43
1:N:23:ILE:O	1:N:25:ALA:N	2.49	0.43
1:G:33:PRO:O	1:HH:39:ARG:NH2	2.52	0.43
1:B:30:LYS:HB2	1:N:22[B]:MET:SD	2.59	0.42
1:D:81:TRP:CD1	1:D:121:SER:HB3	2.54	0.42
1:H:110:GLU:HB2	6:H:202:CL:CL	2.56	0.42
1:C:57:VAL:HG22	1:C:140[A]:VAL:HG22	2.01	0.42
1:G:81:TRP:CD1	1:G:121:SER:HB3	2.55	0.42
1:II:44:GLU:OE2	6:II:203:CL:CL	2.74	0.42
1:L:11:LYS:O	1:L:11:LYS:HG2	2.18	0.42
1:G:128:THR:HG23	1:HH:15:ASP:HB3	2.01	0.42
1:M:80:ALA:O	1:M:121:SER:HA	2.20	0.42
1:A:30:LYS:HG3	1:J:24:ARG:HA	2.01	0.42
1:I:117:ASN:O	1:J:115:ASN:HA	2.20	0.42
3:Y:167[A]:A:C2'	3:Y:168[A]:A:O5'	2.68	0.42
1:C:118[A]:THR:HA	1:D:114:SER:O	2.20	0.42
1:D:18:ASN:CA	1:II:129:ASN:HD21	2.33	0.42
1:N:81:TRP:O	1:N:151:ALA:N	2.51	0.42
1:O:11:LYS:HE3	2:T:168[A]:A:N6	2.33	0.42
1:G:73:VAL:HG22	1:G:156:CYS:HB2	2.01	0.42
1:L:76[B]:MET:SD	1:L:157:CYS:SG	3.18	0.42
1:O:11:LYS:O	1:O:12:SER:HB2	2.20	0.42
1:H:95:ARG:CD	6:H:202:CL:CL	3.04	0.41
1:JJ:45:VAL:HB	1:JJ:53:PHE:CE2	2.55	0.41
1:B:73:VAL:HG22	1:B:156:CYS:HB2	2.02	0.41
1:D:144:ARG:NE	6:D:201:CL:CL	2.88	0.41
1:E:33:PRO:O	1:F:39:ARG:NH2	2.53	0.41
1:F:117:ASN:HB3	1:G:116:ILE:HG12	2.02	0.41
1:I:24:ARG:HA	1:L:30:LYS:HG3	2.01	0.41
1:C:117:ASN:O	1:D:115:ASN:HA	2.20	0.41
1:F:81:TRP:CD1	1:F:121:SER:HB3	2.55	0.41
1:L:13:THR:O	1:L:13:THR:OG1	2.36	0.41
1:M:85:THR:HG22	1:N:116:ILE:HG21	2.02	0.41
1:F:47[B]:VAL:HG23	1:F:147:CYS:O	2.20	0.41
2:T:164[A]:A:H4'	1:HH:17:SER:HA	2.02	0.41
3:TT:164[A]:A:C8	3:TT:164[A]:A:C5'	3.03	0.41
1:A:88:VAL:O	1:A:89:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ALA:HB1	6:C:206:CL:CL	2.57	0.41
1:F:24:ARG:HA	1:II:30:LYS:HG3	2.03	0.41
1:H:57:VAL:HG22	1:H:140:VAL:HG22	2.03	0.41
1:L:11:LYS:HZ1	1:L:14:GLY:HA2	1.85	0.41
1:H:142:GLU:OE1	6:H:201:CL:CL	2.76	0.41
1:A:47:VAL:CG1	1:A:147:CYS:O	2.68	0.41
1:J:17:SER:HB3	2:P:164[A]:A:O3'	2.20	0.41
1:A:131:ARG:O	1:K:129:ASN:ND2	2.43	0.41
1:B:50:GLY:N	8:B:403:HOH:O	2.39	0.41
1:F:16:ASN:O	1:F:17:SER:HB2	2.21	0.41
1:J:39:ARG:NH2	1:K:33:PRO:O	2.54	0.41
1:L:8:PRO:O	6:L:501:CL:CL	2.76	0.41
1:M:91:TYR:CE1	1:M:116:ILE:HG23	2.56	0.41
1:O:11:LYS:NZ	1:O:11:LYS:HB3	2.36	0.41
1:G:152:LEU:O	6:G:301:CL:CL	2.75	0.41
1:JJ:37:TRP:HH2	1:JJ:66:ARG:HD2	1.86	0.41
1:JJ:127:PRO:HB2	1:JJ:129:ASN:OD1	2.21	0.41
1:J:29:PRO:HD3	1:K:81:TRP:CZ2	2.56	0.40
1:N:115:ASN:OD1	1:N:117:ASN:N	2.50	0.40
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.56	0.40
4:WW:173:U:O2'	4:WW:174:U:P	2.79	0.40
1:E:37:TRP:CE2	1:E:39:ARG:HD3	2.56	0.40
1:M:38:VAL:HG22	1:M:157:CYS:SG	2.61	0.40
1:JJ:108:GLU:HB3	6:JJ:302:CL:CL	2.59	0.40
1:F:114:SER:O	1:J:118:THR:HA	2.22	0.40
1:N:110:GLU:OE2	1:N:112:ARG:NE	2.46	0.40
1:B:52:ALA:HB2	1:B:144:ARG:CZ	2.51	0.40
1:B:57:VAL:HG22	1:B:140:VAL:CG2	2.50	0.40
1:H:22[A]:MET:HG3	1:H:23:ILE:N	2.36	0.40
1:II:68:ASP:OD1	1:II:68:ASP:N	2.54	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:308:HOH:O	8:N:202:HOH:O[6_566]	1.91	0.29
4:ll:186[A]:U:OP1	8:II:305:HOH:O[6_566]	1.91	0.29
2:S:164[A]:A:O2'	8:KK:317:HOH:O[12_665]	1.97	0.23
6:TT:201:CL:CL	8:B:420:HOH:O[6_566]	2.07	0.13
1:H:15:ASP:N	4:e:183[A]:U:OP2[6_566]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:N	2:X:164[A]:A:OP1[12_665]	2.11	0.09
1:L:72:SER:OG	1:N:104:ASP:O[6_566]	2.14	0.06
1:L:26:GLY:O	1:M:81:TRP:HE1[6_566]	1.57	0.03
2:bb:164[A]:A:O2'	8:JJ:425:HOH:O[12_665]	2.19	0.01

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	148/159 (93%)	138 (93%)	9 (6%)	1 (1%)	22	52
1	B	143/159 (90%)	134 (94%)	8 (6%)	1 (1%)	22	52
1	C	143/159 (90%)	135 (94%)	8 (6%)	0	100	100
1	D	148/159 (93%)	140 (95%)	8 (5%)	0	100	100
1	E	147/159 (92%)	138 (94%)	9 (6%)	0	100	100
1	F	152/159 (96%)	143 (94%)	8 (5%)	1 (1%)	22	52
1	G	150/159 (94%)	142 (95%)	8 (5%)	0	100	100
1	GG	146/159 (92%)	139 (95%)	7 (5%)	0	100	100
1	H	147/159 (92%)	136 (92%)	11 (8%)	0	100	100
1	HH	150/159 (94%)	144 (96%)	6 (4%)	0	100	100
1	I	145/159 (91%)	139 (96%)	6 (4%)	0	100	100
1	II	149/159 (94%)	139 (93%)	10 (7%)	0	100	100
1	J	152/159 (96%)	143 (94%)	8 (5%)	1 (1%)	22	52
1	JJ	142/159 (89%)	135 (95%)	7 (5%)	0	100	100
1	K	156/159 (98%)	147 (94%)	9 (6%)	0	100	100
1	KK	143/159 (90%)	136 (95%)	7 (5%)	0	100	100
1	L	170/159 (107%)	146 (86%)	17 (10%)	7 (4%)	3	9
1	M	155/159 (98%)	145 (94%)	9 (6%)	1 (1%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	155/159 (98%)	141 (91%)	13 (8%)	1 (1%)	25 56
1	O	150/159 (94%)	138 (92%)	11 (7%)	1 (1%)	22 52
All	All	2991/3180 (94%)	2798 (94%)	179 (6%)	14 (0%)	29 60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	15	ASP
1	L	7	LYS
1	L	8	PRO
1	L	10	ARG
1	M	122	VAL
1	N	122	VAL
1	O	12	SER
1	L	13	THR
1	A	17	SER
1	F	17	SER
1	L	6	VAL
1	L	9	ASN
1	B	37	TRP
1	L	14	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/140 (96%)	134 (100%)	0	100 100
1	B	129/140 (92%)	128 (99%)	1 (1%)	81 93
1	C	129/140 (92%)	127 (98%)	2 (2%)	62 84
1	D	134/140 (96%)	134 (100%)	0	100 100
1	E	133/140 (95%)	133 (100%)	0	100 100
1	F	138/140 (99%)	138 (100%)	0	100 100
1	G	135/140 (96%)	135 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	GG	132/140 (94%)	132 (100%)	0	100 100
1	H	133/140 (95%)	133 (100%)	0	100 100
1	HH	136/140 (97%)	136 (100%)	0	100 100
1	I	131/140 (94%)	131 (100%)	0	100 100
1	II	135/140 (96%)	135 (100%)	0	100 100
1	J	137/140 (98%)	137 (100%)	0	100 100
1	JJ	128/140 (91%)	128 (100%)	0	100 100
1	K	142/140 (101%)	142 (100%)	0	100 100
1	KK	129/140 (92%)	128 (99%)	1 (1%)	81 93
1	L	154/140 (110%)	154 (100%)	0	100 100
1	M	141/140 (101%)	140 (99%)	1 (1%)	84 94
1	N	141/140 (101%)	141 (100%)	0	100 100
1	O	135/140 (96%)	135 (100%)	0	100 100
All	All	2706/2800 (97%)	2701 (100%)	5 (0%)	93 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	TRP
1	C	24	ARG
1	C	106	THR
1	M	122	VAL
1	KK	155[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	B	117	ASN
1	D	18	ASN
1	E	117	ASN
1	F	117	ASN
1	I	117	ASN
1	K	117	ASN
1	N	117	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	6/12 (50%)	1 (16%)	0
2	S	6/12 (50%)	1 (16%)	0
2	T	4/12 (33%)	1 (25%)	0
2	UU	6/12 (50%)	1 (16%)	0
2	V	7/12 (58%)	2 (28%)	0
2	X	7/12 (58%)	0	0
2	bb	10/12 (83%)	5 (50%)	0
3	TT	5/11 (45%)	3 (60%)	1 (20%)
3	Y	8/11 (72%)	4 (50%)	0
3	a	4/11 (36%)	2 (50%)	0
4	WW	9/13 (69%)	5 (55%)	1 (11%)
4	e	10/13 (76%)	5 (50%)	0
4	h	6/13 (46%)	2 (33%)	0
4	i	4/13 (30%)	1 (25%)	0
4	kk	5/13 (38%)	3 (60%)	0
4	ll	4/13 (30%)	0	0
4	n	6/13 (46%)	0	0
4	qq	5/13 (38%)	3 (60%)	0
5	m	8/11 (72%)	3 (37%)	0
All	All	120/232 (51%)	42 (35%)	2 (1%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	P	164[A]	A
2	S	163[A]	A
2	T	168[A]	A
2	V	163	A
2	V	169[A]	A
3	Y	168[A]	A
3	Y	169	A
3	Y	170	A
3	Y	171	A
3	a	165[A]	A
3	a	168[A]	A
4	e	181[A]	U
4	e	183[A]	U
4	e	184[A]	U
4	e	185[A]	U
4	e	186[A]	U
4	h	186[A]	U

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Mol	Chain	Res	Type
4	h	187[A]	U
4	i	185[A]	U
5	m	183[A]	U
5	m	188[A]	U
5	m	189[A]	U
3	TT	165	A
3	TT	166[A]	A
3	TT	168[A]	A
2	UU	164[A]	A
4	WW	167[A]	U
4	WW	169	U
4	WW	172	U
4	WW	173	U
4	WW	174	U
2	bb	159	A
2	bb	160	A
2	bb	161[A]	A
2	bb	163[A]	A
2	bb	168[A]	A
4	kk	185[A]	U
4	kk	188[A]	U
4	kk	189	U
4	qq	186[A]	U
4	qq	187[A]	U
4	qq	188	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	TT	164[A]	A
4	WW	173	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 53 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	145/159 (91%)	0.32	5 (3%) 45 43	31, 50, 76, 148	1 (0%)
1	B	143/159 (89%)	0.13	1 (0%) 87 88	33, 48, 68, 93	1 (0%)
1	C	142/159 (89%)	0.04	0 100 100	29, 39, 56, 87	3 (2%)
1	D	144/159 (90%)	0.08	4 (2%) 53 53	27, 36, 62, 114	2 (1%)
1	E	144/159 (90%)	0.21	3 (2%) 63 64	31, 40, 72, 122	2 (1%)
1	F	144/159 (90%)	0.27	4 (2%) 53 53	39, 51, 73, 140	1 (0%)
1	G	146/159 (91%)	0.34	5 (3%) 45 43	33, 44, 78, 167	1 (0%)
1	GG	145/159 (91%)	0.02	2 (1%) 75 77	23, 31, 55, 211	1 (0%)
1	H	145/159 (91%)	0.17	3 (2%) 63 64	37, 44, 65, 184	1 (0%)
1	HH	145/159 (91%)	0.16	4 (2%) 53 53	28, 36, 61, 119	0
1	I	144/159 (90%)	0.35	3 (2%) 63 64	41, 56, 74, 113	2 (1%)
1	II	143/159 (89%)	0.27	2 (1%) 75 77	27, 37, 56, 86	0
1	J	147/159 (92%)	0.60	7 (4%) 30 30	43, 62, 86, 162	4 (2%)
1	JJ	144/159 (90%)	-0.06	2 (1%) 75 77	24, 31, 56, 124	3 (2%)
1	K	145/159 (91%)	0.61	7 (4%) 30 30	47, 61, 86, 141	3 (2%)
1	KK	144/159 (90%)	-0.05	1 (0%) 87 88	23, 30, 52, 110	2 (1%)
1	L	157/159 (98%)	0.73	14 (8%) 9 8	56, 72, 120, 150	0
1	M	144/159 (90%)	0.82	8 (5%) 24 23	58, 75, 101, 120	0
1	N	144/159 (90%)	0.46	5 (3%) 44 42	47, 68, 110, 144	0
1	O	150/159 (94%)	0.88	14 (9%) 8 7	37, 60, 102, 145	5 (3%)
2	P	7/12 (58%)	2.82	6 (85%) 0 0	88, 102, 143, 152	6 (85%)
2	S	7/12 (58%)	2.84	4 (57%) 0 0	62, 78, 146, 166	5 (71%)
2	T	5/12 (41%)	1.37	0 100 100	67, 69, 82, 99	4 (80%)
2	UU	7/12 (58%)	2.01	3 (42%) 0 0	57, 69, 94, 98	7 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	V	8/12 (66%)	3.21	6 (75%)	0	0	71, 110, 160, 180	4 (50%)
2	X	8/12 (66%)	4.46	8 (100%)	0	0	82, 97, 146, 151	8 (100%)
2	bb	11/12 (91%)	7.03	8 (72%)	0	0	64, 102, 138, 158	8 (72%)
3	TT	6/11 (54%)	4.85	5 (83%)	0	0	97, 128, 163, 245	1 (16%)
3	Y	9/11 (81%)	3.81	7 (77%)	0	0	81, 89, 137, 137	9 (100%)
3	a	5/11 (45%)	5.26	4 (80%)	0	0	92, 98, 133, 138	4 (80%)
4	WW	10/13 (76%)	4.72	9 (90%)	0	0	94, 138, 183, 185	6 (60%)
4	e	11/13 (84%)	5.60	8 (72%)	0	0	92, 120, 173, 174	11 (100%)
4	h	7/13 (53%)	2.59	3 (42%)	0	0	60, 79, 105, 113	7 (100%)
4	i	5/13 (38%)	2.34	2 (40%)	0	0	67, 78, 120, 122	3 (60%)
4	kk	6/13 (46%)	2.82	4 (66%)	0	0	89, 98, 131, 145	6 (100%)
4	ll	5/13 (38%)	1.52	0	100	100	58, 64, 74, 91	3 (60%)
4	n	7/13 (53%)	2.68	4 (57%)	0	0	76, 82, 105, 147	7 (100%)
4	qq	6/13 (46%)	1.62	3 (50%)	0	0	64, 84, 128, 156	1 (16%)
5	m	9/11 (81%)	3.56	8 (88%)	0	0	83, 102, 148, 156	9 (100%)
All	All	3044/3412 (89%)	0.47	186 (6%)	21	19	23, 50, 99, 245	141 (4%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	bb	160	A	18.0
4	e	181[A]	U	16.8
2	bb	161[A]	A	12.3
3	TT	171	A	12.2
2	bb	158	A	11.3
4	e	180	U	11.2
2	bb	162[A]	A	11.0
1	GG	15	ASP	10.9
2	X	169[A]	A	10.8
1	G	15	ASP	10.3
3	a	164[A]	A	10.0
1	O	15	ASP	9.8
1	H	15	ASP	9.2
4	WW	172	U	8.9
4	WW	173	U	8.5
1	G	14	GLY	8.5
2	bb	159	A	8.4

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Mol	Chain	Res	Type	RSRZ
2	V	169[A]	A	7.3
3	Y	170	A	7.2
3	a	168[A]	A	7.2
4	e	182[A]	U	6.9
4	n	188[A]	U	6.7
1	O	16	ASN	6.5
1	H	16	ASN	6.4
4	WW	171	U	6.4
4	WW	174	U	6.2
4	e	190[A]	U	6.1
5	m	190[A]	U	5.9
5	m	182[A]	U	5.7
4	e	189[A]	U	5.6
1	A	15	ASP	5.5
4	WW	170	U	5.4
1	K	15	ASP	5.4
2	S	162	A	5.3
3	Y	171	A	5.3
2	P	163[A]	A	5.3
1	J	15	ASP	5.3
2	X	162[A]	A	5.3
4	e	188[A]	U	5.2
3	Y	169	A	5.1
1	HH	15	ASP	5.0
1	G	16	ASN	5.0
2	S	163[A]	A	5.0
4	kk	189	U	4.9
2	bb	163[A]	A	4.8
2	X	168[A]	A	4.8
2	V	162	A	4.7
4	h	190[A]	U	4.7
5	m	189[A]	U	4.7
3	TT	164[A]	A	4.6
1	L	16	ASN	4.5
1	N	16	ASN	4.5
4	h	184[A]	U	4.4
1	O	10	ARG	4.4
1	O	13	THR	4.3
1	L	3	ARG	4.3
3	Y	168[A]	A	4.2
4	i	188[A]	U	4.2
3	TT	165	A	4.1

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Mol	Chain	Res	Type	RSRZ
3	Y	163[A]	A	4.1
5	m	188[A]	U	4.0
1	M	24	ARG	4.0
2	bb	168[A]	A	3.9
3	a	165[A]	A	3.9
1	L	10	ARG	3.9
1	O	12	SER	3.8
4	i	184[A]	U	3.8
1	KK	16	ASN	3.8
3	TT	168[A]	A	3.7
1	D	148	ARG	3.7
2	X	165[A]	A	3.6
3	a	167[A]	A	3.6
1	HH	16	ASN	3.6
1	A	16	ASN	3.5
2	P	169[A]	A	3.5
1	J	13	THR	3.5
2	X	163[A]	A	3.5
1	O	14	GLY	3.4
1	L	15	ASP	3.4
1	O	11	LYS	3.4
3	TT	166[A]	A	3.3
1	I	24	ARG	3.3
4	h	189[A]	U	3.2
3	Y	167[A]	A	3.2
1	K	16	ASN	3.2
2	V	163	A	3.2
1	M	16	ASN	3.1
1	F	24	ARG	3.1
4	qq	188	U	3.1
5	m	184[A]	U	3.1
1	L	8	PRO	3.1
1	L	7	LYS	3.1
1	K	116	ILE	3.1
1	G	24	ARG	3.1
1	L	11	LYS	3.0
1	M	121	SER	3.0
4	kk	184[A]	U	3.0
4	WW	166[A]	U	3.0
2	S	167[A]	A	3.0
1	F	92	SER	2.9
1	L	50	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	24	ARG	2.9
1	L	18[A]	ASN	2.9
5	m	183[A]	U	2.8
1	O	148	ARG	2.8
2	V	168[A]	A	2.8
1	F	16	ASN	2.8
1	L	120	ALA	2.8
4	e	187[A]	U	2.8
4	kk	185[A]	U	2.8
1	M	128[A]	THR	2.8
1	O	153	VAL	2.8
1	J	16	ASN	2.8
1	JJ	16	ASN	2.8
2	X	166[A]	A	2.7
1	E	24	ARG	2.7
1	O	24	ARG	2.7
2	UU	168[A]	A	2.7
2	X	164[A]	A	2.7
4	kk	188[A]	U	2.7
2	P	168[A]	A	2.6
1	GG	16	ASN	2.6
1	II	24	ARG	2.6
4	n	185[A]	U	2.6
1	D	16	ASN	2.6
3	Y	166[A]	A	2.6
1	D	22[A]	MET	2.6
4	e	186[A]	U	2.6
4	n	182[A]	U	2.6
1	J	14	GLY	2.5
4	WW	165	U	2.5
1	G	48[A]	GLN	2.5
1	N	24	ARG	2.5
1	K	88	VAL	2.5
1	N	123	GLY	2.5
1	J	105	SER	2.5
1	K	51	ILE	2.5
4	WW	167[A]	U	2.5
4	n	183[A]	U	2.4
2	bb	167[A]	A	2.4
1	L	118	THR	2.4
1	L	19[A]	VAL	2.4
1	D	24	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	16	ASN	2.4
1	M	157	CYS	2.4
2	UU	167[A]	A	2.4
1	O	152	LEU	2.4
1	I	23	ILE	2.4
1	A	22[A]	MET	2.3
2	V	164[A]	A	2.3
4	WW	169	U	2.3
1	O	84	LEU	2.3
1	L	14	GLY	2.3
2	X	167[A]	A	2.3
2	P	164[A]	A	2.3
1	M	134	THR	2.3
1	A	31	VAL	2.2
1	B	21	THR	2.2
1	HH	27[A]	SER	2.2
1	F	113	ALA	2.2
2	UU	162[A]	A	2.2
1	M	31	VAL	2.2
1	M	102	THR	2.2
2	V	167[A]	A	2.2
1	N	125	ARG	2.2
4	qq	187[A]	U	2.2
1	JJ	50	GLY	2.2
5	m	187[A]	U	2.2
1	J	38	VAL	2.2
1	HH	24	ARG	2.2
5	m	185[A]	U	2.1
1	A	24	ARG	2.1
1	E	17	SER	2.1
2	P	165[A]	A	2.1
2	P	166[A]	A	2.1
2	S	168[A]	A	2.1
4	qq	183	U	2.1
1	O	120	ALA	2.1
1	I	16	ASN	2.1
1	J	22[A]	MET	2.1
1	K	81	TRP	2.1
1	O	49[A]	SER	2.0
1	II	146	ASN	2.0
1	N	148	ARG	2.0
1	L	24	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	24	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	E	201	1/1	0.23	1.11	71,71,71,71	0
6	CL	L	501	1/1	0.37	0.39	111,111,111,111	0
6	CL	JJ	301	1/1	0.45	1.52	100,100,100,100	0
6	CL	KK	203	1/1	0.57	0.36	86,86,86,86	0
6	CL	HH	402	1/1	0.71	1.00	115,115,115,115	0
6	CL	B	301	1/1	0.74	0.46	68,68,68,68	0
6	CL	T	201	1/1	0.74	0.23	82,82,82,82	0
6	CL	H	201	1/1	0.74	0.26	74,74,74,74	0
6	CL	B	302	1/1	0.77	0.51	82,82,82,82	0
7	MG	F	203	1/1	0.77	1.19	71,71,71,71	0
6	CL	C	204	1/1	0.78	0.75	91,91,91,91	0
6	CL	F	201	1/1	0.78	0.95	91,91,91,91	0
6	CL	B	303	1/1	0.79	0.35	89,89,89,89	0
6	CL	K	302	1/1	0.80	0.34	90,90,90,90	0
6	CL	TT	201	1/1	0.81	0.42	117,117,117,117	0
6	CL	KK	204	1/1	0.83	0.15	87,87,87,87	0
6	CL	II	203	1/1	0.83	0.94	93,93,93,93	0
6	CL	JJ	302	1/1	0.84	0.42	57,57,57,57	0
6	CL	KK	202	1/1	0.86	0.52	56,56,56,56	0
6	CL	GG	201	1/1	0.87	0.82	82,82,82,82	0
6	CL	HH	401	1/1	0.87	0.95	68,68,68,68	0
6	CL	H	202	1/1	0.87	0.86	88,88,88,88	0

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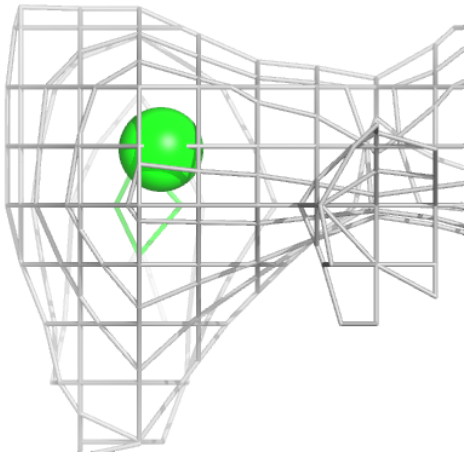
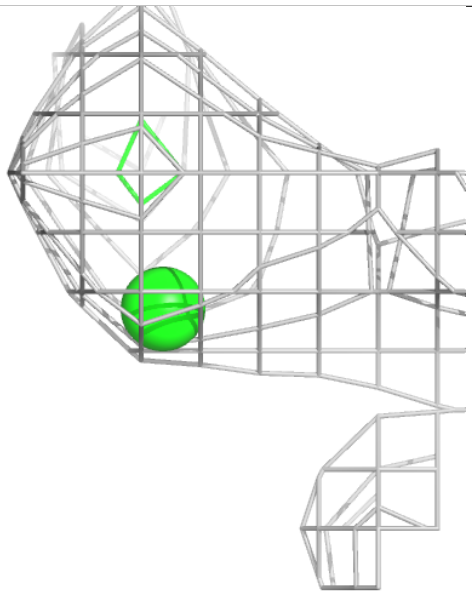
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	C	202	1/1	0.87	0.28	74,74,74,74	0
6	CL	JJ	303	1/1	0.88	0.29	52,52,52,52	0
7	MG	HH	403	1/1	0.88	0.56	35,35,35,35	0
7	MG	I	201	1/1	0.89	0.72	49,49,49,49	0
7	MG	K	303	1/1	0.90	0.70	79,79,79,79	0
7	MG	GG	202	1/1	0.90	0.29	26,26,26,26	0
6	CL	II	202	1/1	0.90	0.42	42,42,42,42	0
6	CL	JJ	304	1/1	0.91	0.57	83,83,83,83	0
6	CL	KK	205	1/1	0.91	0.22	72,72,72,72	0
6	CL	C	203	1/1	0.91	0.12	57,57,57,57	0
6	CL	ll	201	1/1	0.91	0.15	78,78,78,78	0
6	CL	D	202	1/1	0.91	0.41	71,71,71,71	0
6	CL	C	205	1/1	0.92	0.65	59,59,59,59	0
6	CL	G	302	1/1	0.92	0.29	59,59,59,59	0
7	MG	JJ	307	1/1	0.92	0.39	30,30,30,30	0
6	CL	C	201	1/1	0.93	0.41	51,51,51,51	0
6	CL	D	201	1/1	0.93	0.59	59,59,59,59	0
7	MG	G	303	1/1	0.94	0.32	43,43,43,43	0
7	MG	E	202	1/1	0.94	0.32	39,39,39,39	0
6	CL	II	201	1/1	0.95	0.33	66,66,66,66	0
6	CL	G	301	1/1	0.95	0.68	104,104,104,104	0
6	CL	JJ	305	1/1	0.96	0.50	47,47,47,47	0
6	CL	KK	201	1/1	0.96	0.08	11,11,11,11	0
6	CL	K	301	1/1	0.96	0.22	45,45,45,45	0
7	MG	F	204	1/1	0.96	0.95	128,128,128,128	0
6	CL	F	202	1/1	0.96	0.16	38,38,38,38	0
6	CL	B	304	1/1	0.97	0.14	29,29,29,29	0
7	MG	HH	404	1/1	0.97	0.40	40,40,40,40	0
6	CL	C	206	1/1	0.97	0.77	82,82,82,82	0
7	MG	KK	206	1/1	0.97	0.12	25,25,25,25	0
7	MG	JJ	306	1/1	0.98	0.57	149,149,149,149	0

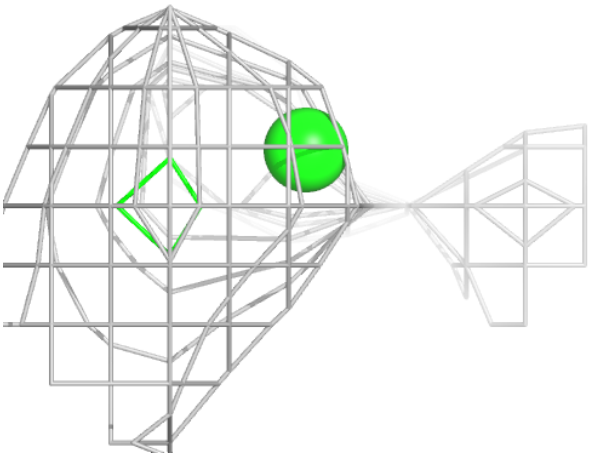
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CL L 501:

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

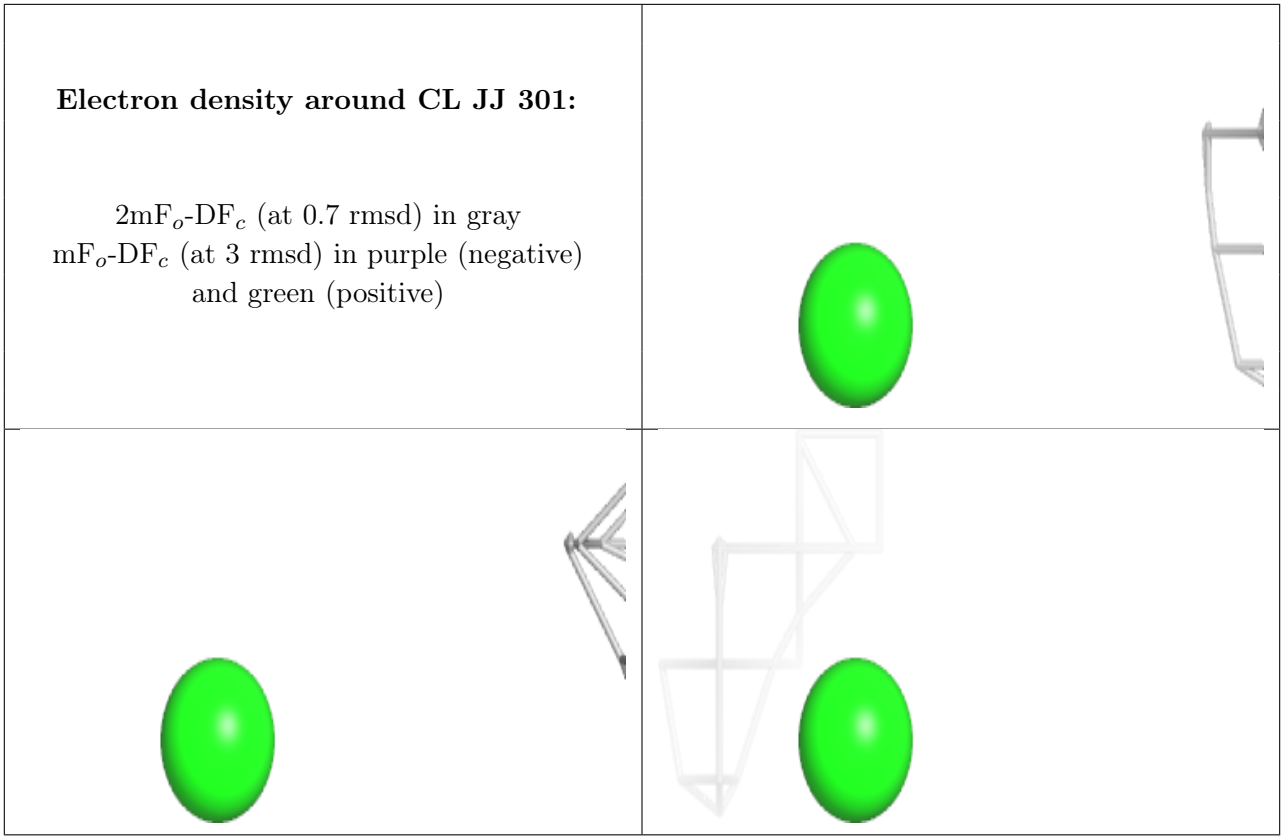






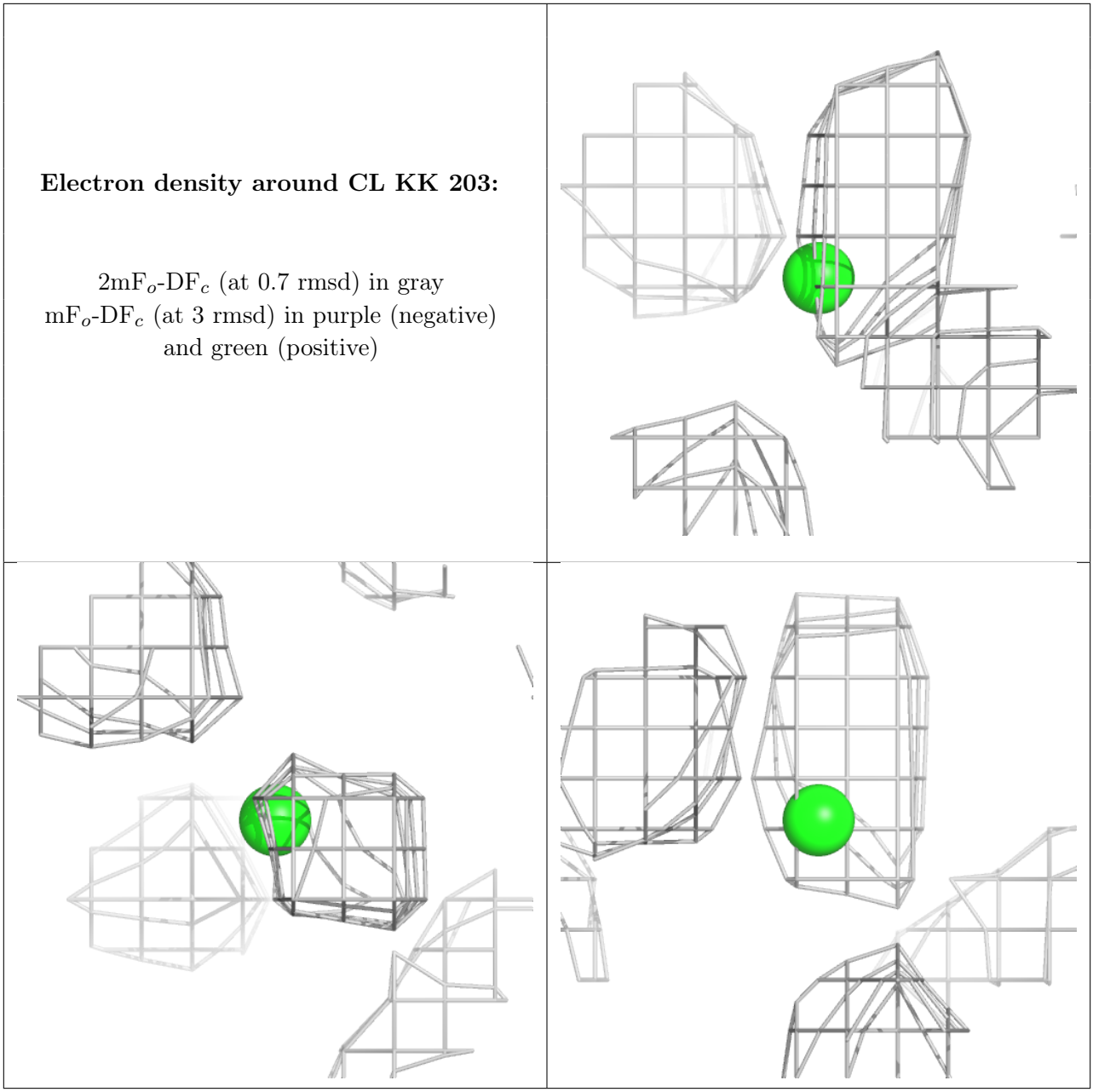
Electron density around CL JJ 301:

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



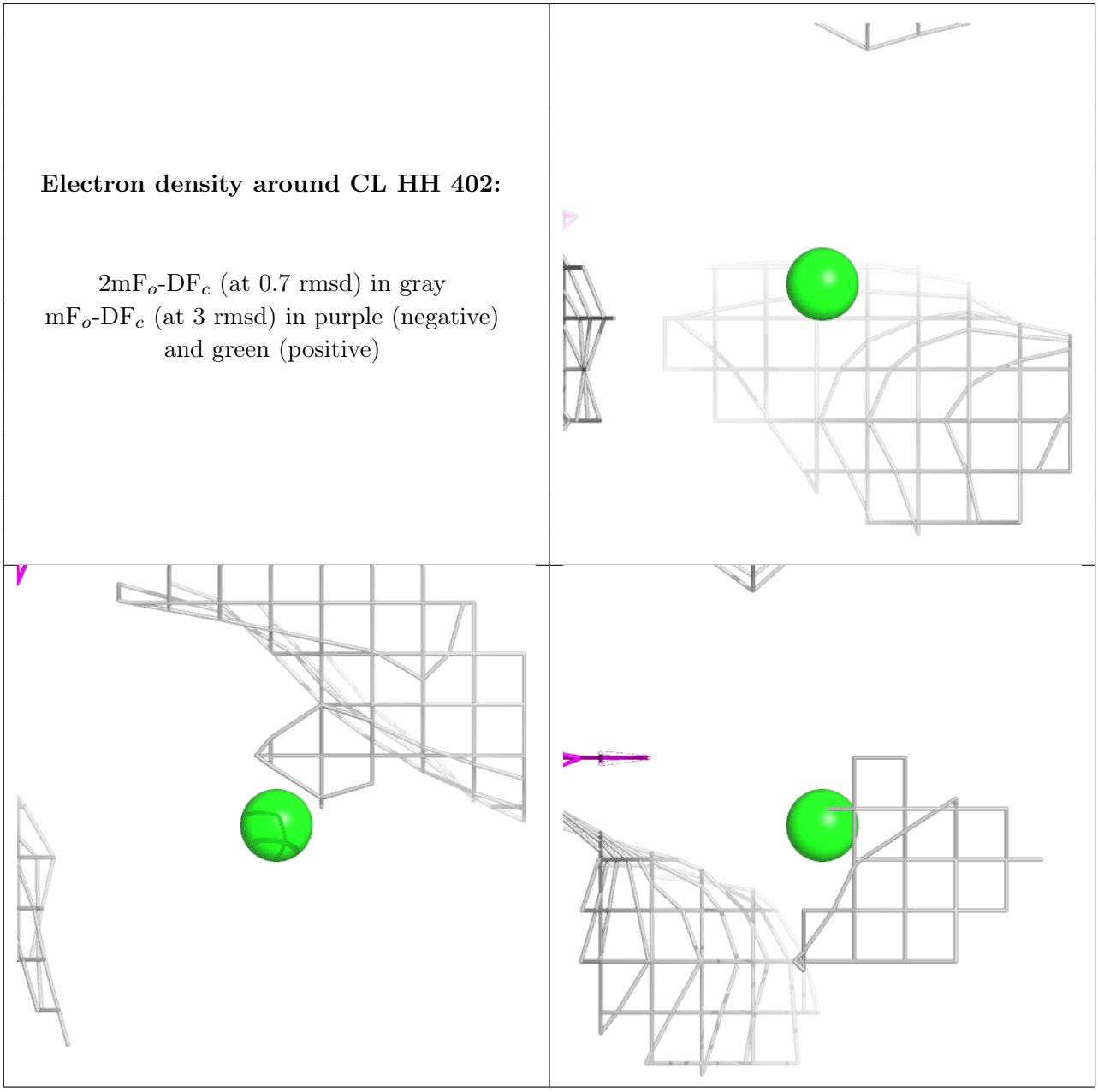
Electron density around CL KK 203:

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



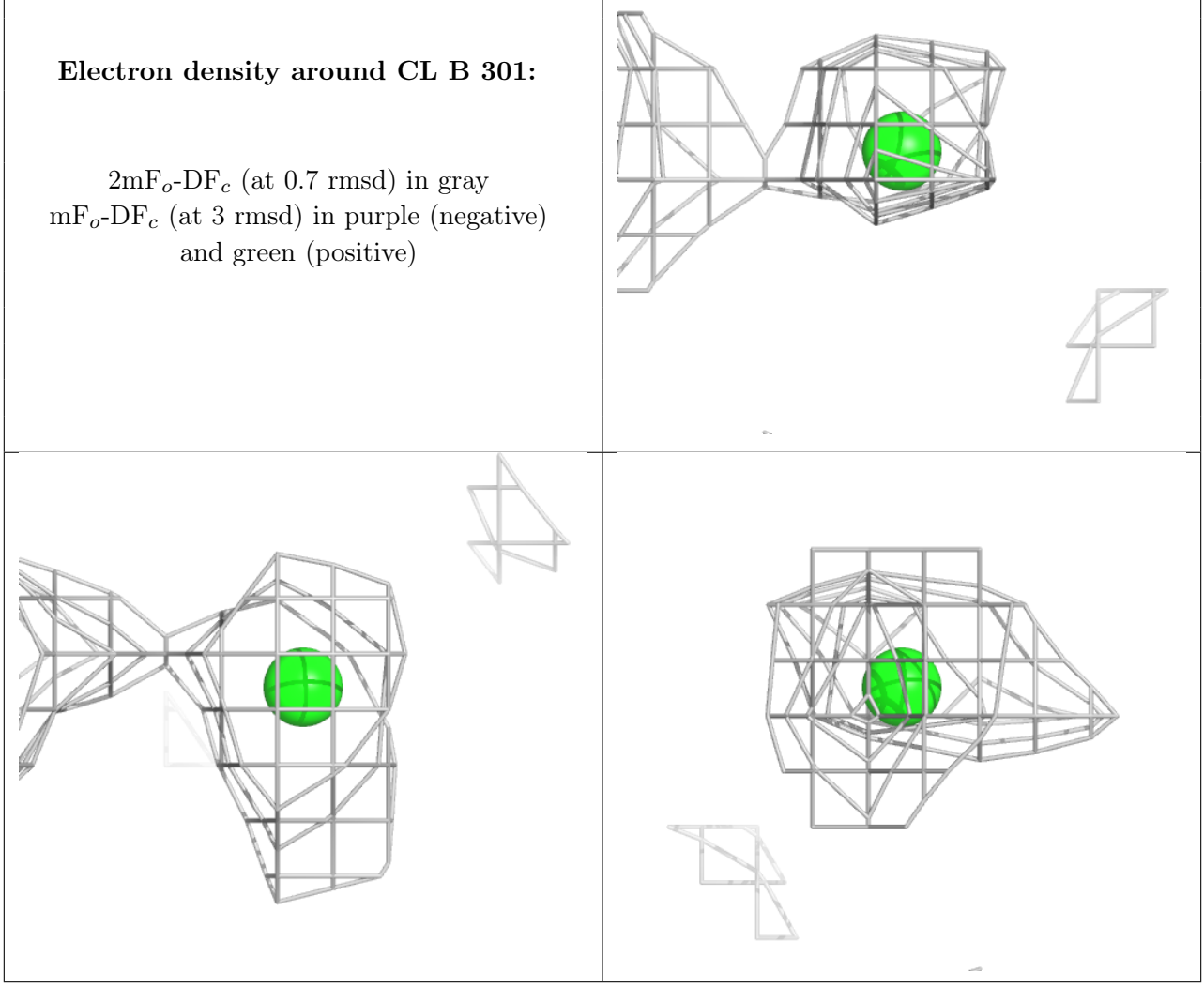
Electron density around CL HH 402:

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



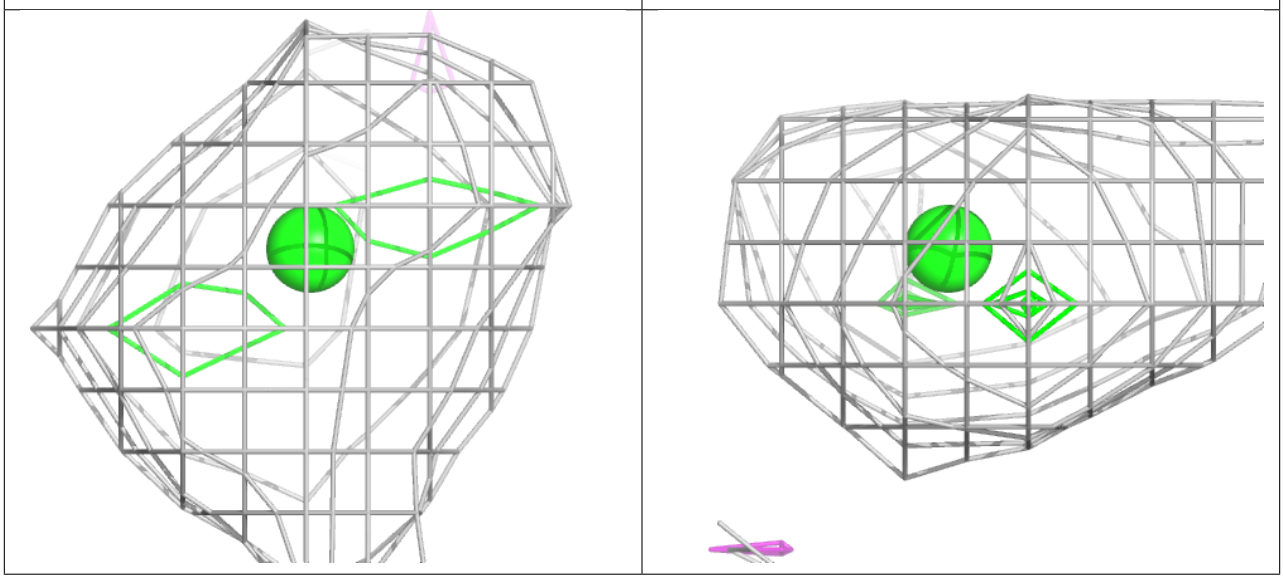
Electron density around CL B 301:

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



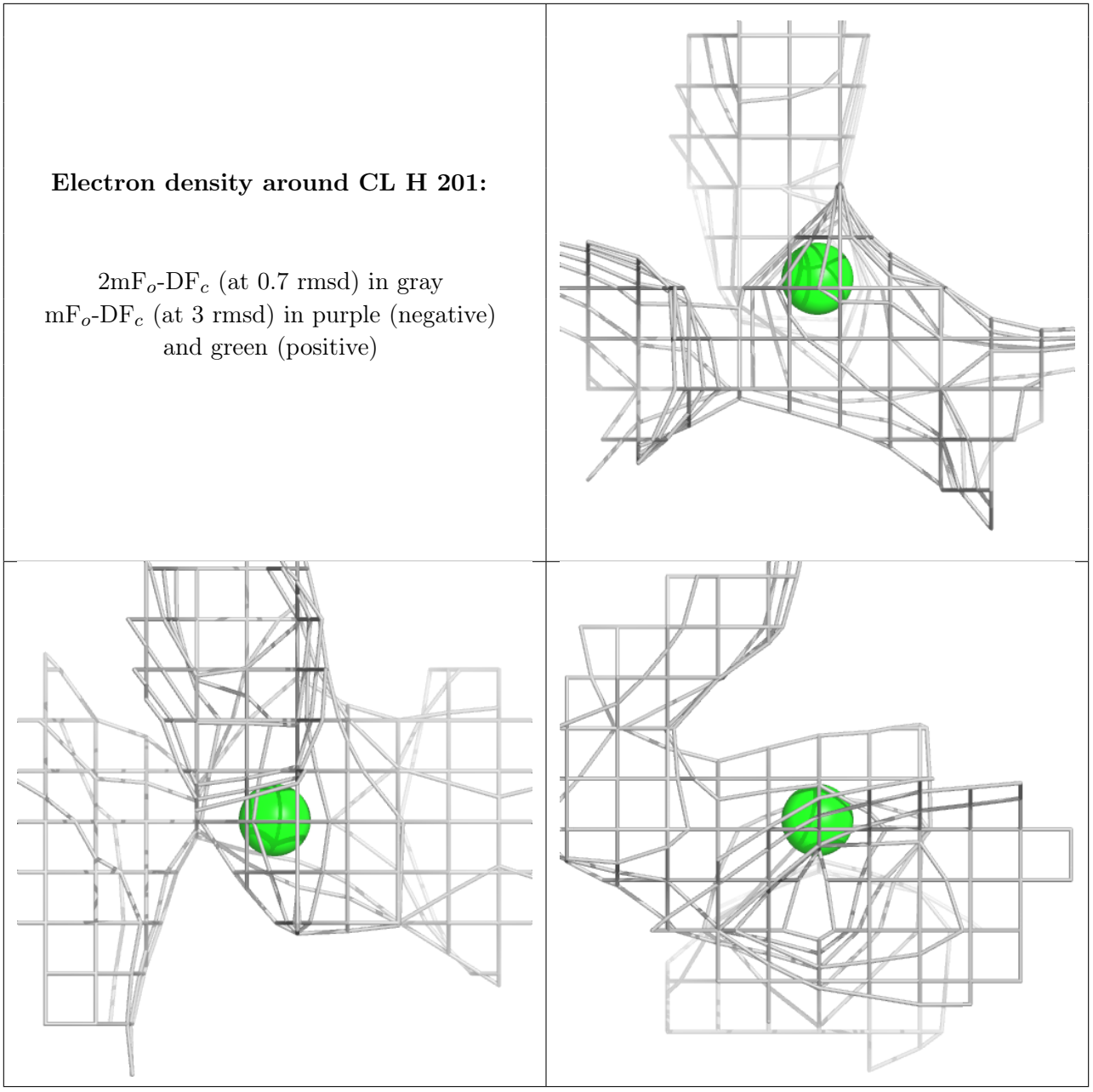
Electron density around CL T 201:

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



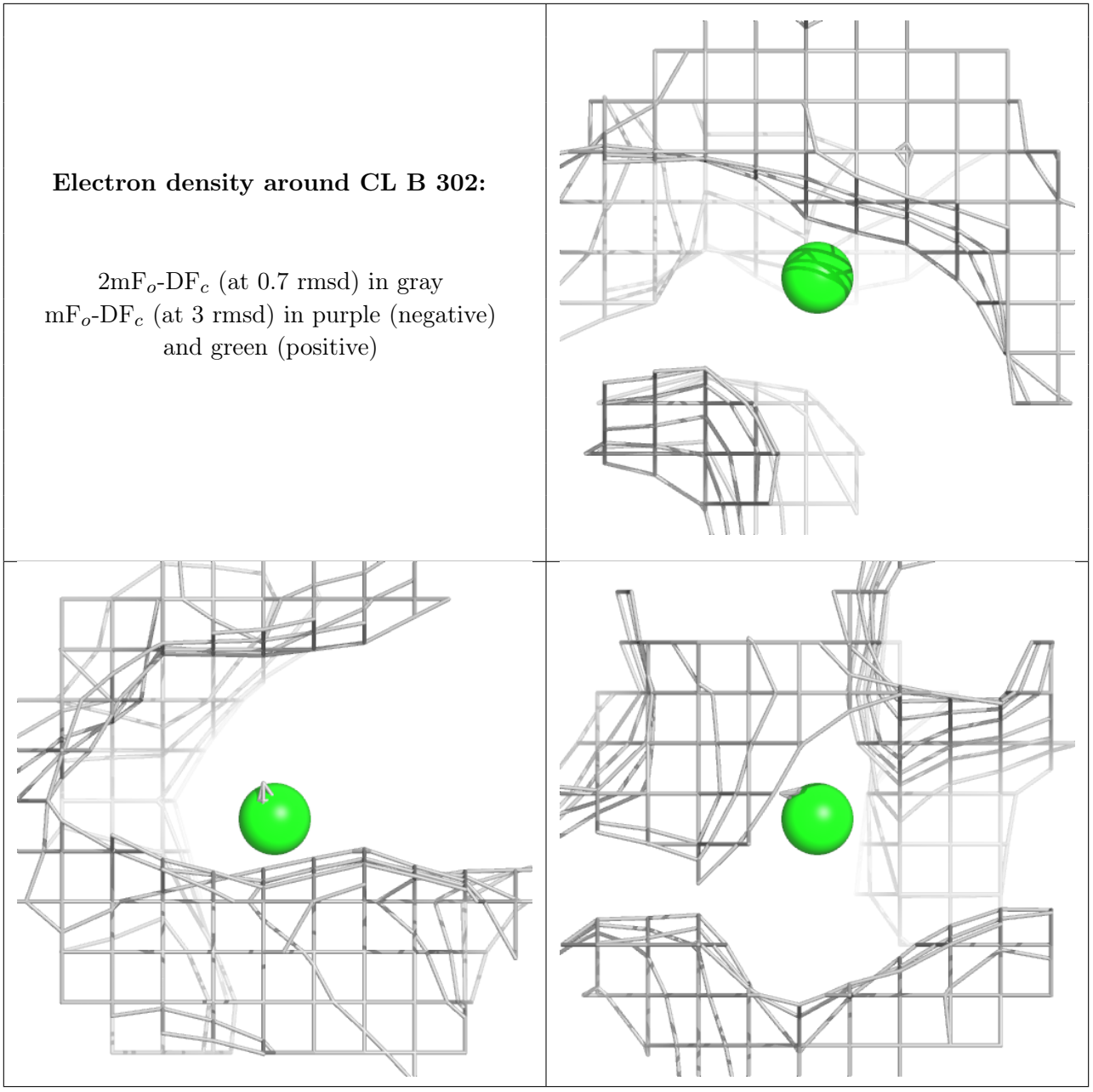
Electron density around CL H 201:

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



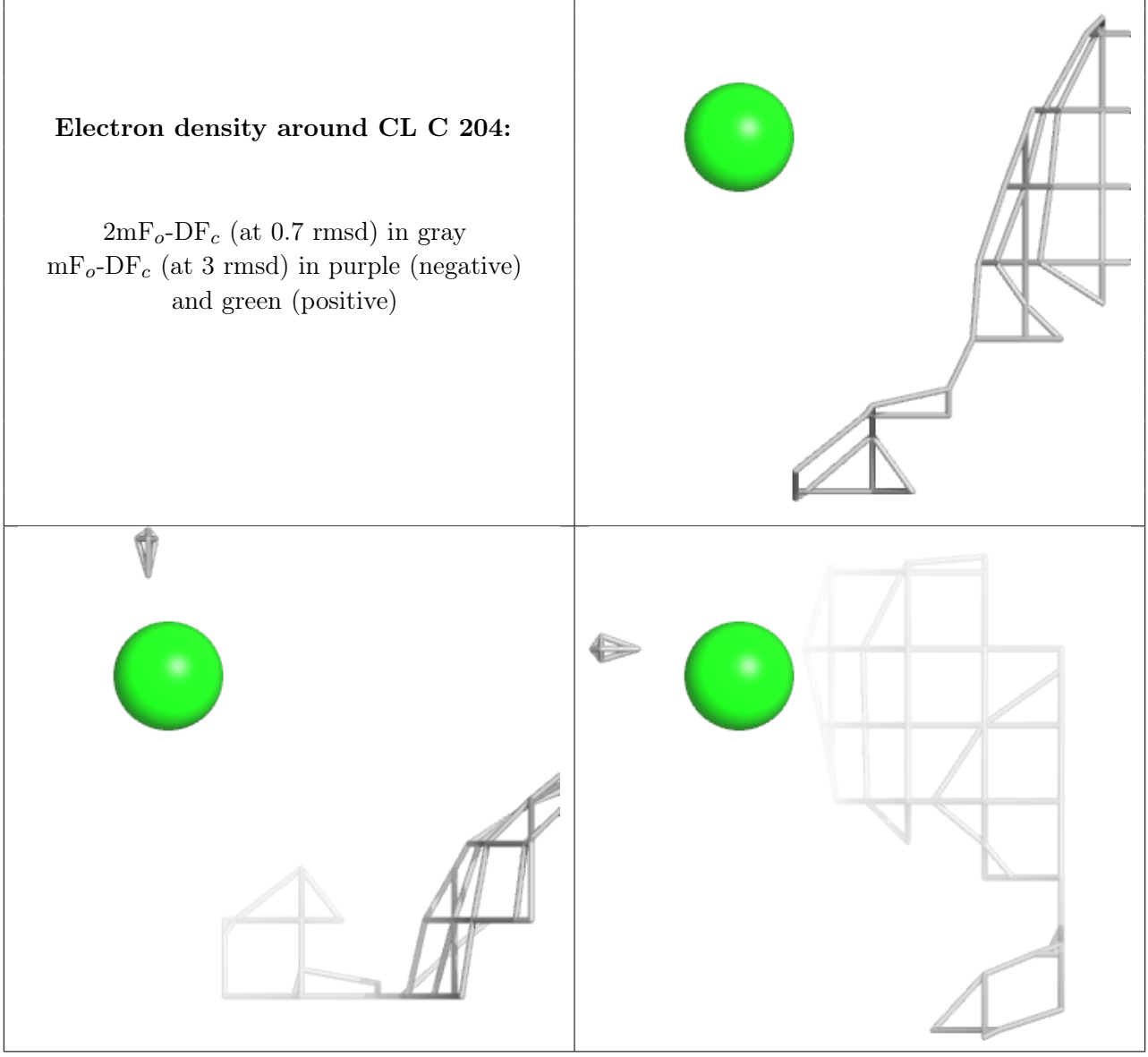
Electron density around CL B 302:

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



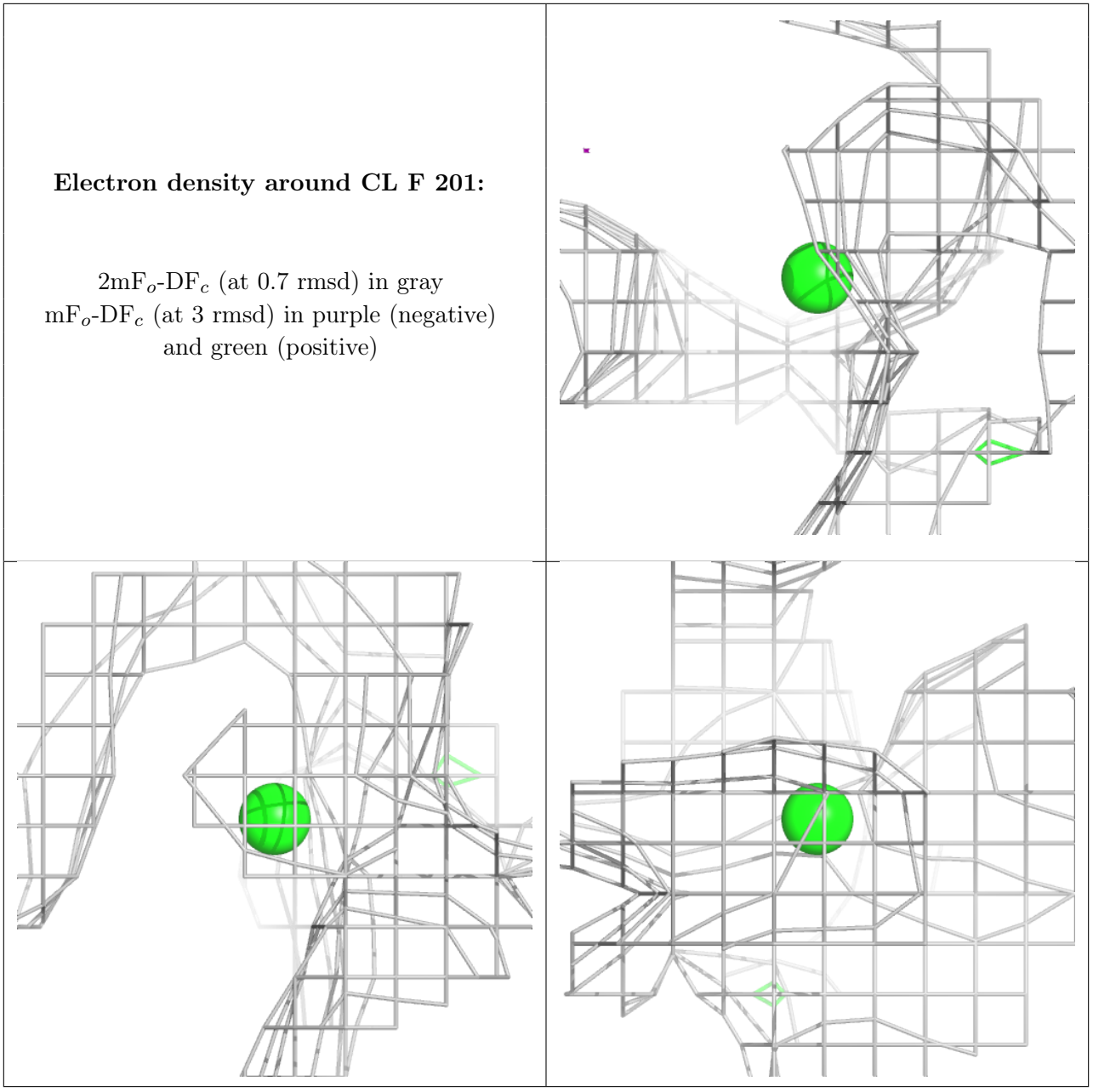
Electron density around CL C 204:

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



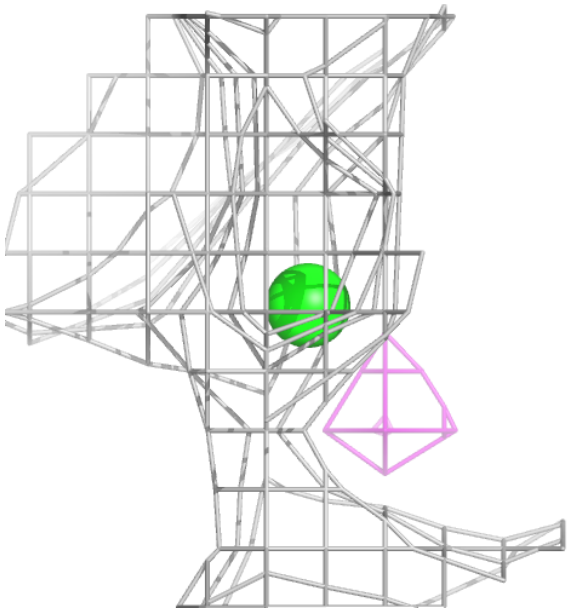
Electron density around CL F 201:

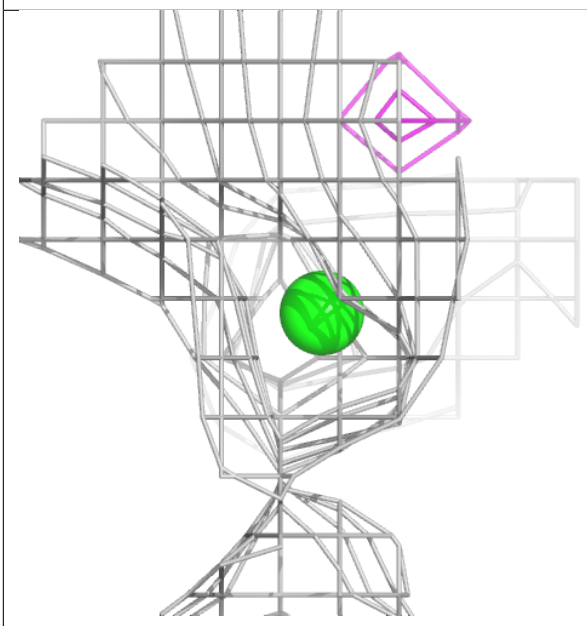
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

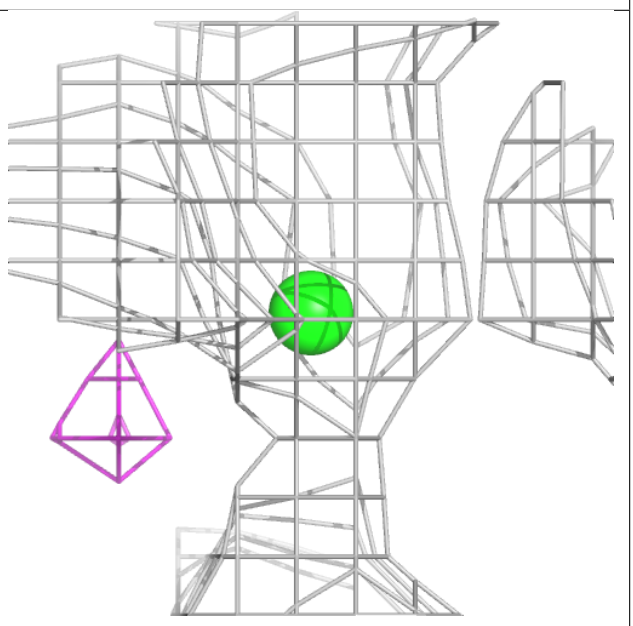


Electron density around CL B 303:

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

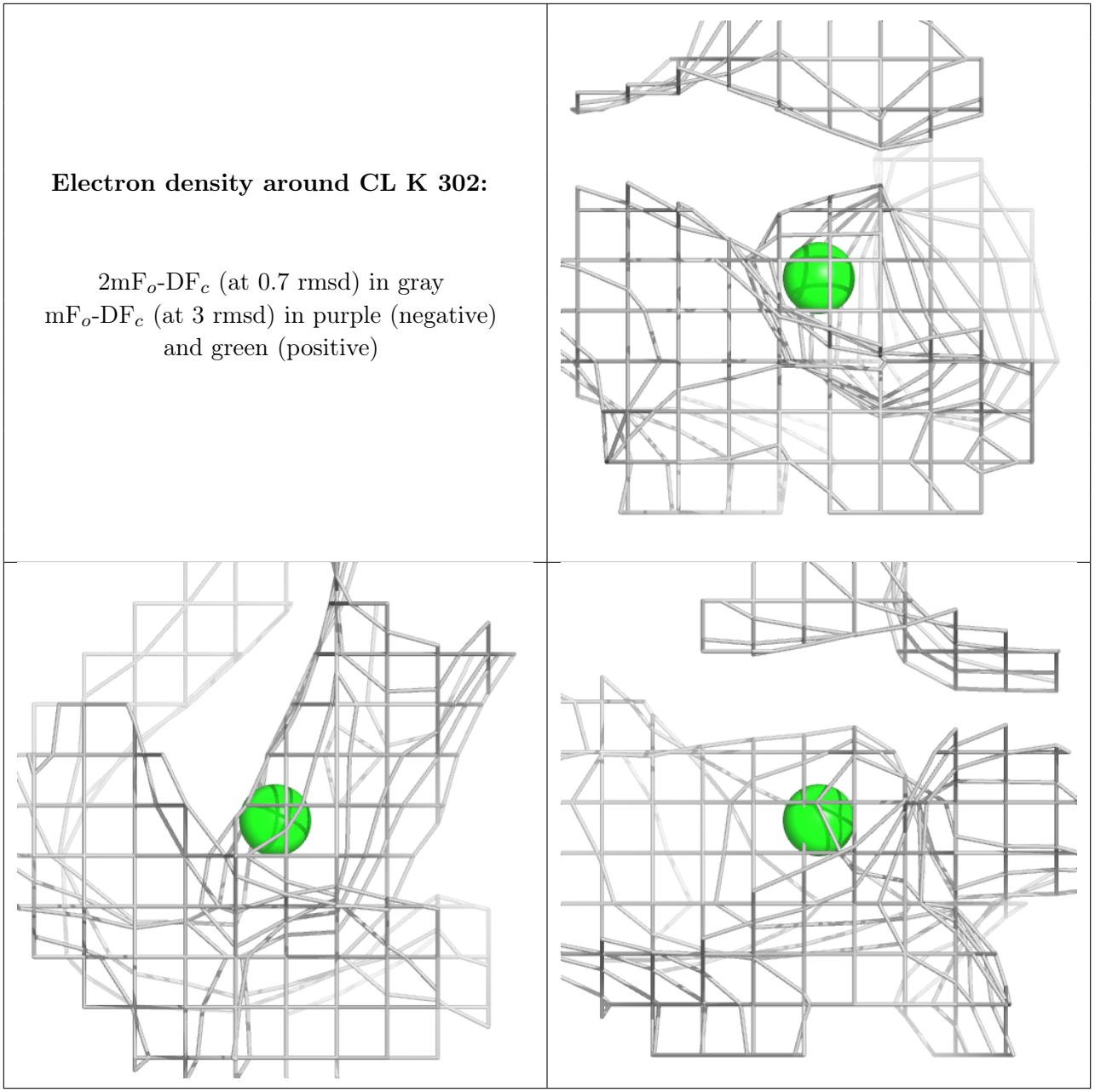






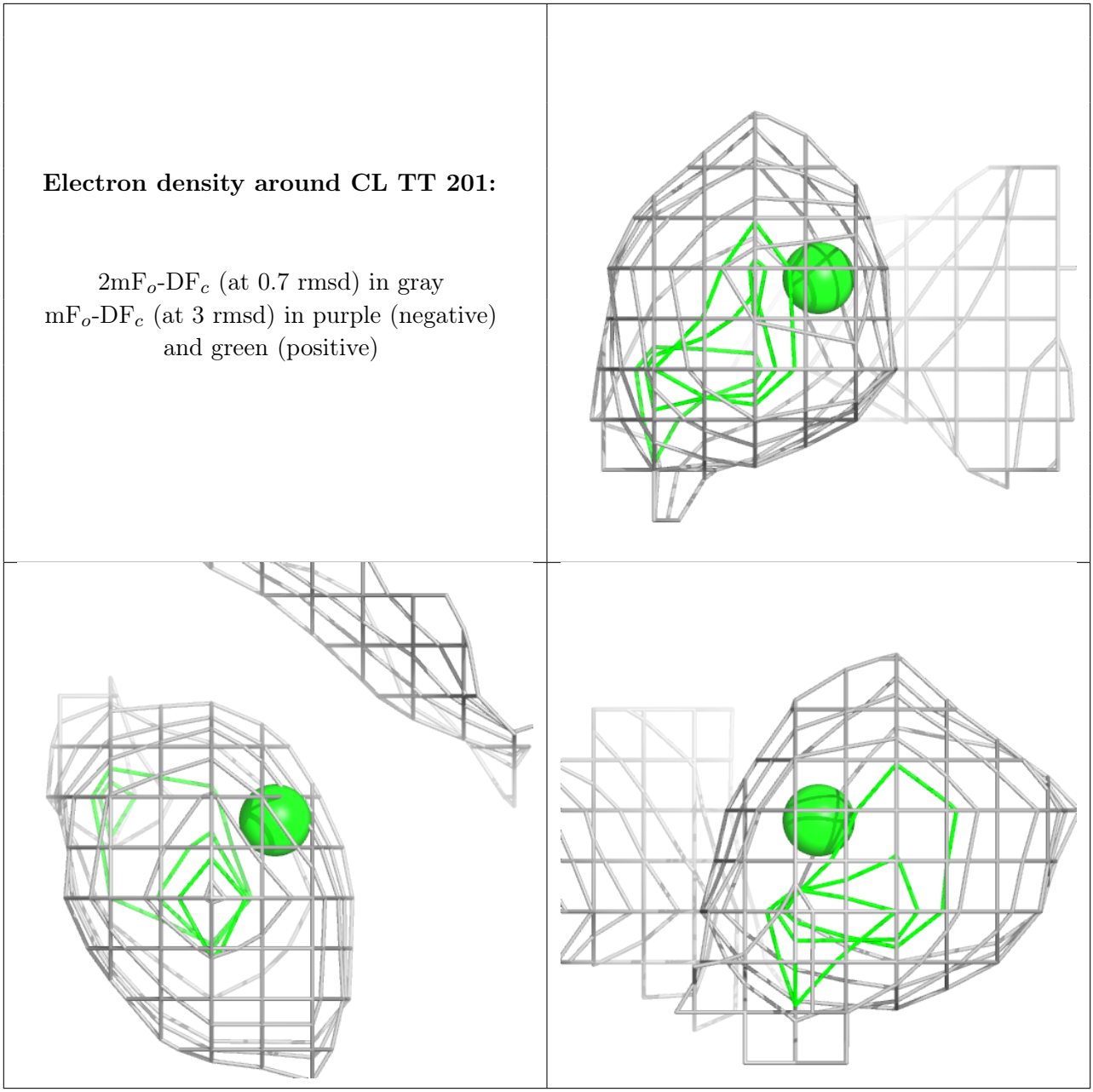
Electron density around CL K 302:

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



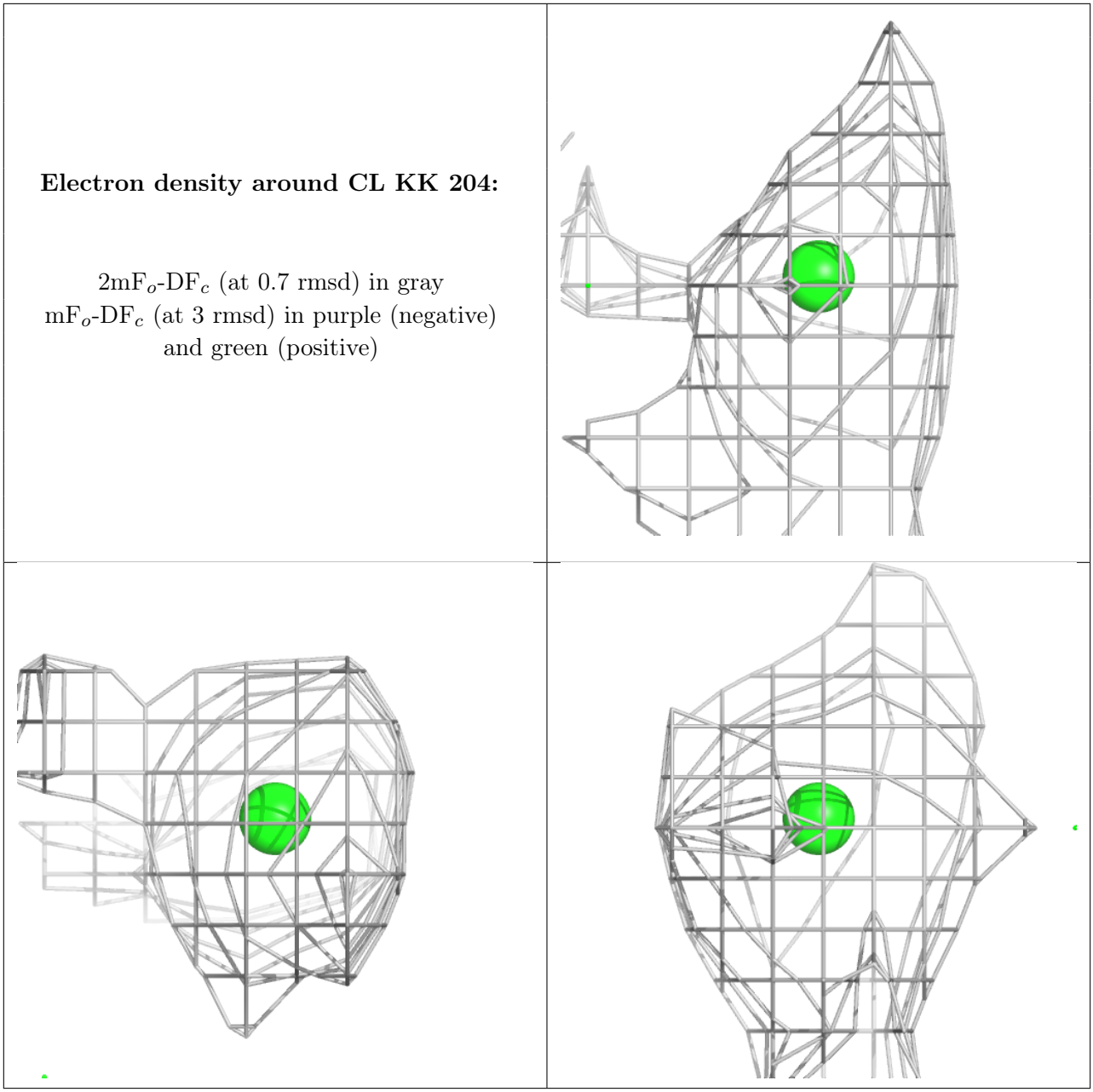
Electron density around CL TT 201:

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



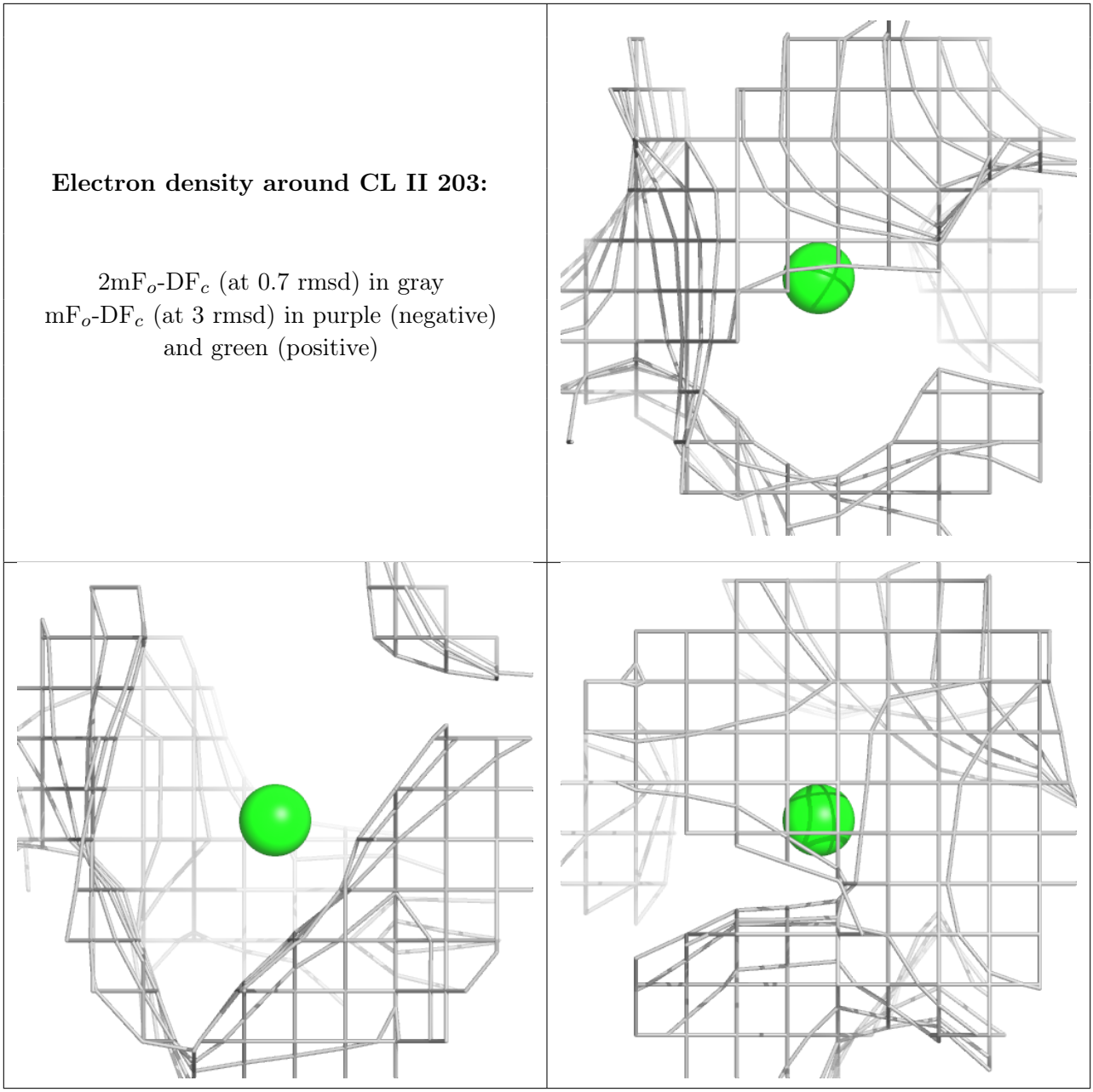
Electron density around CL KK 204:

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



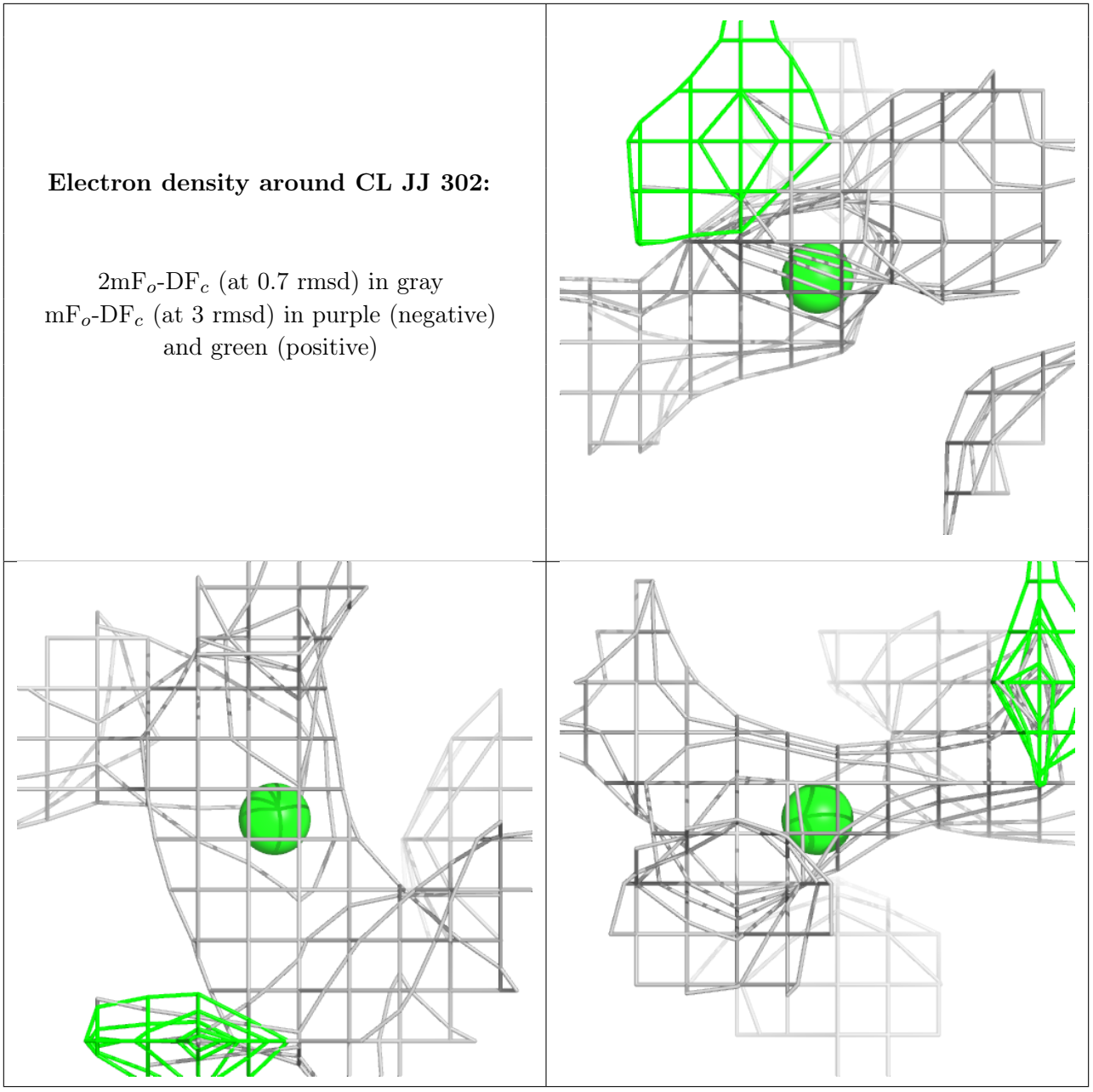
Electron density around CL II 203:

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



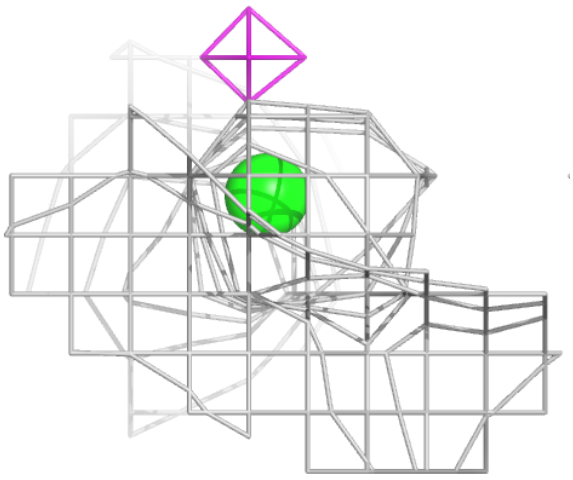
Electron density around CL JJ 302:

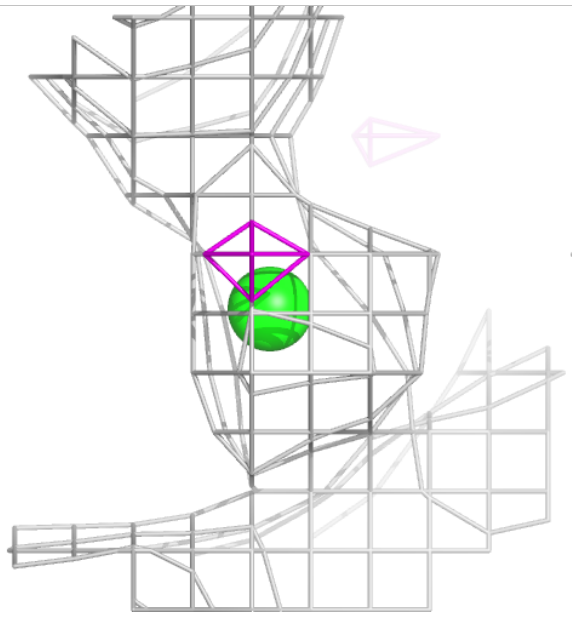
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

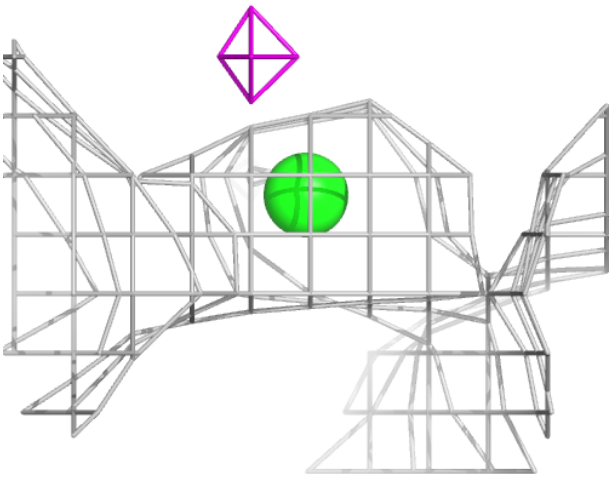


Electron density around CL KK 202:

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

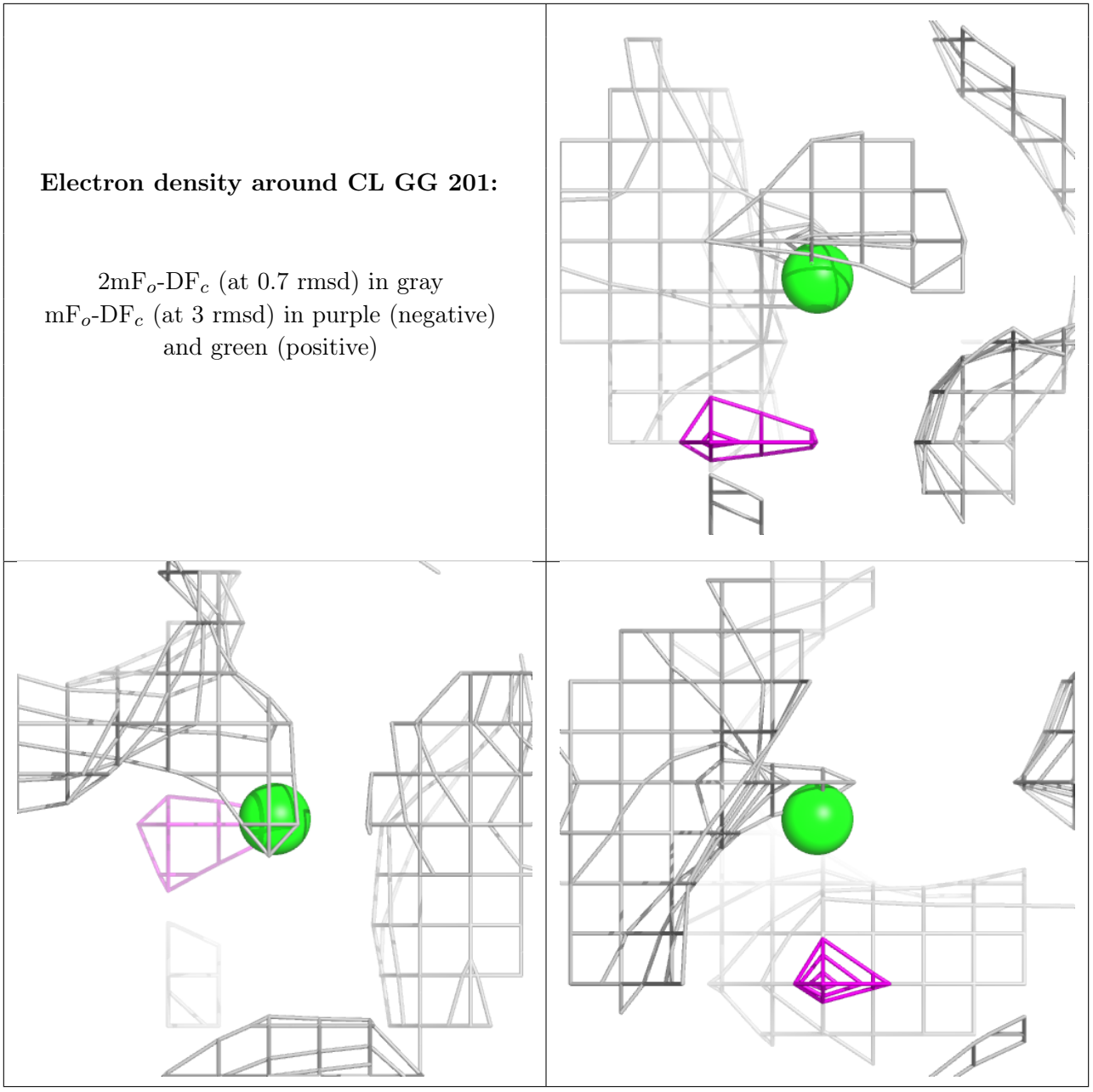






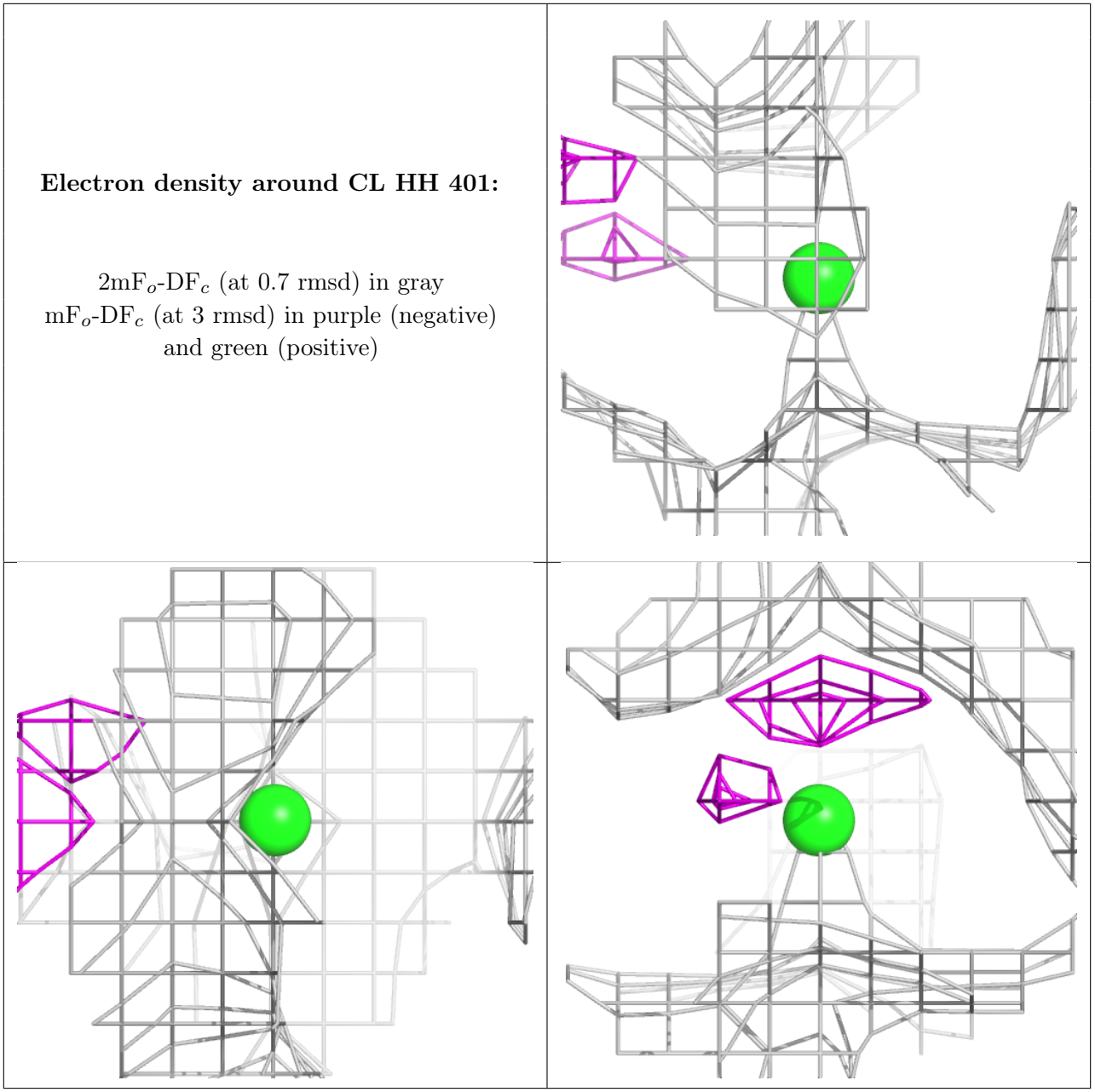
Electron density around CL GG 201:

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



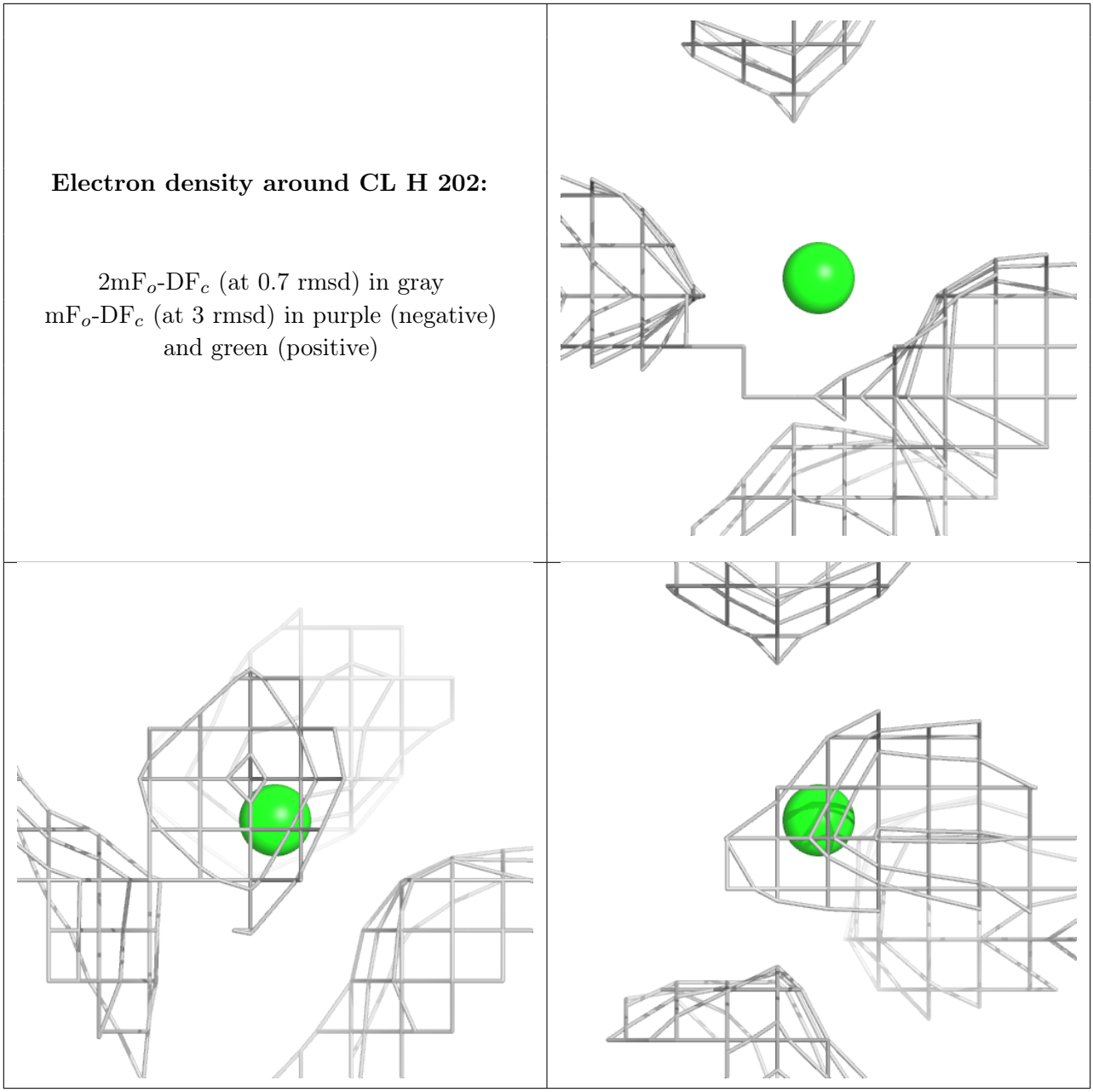
Electron density around CL HH 401:

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



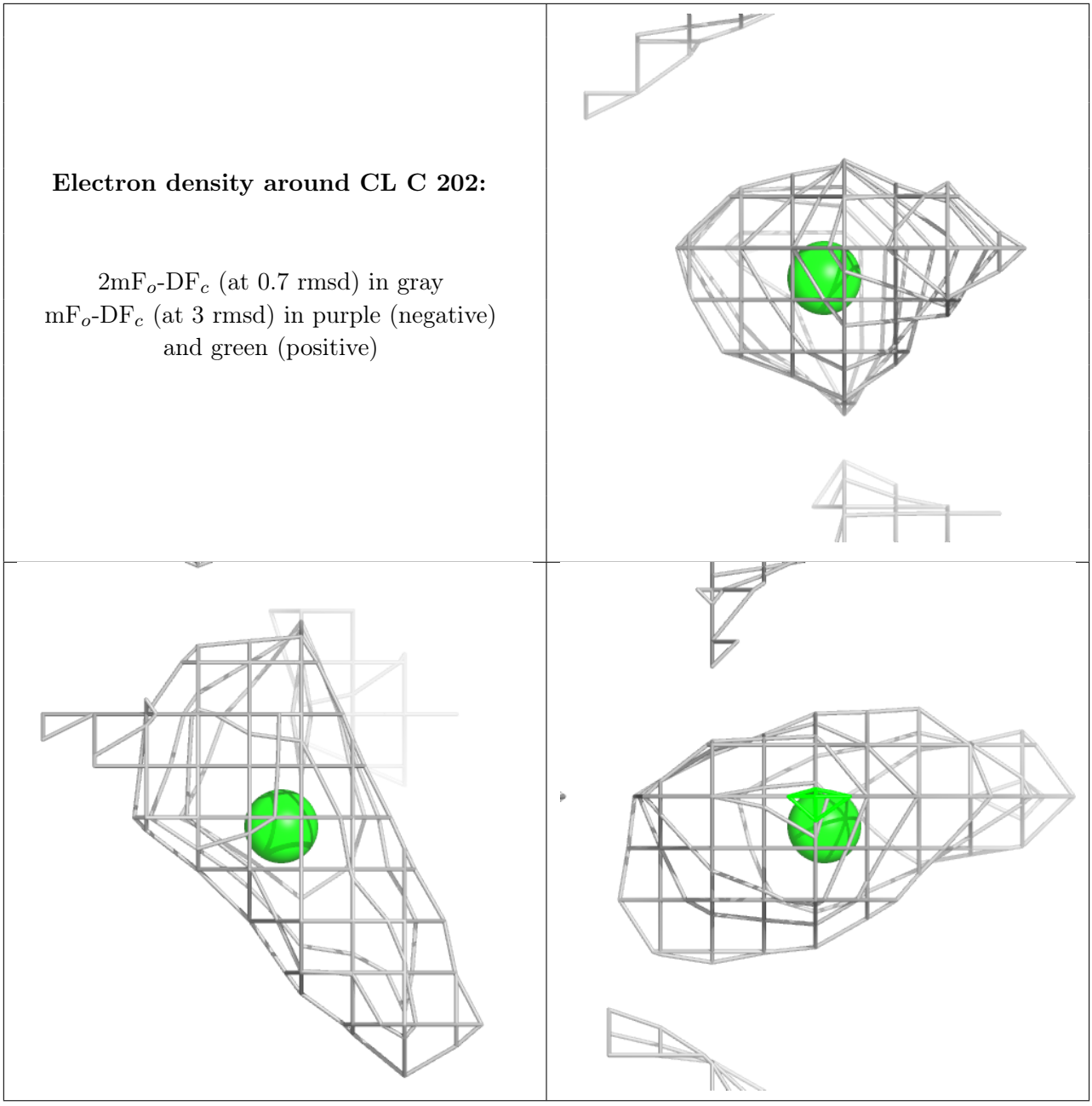
Electron density around CL H 202:

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



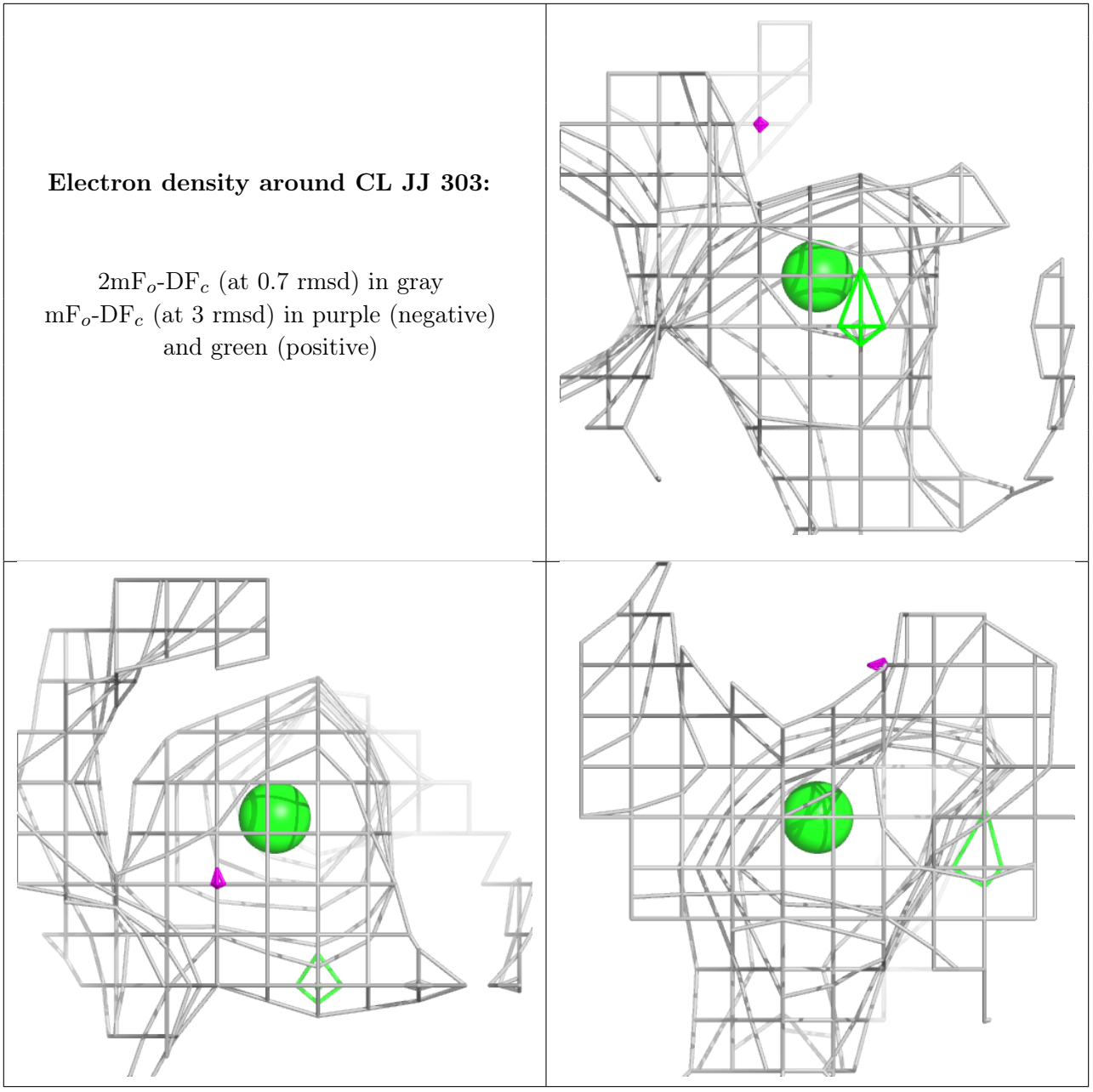
Electron density around CL C 202:

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



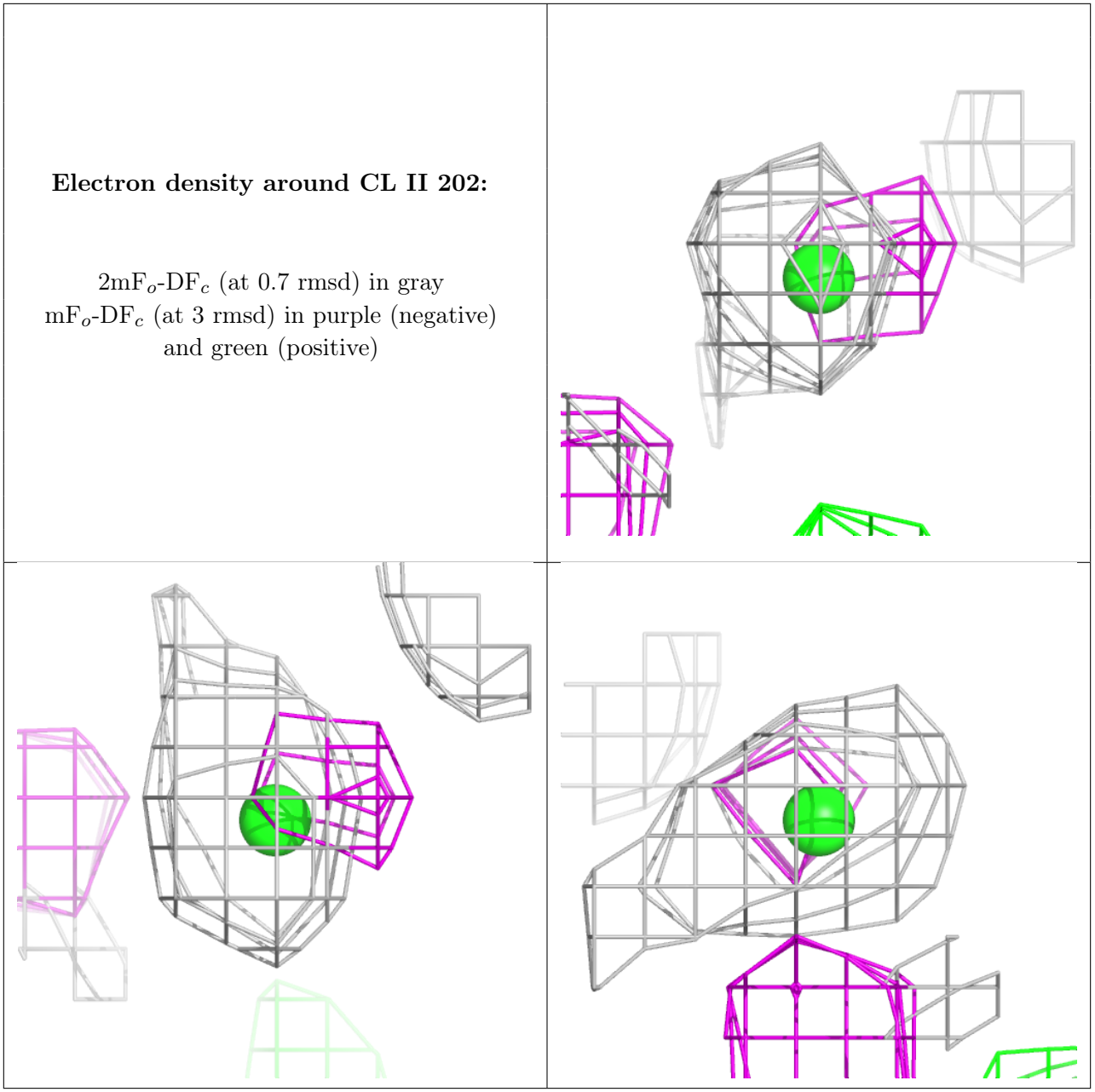
Electron density around CL JJ 303:

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



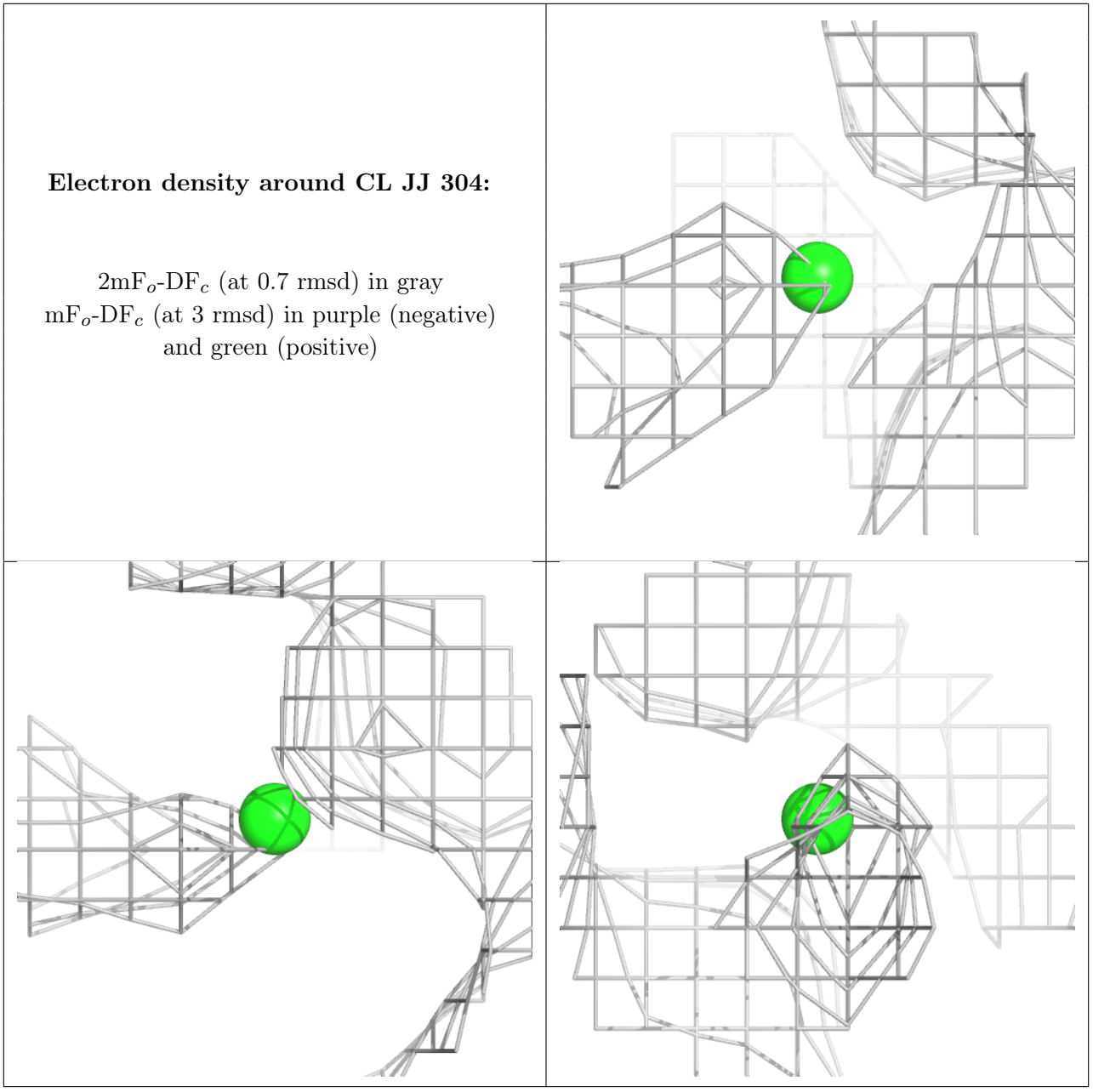
Electron density around CL II 202:

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



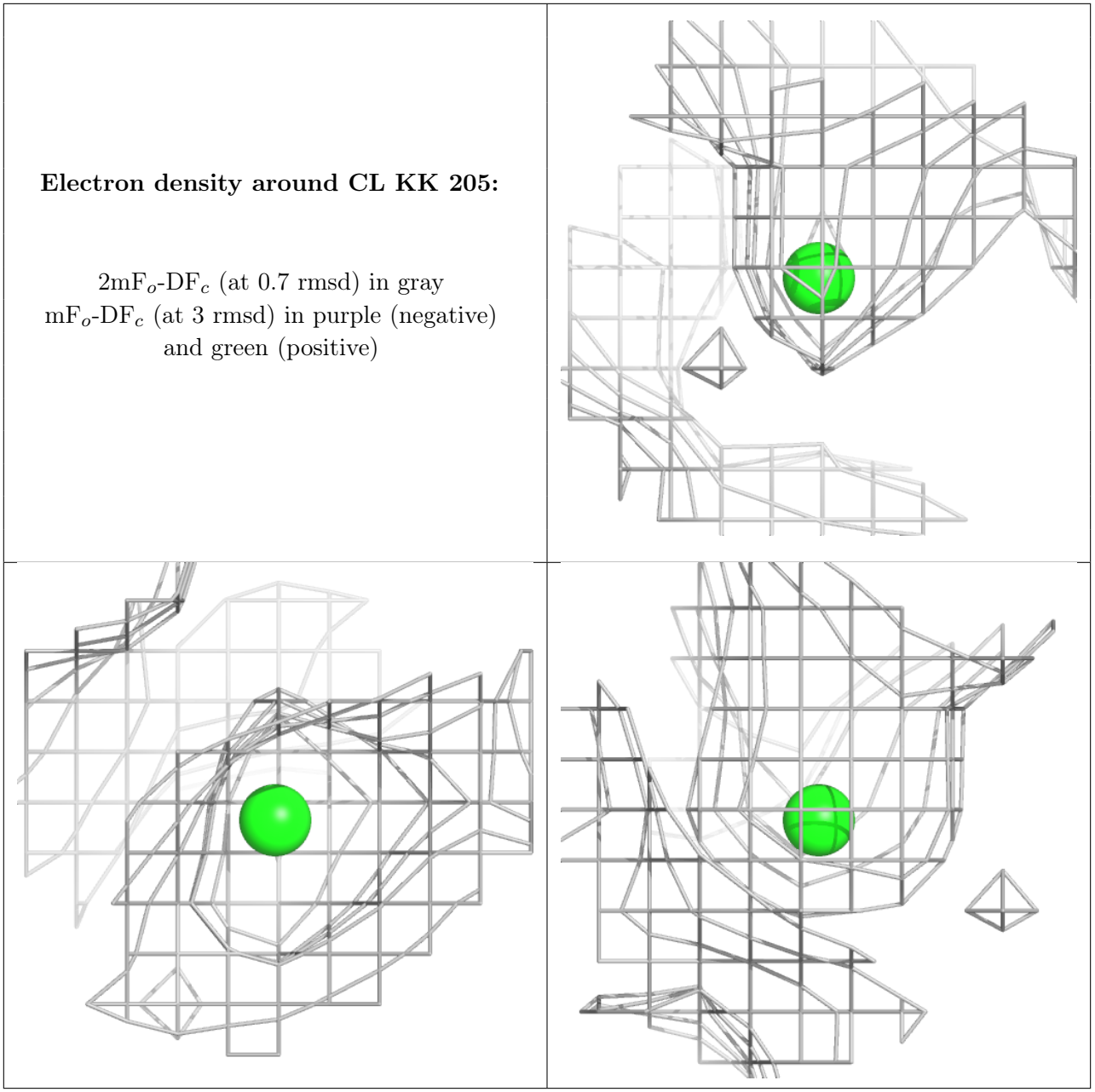
Electron density around CL JJ 304:

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



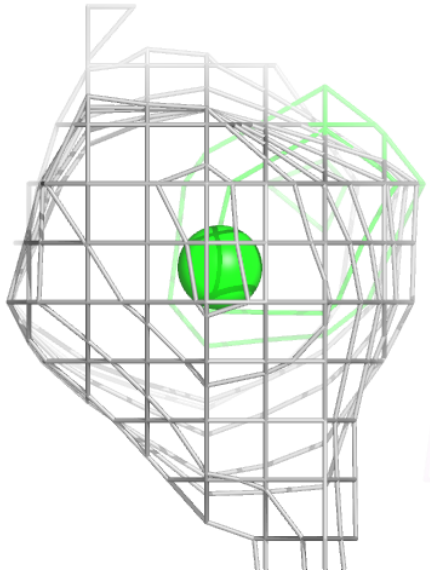
Electron density around CL KK 205:

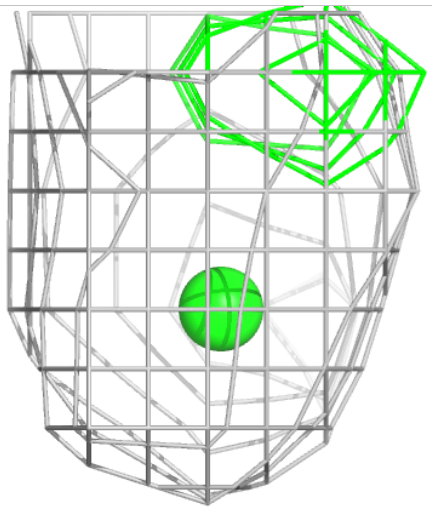
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

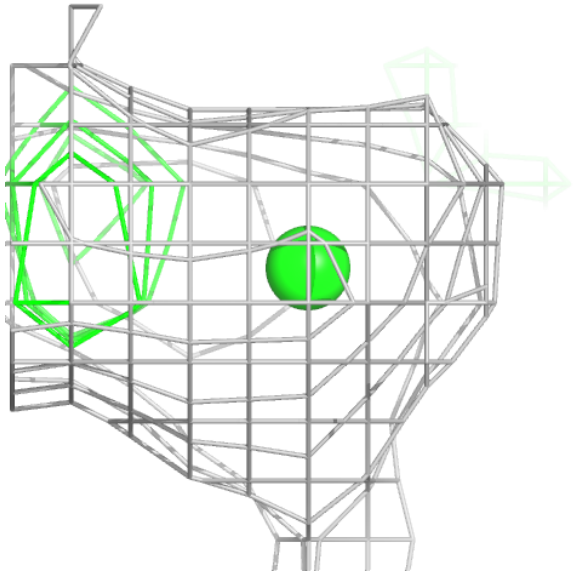


Electron density around CL C 203:

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

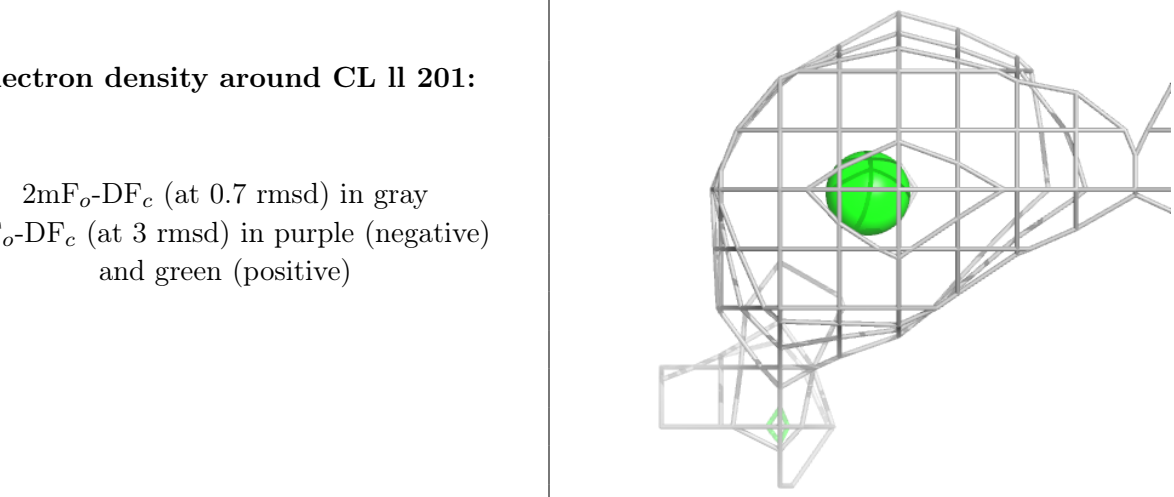


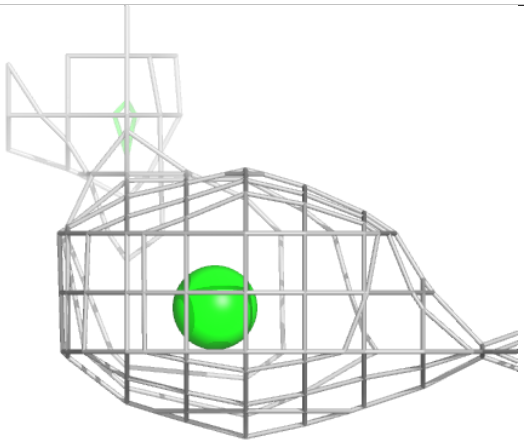


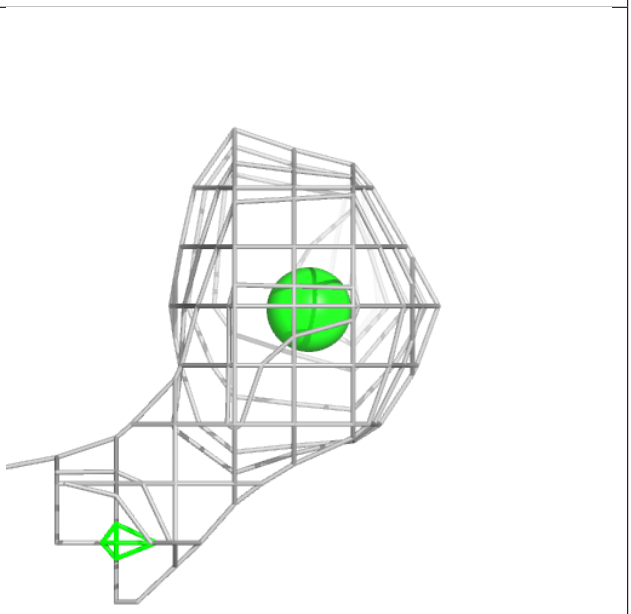


Electron density around CL ll 201:

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

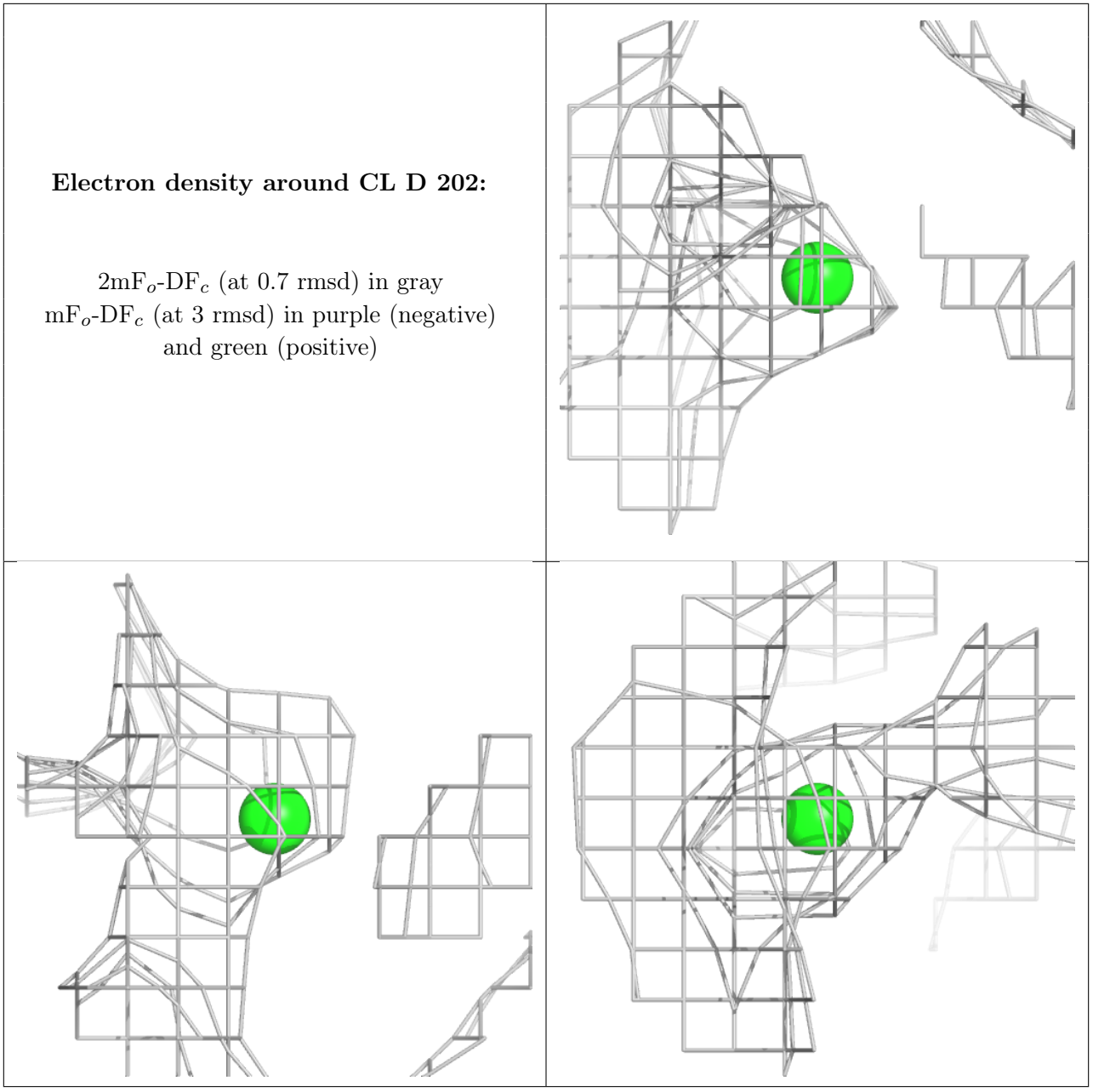






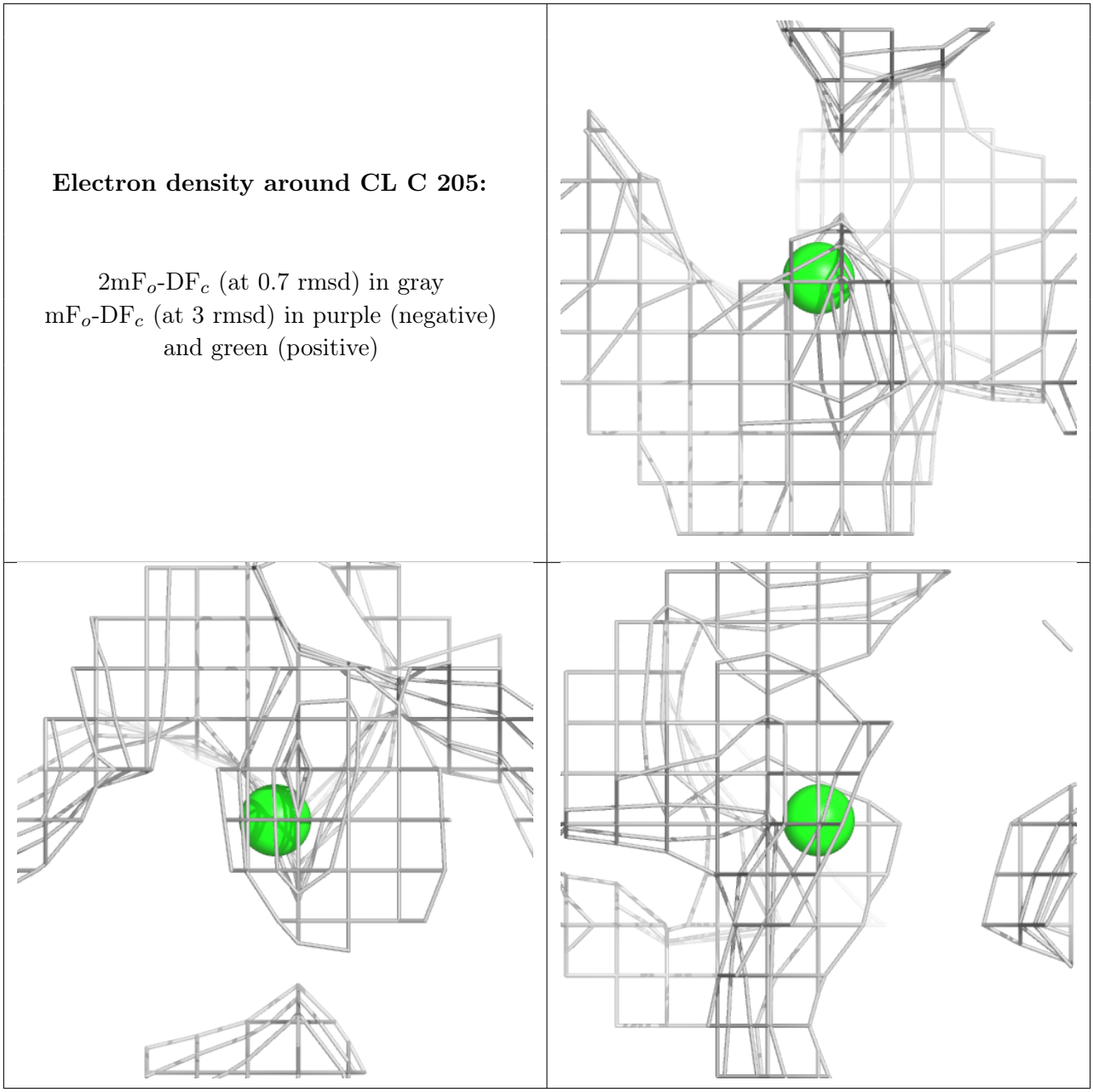
Electron density around CL D 202:

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



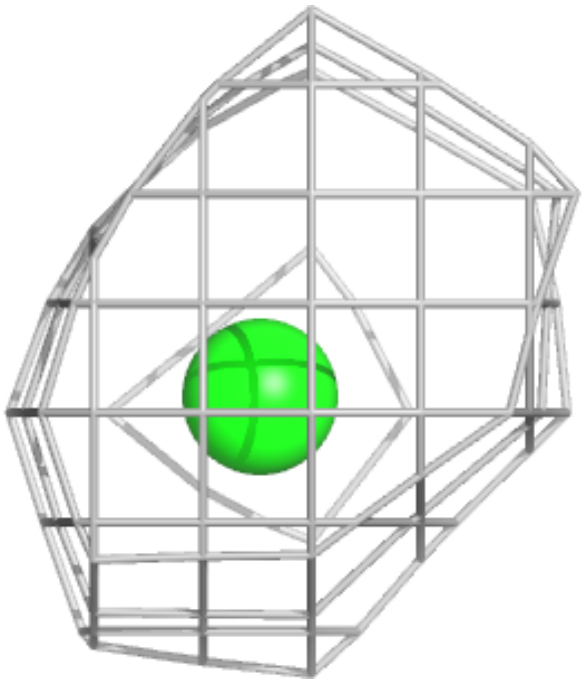
Electron density around CL C 205:

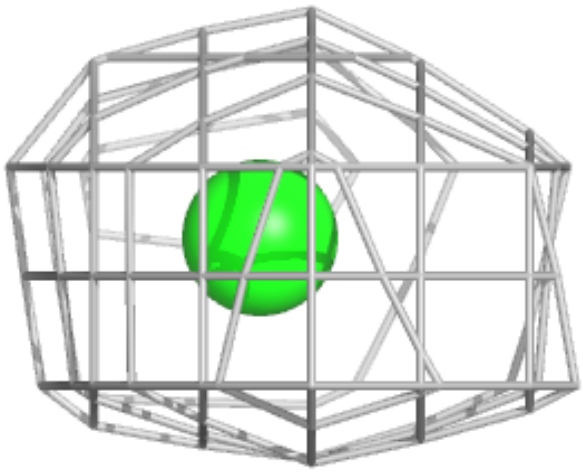
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

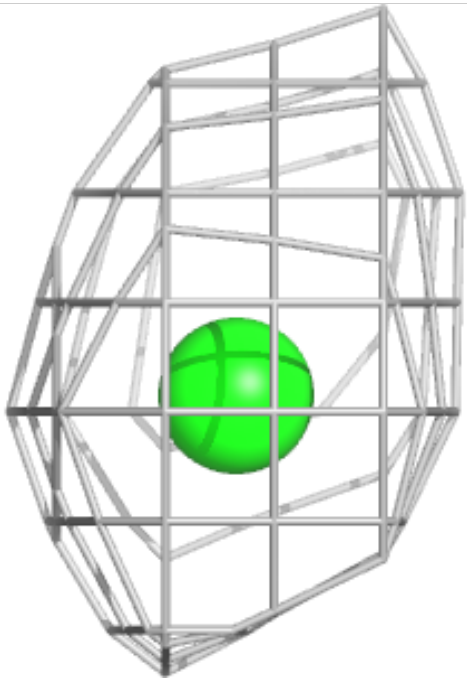


Electron density around CL G 302:

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

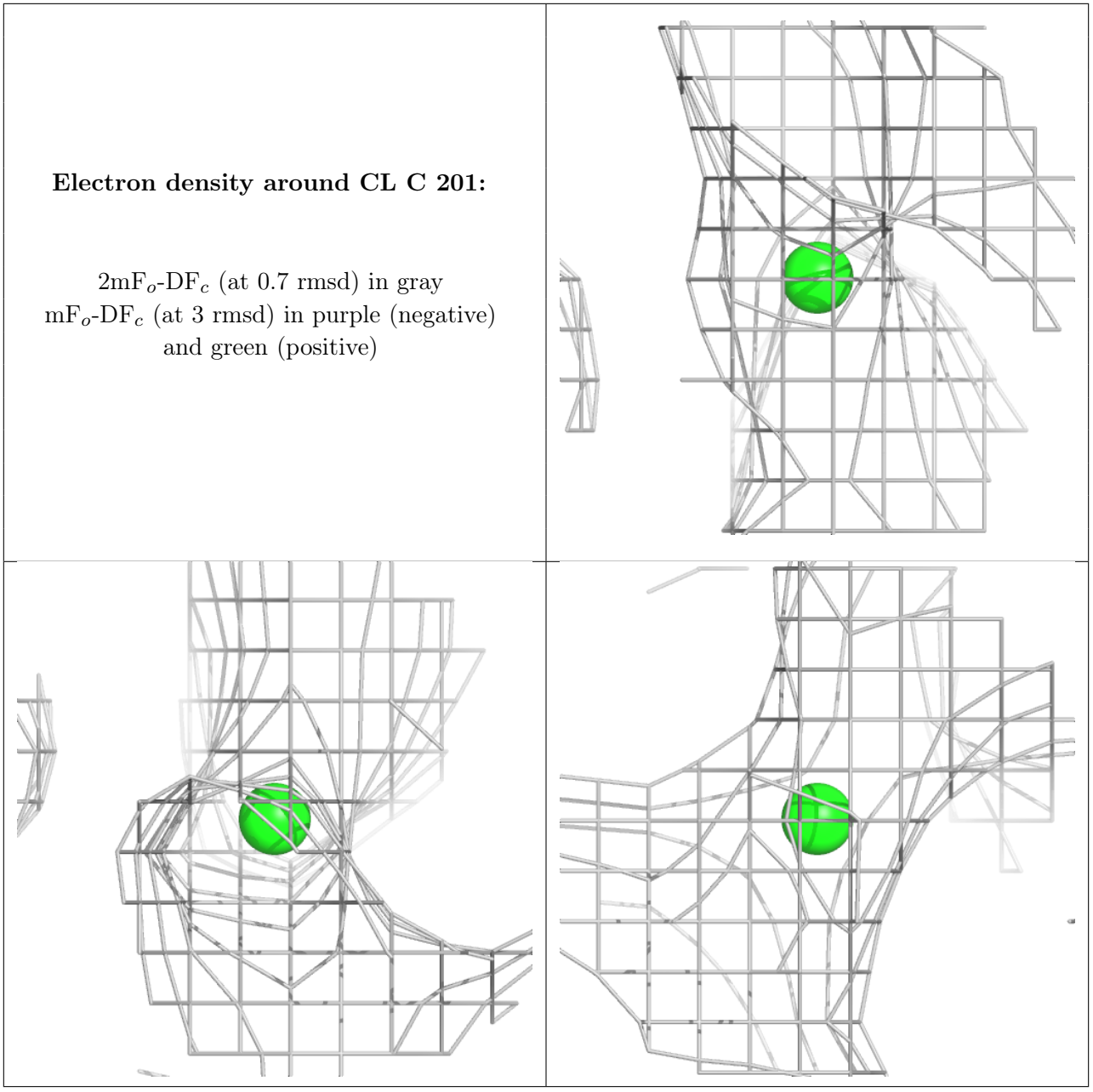






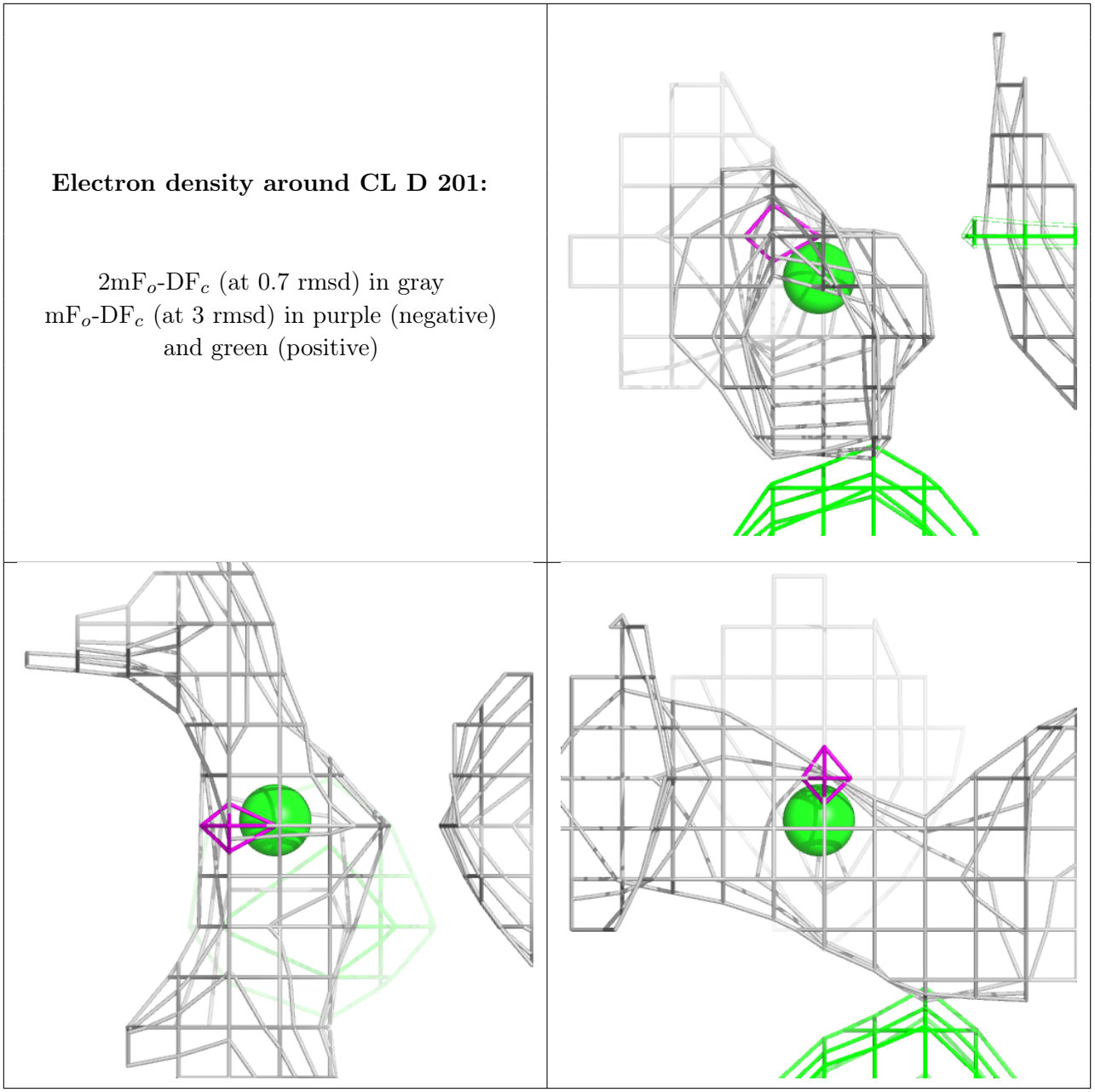
Electron density around CL C 201:

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



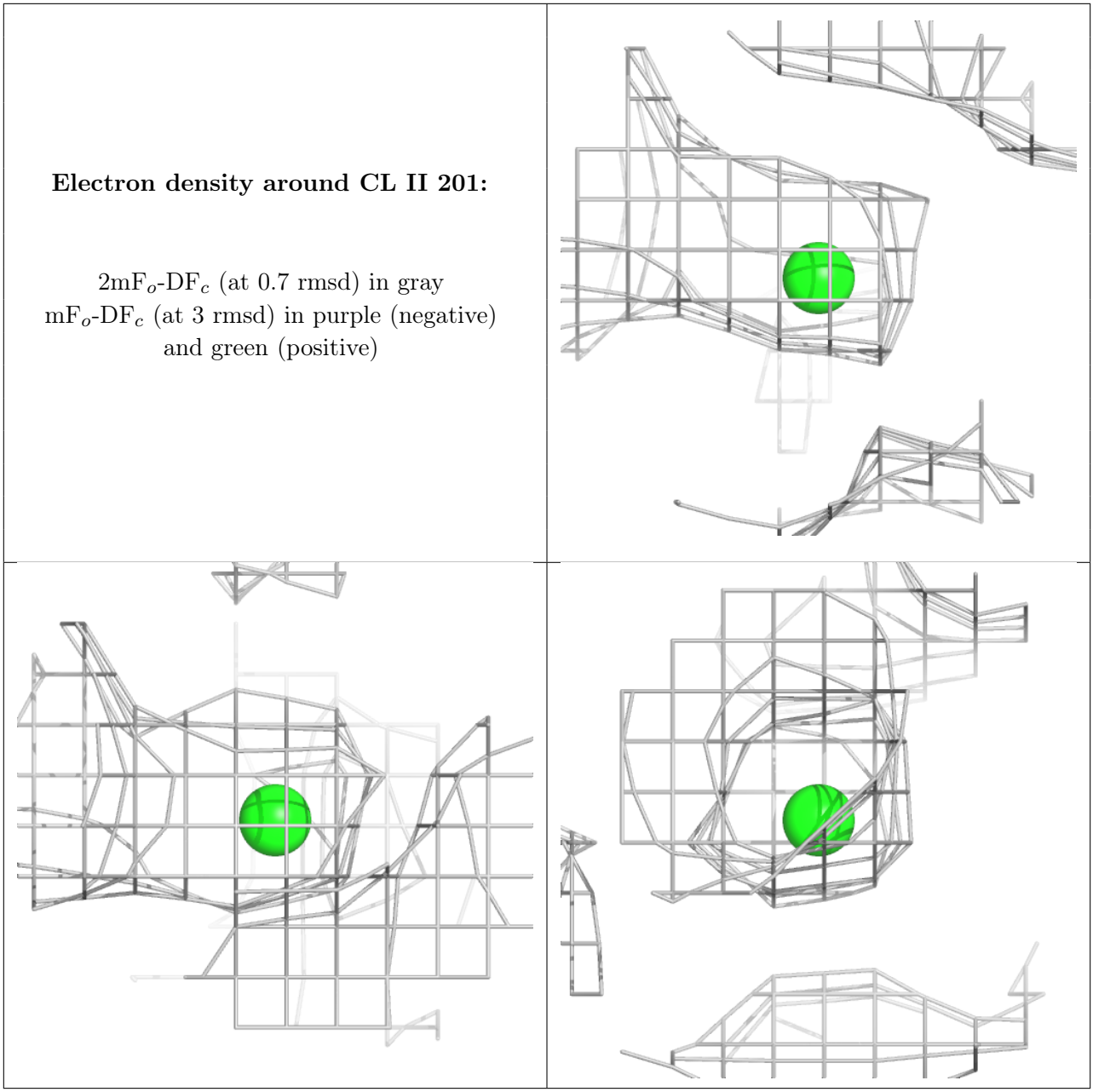
Electron density around CL D 201:

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



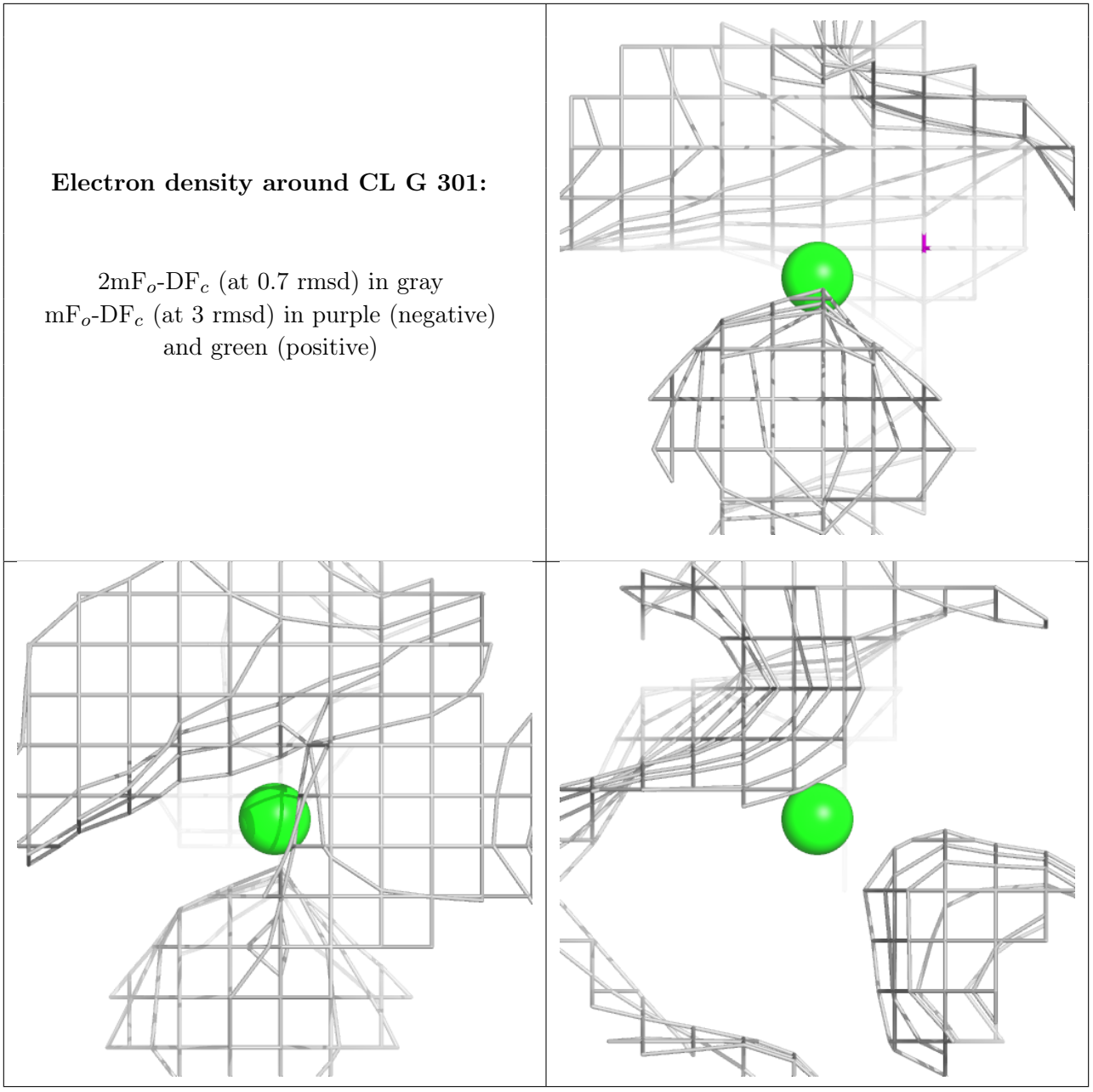
Electron density around CL II 201:

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



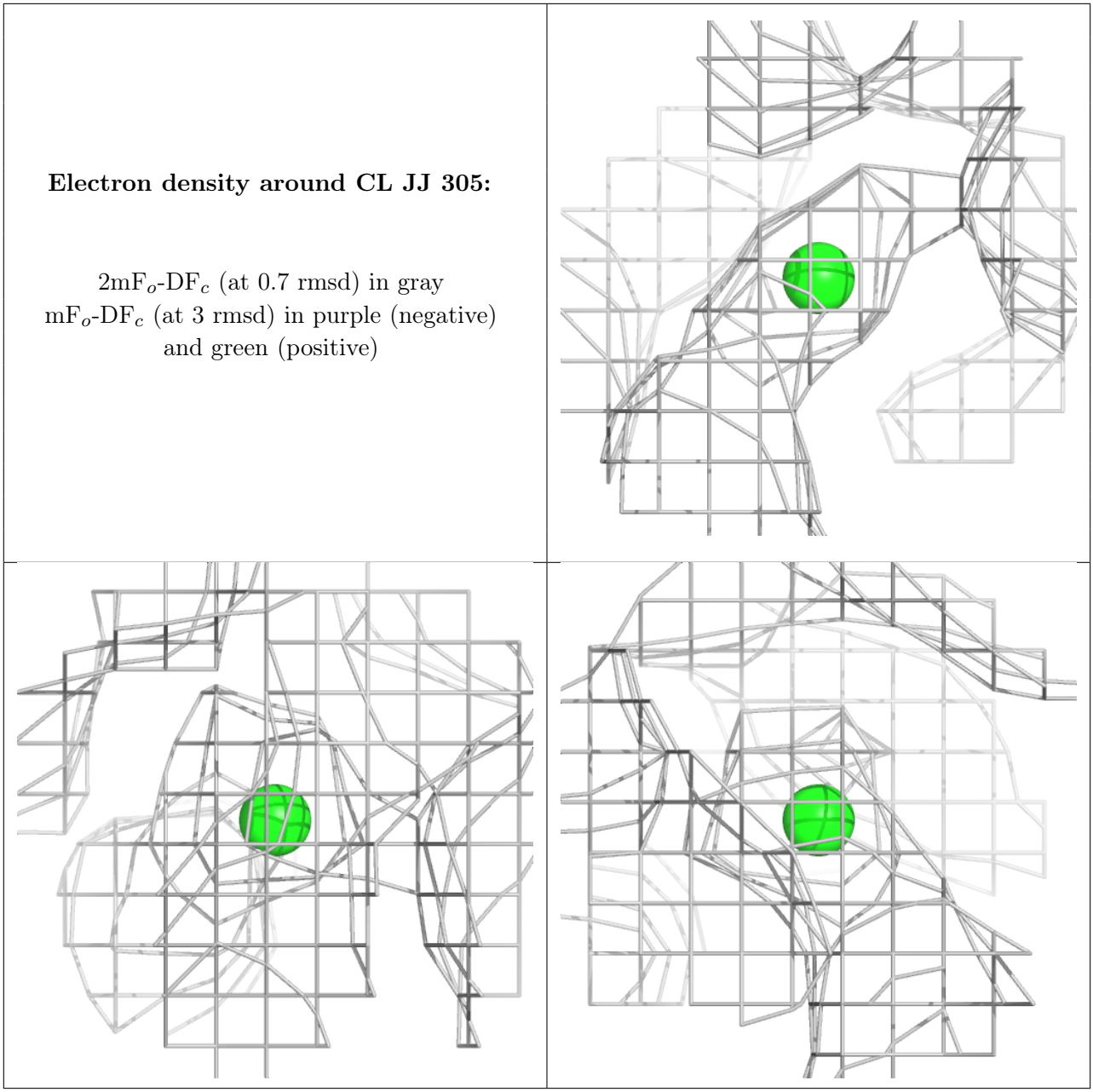
Electron density around CL G 301:

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



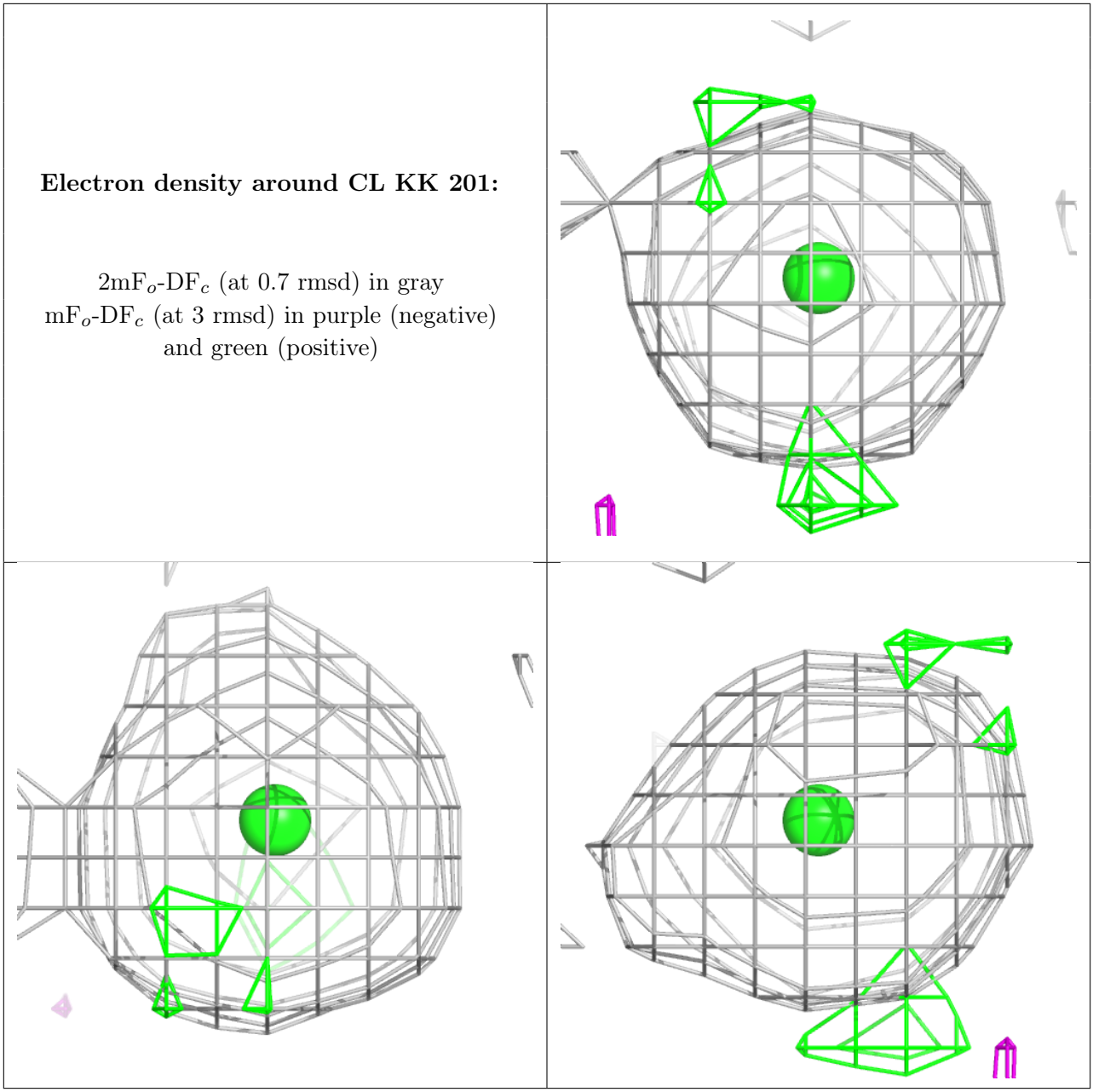
Electron density around CL JJ 305:

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



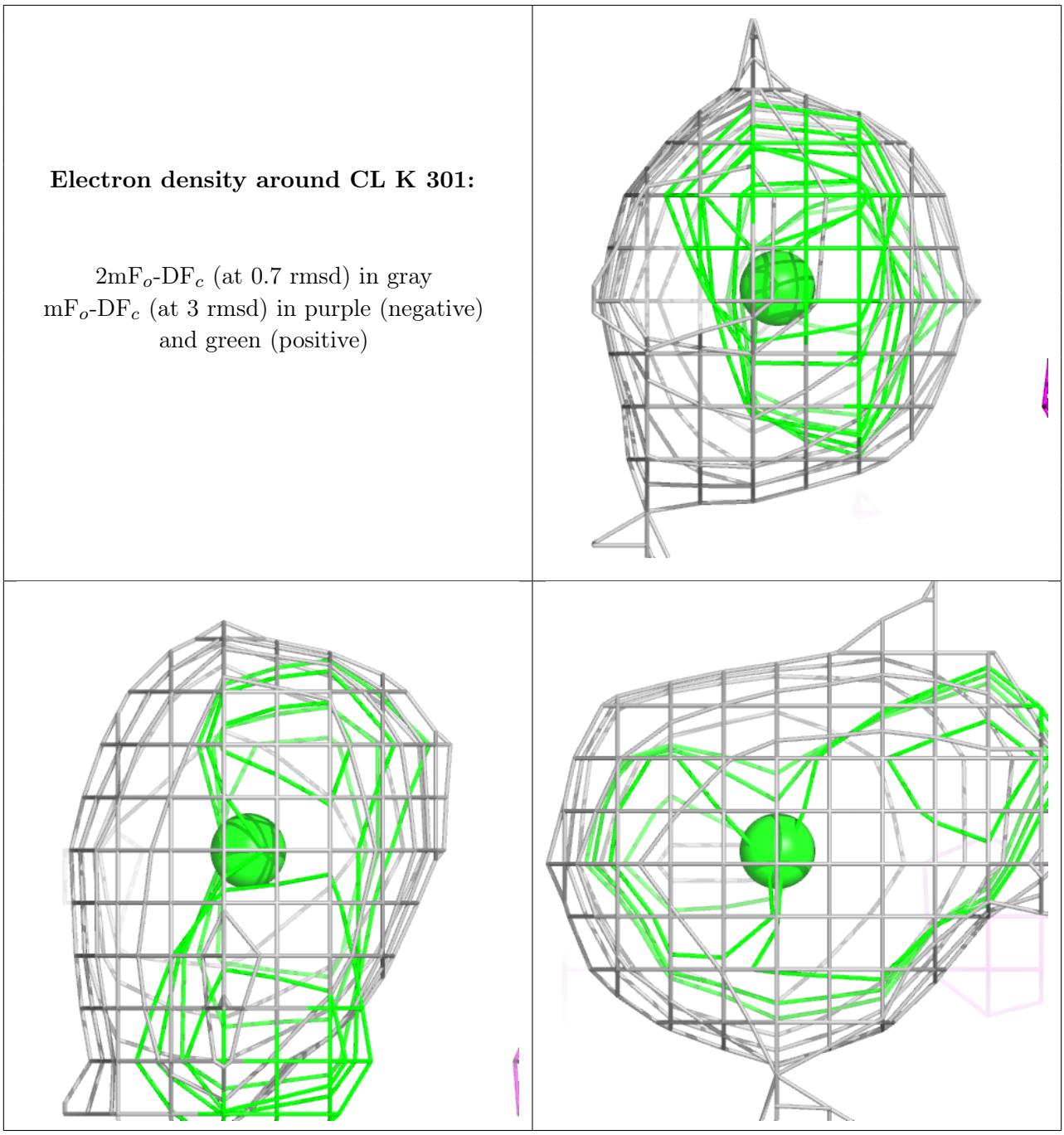
Electron density around CL KK 201:

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



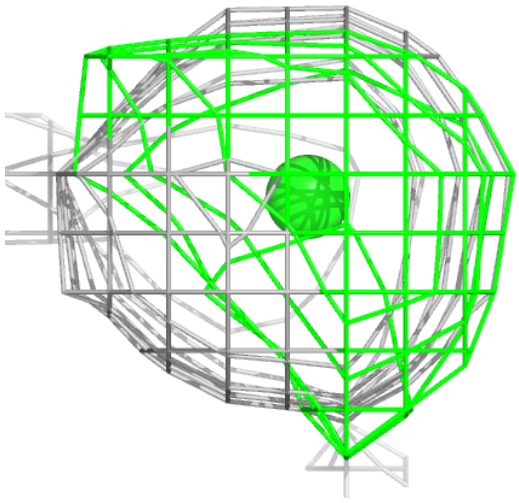
Electron density around CL K 301:

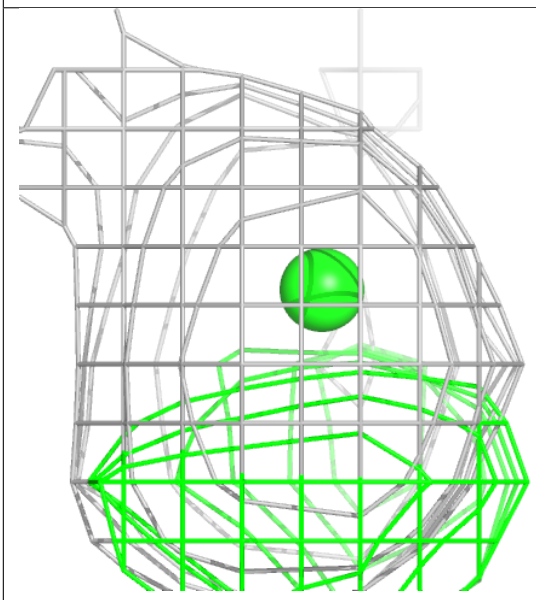
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

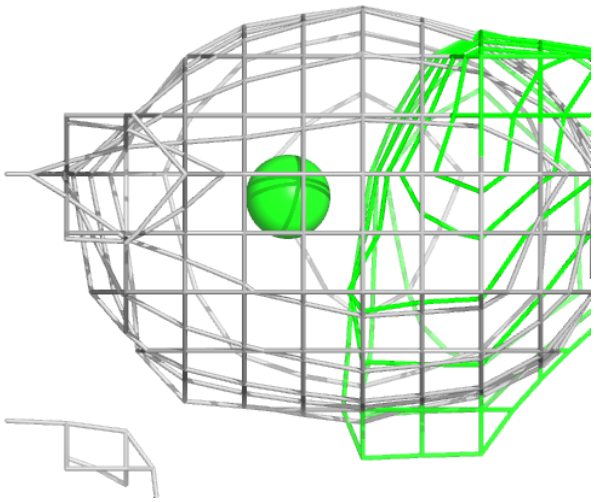


Electron density around CL F 202:

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

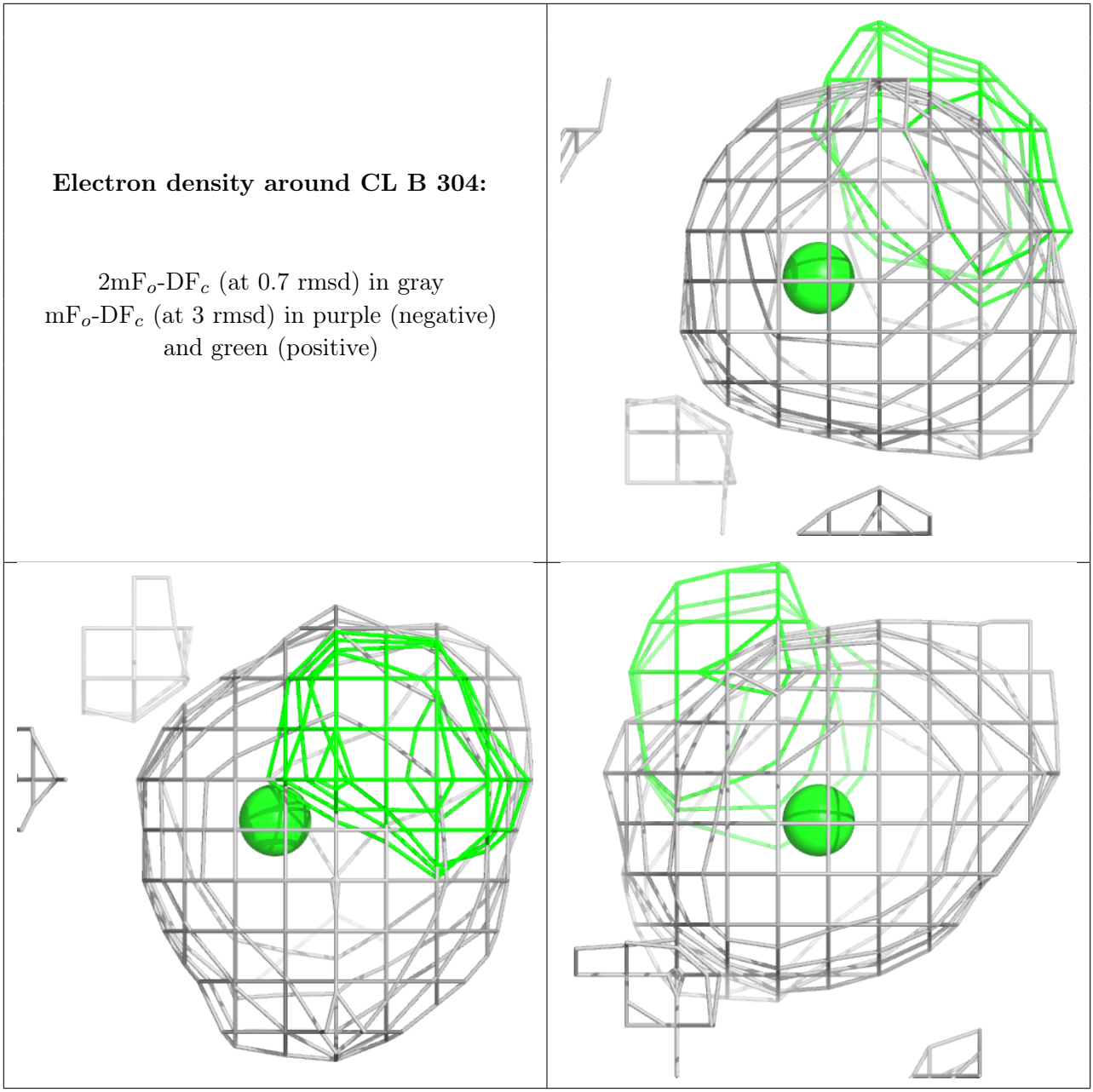






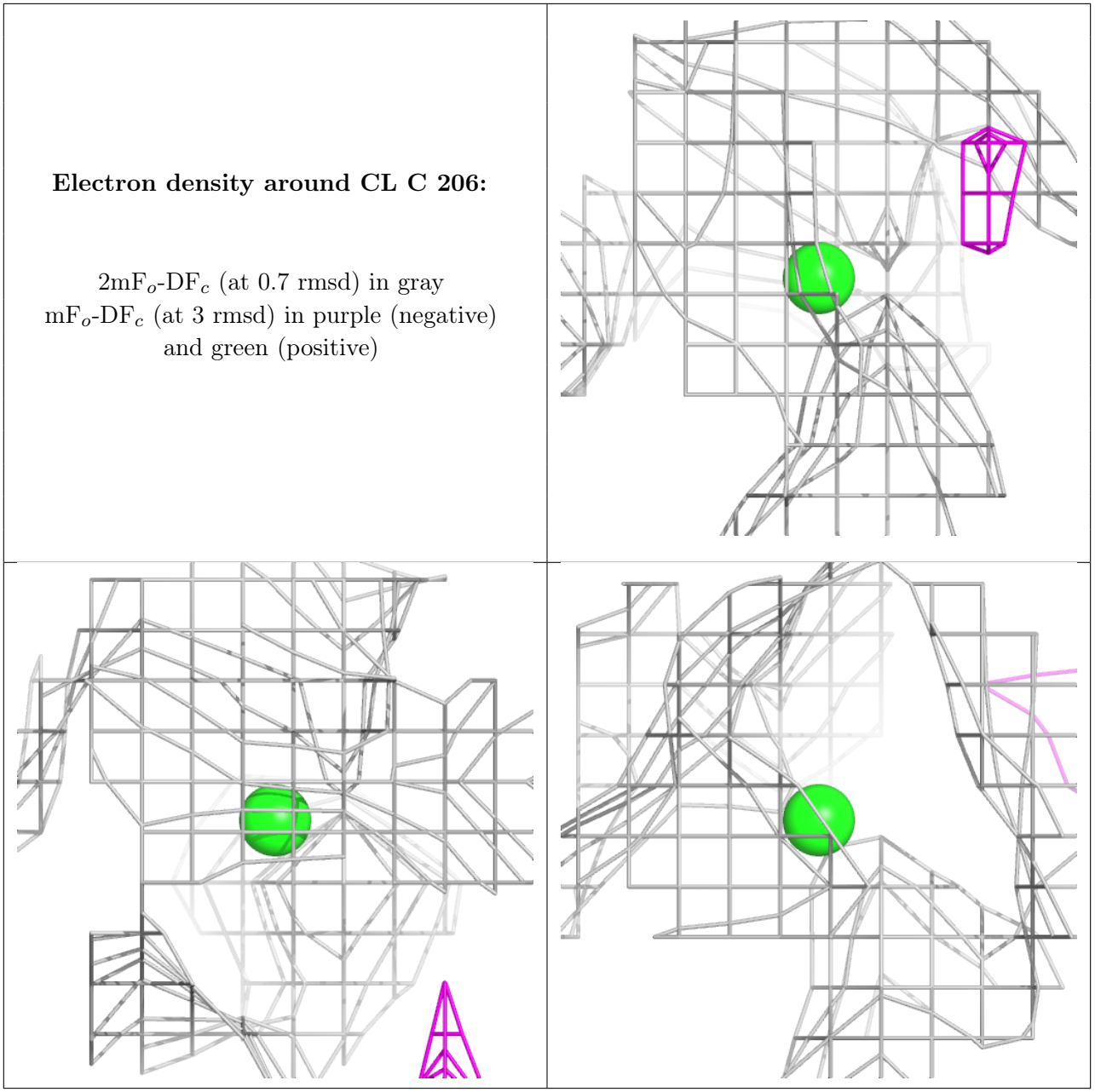
Electron density around CL B 304:

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



Electron density around CL C 206:

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



6.5 Other polymers (i)

There are no such residues in this entry.