wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 06:11 pm BST

PDB ID	:	8AQ6
Title	:	NanoLuc luciferase with bound furimamide in surface allosteric site
Authors	:	Nemergut, M.; Marek, M.
Deposited on	:	2022-08-11
Resolution	:	1.69 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.69 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.219
Clashscore		14
Ramachandran outliers		1.3%
Sidechain outliers		6.0%
RSRZ outliers		6.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
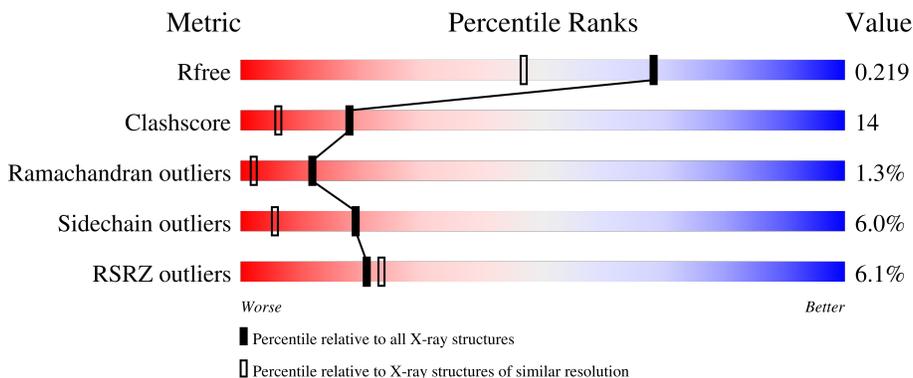
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	181	6% 61% 27% 6% · 6%
1	B	181	4% 72% 20% · 6%
1	C	181	% 69% 21% · 6%
1	D	181	9% 74% 17% ·· 6%
1	E	181	8% 62% 27% ·· 6%

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Mol	Chain	Length	Quality of chain
1	F	181	4% ... 77% ... 17% · 6%
1	G	181	9% ... 73% ... 15% 6% 6%
1	H	181	6% ... 76% ... 13% · · 5%

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
2	GOL	H	201	-	-	X	-
3	PG4	A	204	-	-	X	-
3	PG4	E	201	-	-	X	-
4	OXY	A	205	-	-	X	-
7	NT0	G	301	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11762 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 NanoLuc luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total 1355	C 874	N 226	O 250	S 5	0	1	0
1	B	171	Total 1349	C 871	N 225	O 249	S 4	0	0	0
1	C	171	Total 1349	C 871	N 225	O 249	S 4	0	0	0
1	D	171	Total 1355	C 874	N 226	O 250	S 5	0	1	0
1	E	171	Total 1349	C 871	N 225	O 249	S 4	0	0	0
1	F	171	Total 1357	C 876	N 228	O 249	S 4	0	1	0
1	G	171	Total 1355	C 874	N 226	O 250	S 5	0	1	0
1	H	172	Total 1357	C 875	N 227	O 251	S 4	0	0	0

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9GV45
A	-10	HIS	-	expression tag	UNP Q9GV45
A	-9	HIS	-	expression tag	UNP Q9GV45
A	-8	HIS	-	expression tag	UNP Q9GV45
A	-7	HIS	-	expression tag	UNP Q9GV45
A	-6	HIS	-	expression tag	UNP Q9GV45
A	-5	HIS	-	expression tag	UNP Q9GV45
A	-4	SER	-	expression tag	UNP Q9GV45
A	-3	ASP	-	expression tag	UNP Q9GV45
A	-2	ASN	-	expression tag	UNP Q9GV45
A	-1	MET	-	expression tag	UNP Q9GV45
A	0	VAL	-	expression tag	UNP Q9GV45
A	4	GLU	ALA	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ARG	GLN	engineered mutation	UNP Q9GV45
A	18	LEU	GLN	engineered mutation	UNP Q9GV45
A	27	VAL	LEU	engineered mutation	UNP Q9GV45
A	33	ASN	ALA	engineered mutation	UNP Q9GV45
A	43	ARG	LYS	engineered mutation	UNP Q9GV45
A	44	ILE	VAL	engineered mutation	UNP Q9GV45
A	54	ILE	ALA	engineered mutation	UNP Q9GV45
A	68	ASP	PHE	engineered mutation	UNP Q9GV45
A	72	GLN	LEU	engineered mutation	UNP Q9GV45
A	75	LYS	MET	engineered mutation	UNP Q9GV45
A	90	VAL	ILE	engineered mutation	UNP Q9GV45
A	115	GLU	PRO	engineered mutation	UNP Q9GV45
A	124	LYS	GLN	engineered mutation	UNP Q9GV45
A	138	ILE	TYR	engineered mutation	UNP Q9GV45
A	166	ARG	ASN	engineered mutation	UNP Q9GV45
B	-11	MET	-	initiating methionine	UNP Q9GV45
B	-10	HIS	-	expression tag	UNP Q9GV45
B	-9	HIS	-	expression tag	UNP Q9GV45
B	-8	HIS	-	expression tag	UNP Q9GV45
B	-7	HIS	-	expression tag	UNP Q9GV45
B	-6	HIS	-	expression tag	UNP Q9GV45
B	-5	HIS	-	expression tag	UNP Q9GV45
B	-4	SER	-	expression tag	UNP Q9GV45
B	-3	ASP	-	expression tag	UNP Q9GV45
B	-2	ASN	-	expression tag	UNP Q9GV45
B	-1	MET	-	expression tag	UNP Q9GV45
B	0	VAL	-	expression tag	UNP Q9GV45
B	4	GLU	ALA	engineered mutation	UNP Q9GV45
B	11	ARG	GLN	engineered mutation	UNP Q9GV45
B	18	LEU	GLN	engineered mutation	UNP Q9GV45
B	27	VAL	LEU	engineered mutation	UNP Q9GV45
B	33	ASN	ALA	engineered mutation	UNP Q9GV45
B	43	ARG	LYS	engineered mutation	UNP Q9GV45
B	44	ILE	VAL	engineered mutation	UNP Q9GV45
B	54	ILE	ALA	engineered mutation	UNP Q9GV45
B	68	ASP	PHE	engineered mutation	UNP Q9GV45
B	72	GLN	LEU	engineered mutation	UNP Q9GV45
B	75	LYS	MET	engineered mutation	UNP Q9GV45
B	90	VAL	ILE	engineered mutation	UNP Q9GV45
B	115	GLU	PRO	engineered mutation	UNP Q9GV45
B	124	LYS	GLN	engineered mutation	UNP Q9GV45
B	138	ILE	TYR	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
B	166	ARG	ASN	engineered mutation	UNP Q9GV45
C	-11	MET	-	initiating methionine	UNP Q9GV45
C	-10	HIS	-	expression tag	UNP Q9GV45
C	-9	HIS	-	expression tag	UNP Q9GV45
C	-8	HIS	-	expression tag	UNP Q9GV45
C	-7	HIS	-	expression tag	UNP Q9GV45
C	-6	HIS	-	expression tag	UNP Q9GV45
C	-5	HIS	-	expression tag	UNP Q9GV45
C	-4	SER	-	expression tag	UNP Q9GV45
C	-3	ASP	-	expression tag	UNP Q9GV45
C	-2	ASN	-	expression tag	UNP Q9GV45
C	-1	MET	-	expression tag	UNP Q9GV45
C	0	VAL	-	expression tag	UNP Q9GV45
C	4	GLU	ALA	engineered mutation	UNP Q9GV45
C	11	ARG	GLN	engineered mutation	UNP Q9GV45
C	18	LEU	GLN	engineered mutation	UNP Q9GV45
C	27	VAL	LEU	engineered mutation	UNP Q9GV45
C	33	ASN	ALA	engineered mutation	UNP Q9GV45
C	43	ARG	LYS	engineered mutation	UNP Q9GV45
C	44	ILE	VAL	engineered mutation	UNP Q9GV45
C	54	ILE	ALA	engineered mutation	UNP Q9GV45
C	68	ASP	PHE	engineered mutation	UNP Q9GV45
C	72	GLN	LEU	engineered mutation	UNP Q9GV45
C	75	LYS	MET	engineered mutation	UNP Q9GV45
C	90	VAL	ILE	engineered mutation	UNP Q9GV45
C	115	GLU	PRO	engineered mutation	UNP Q9GV45
C	124	LYS	GLN	engineered mutation	UNP Q9GV45
C	138	ILE	TYR	engineered mutation	UNP Q9GV45
C	166	ARG	ASN	engineered mutation	UNP Q9GV45
D	-11	MET	-	initiating methionine	UNP Q9GV45
D	-10	HIS	-	expression tag	UNP Q9GV45
D	-9	HIS	-	expression tag	UNP Q9GV45
D	-8	HIS	-	expression tag	UNP Q9GV45
D	-7	HIS	-	expression tag	UNP Q9GV45
D	-6	HIS	-	expression tag	UNP Q9GV45
D	-5	HIS	-	expression tag	UNP Q9GV45
D	-4	SER	-	expression tag	UNP Q9GV45
D	-3	ASP	-	expression tag	UNP Q9GV45
D	-2	ASN	-	expression tag	UNP Q9GV45
D	-1	MET	-	expression tag	UNP Q9GV45
D	0	VAL	-	expression tag	UNP Q9GV45
D	4	GLU	ALA	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
D	11	ARG	GLN	engineered mutation	UNP Q9GV45
D	18	LEU	GLN	engineered mutation	UNP Q9GV45
D	27	VAL	LEU	engineered mutation	UNP Q9GV45
D	33	ASN	ALA	engineered mutation	UNP Q9GV45
D	43	ARG	LYS	engineered mutation	UNP Q9GV45
D	44	ILE	VAL	engineered mutation	UNP Q9GV45
D	54	ILE	ALA	engineered mutation	UNP Q9GV45
D	68	ASP	PHE	engineered mutation	UNP Q9GV45
D	72	GLN	LEU	engineered mutation	UNP Q9GV45
D	75	LYS	MET	engineered mutation	UNP Q9GV45
D	90	VAL	ILE	engineered mutation	UNP Q9GV45
D	115	GLU	PRO	engineered mutation	UNP Q9GV45
D	124	LYS	GLN	engineered mutation	UNP Q9GV45
D	138	ILE	TYR	engineered mutation	UNP Q9GV45
D	166	ARG	ASN	engineered mutation	UNP Q9GV45
E	-11	MET	-	initiating methionine	UNP Q9GV45
E	-10	HIS	-	expression tag	UNP Q9GV45
E	-9	HIS	-	expression tag	UNP Q9GV45
E	-8	HIS	-	expression tag	UNP Q9GV45
E	-7	HIS	-	expression tag	UNP Q9GV45
E	-6	HIS	-	expression tag	UNP Q9GV45
E	-5	HIS	-	expression tag	UNP Q9GV45
E	-4	SER	-	expression tag	UNP Q9GV45
E	-3	ASP	-	expression tag	UNP Q9GV45
E	-2	ASN	-	expression tag	UNP Q9GV45
E	-1	MET	-	expression tag	UNP Q9GV45
E	0	VAL	-	expression tag	UNP Q9GV45
E	4	GLU	ALA	engineered mutation	UNP Q9GV45
E	11	ARG	GLN	engineered mutation	UNP Q9GV45
E	18	LEU	GLN	engineered mutation	UNP Q9GV45
E	27	VAL	LEU	engineered mutation	UNP Q9GV45
E	33	ASN	ALA	engineered mutation	UNP Q9GV45
E	43	ARG	LYS	engineered mutation	UNP Q9GV45
E	44	ILE	VAL	engineered mutation	UNP Q9GV45
E	54	ILE	ALA	engineered mutation	UNP Q9GV45
E	68	ASP	PHE	engineered mutation	UNP Q9GV45
E	72	GLN	LEU	engineered mutation	UNP Q9GV45
E	75	LYS	MET	engineered mutation	UNP Q9GV45
E	90	VAL	ILE	engineered mutation	UNP Q9GV45
E	115	GLU	PRO	engineered mutation	UNP Q9GV45
E	124	LYS	GLN	engineered mutation	UNP Q9GV45
E	138	ILE	TYR	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
E	166	ARG	ASN	engineered mutation	UNP Q9GV45
F	-11	MET	-	initiating methionine	UNP Q9GV45
F	-10	HIS	-	expression tag	UNP Q9GV45
F	-9	HIS	-	expression tag	UNP Q9GV45
F	-8	HIS	-	expression tag	UNP Q9GV45
F	-7	HIS	-	expression tag	UNP Q9GV45
F	-6	HIS	-	expression tag	UNP Q9GV45
F	-5	HIS	-	expression tag	UNP Q9GV45
F	-4	SER	-	expression tag	UNP Q9GV45
F	-3	ASP	-	expression tag	UNP Q9GV45
F	-2	ASN	-	expression tag	UNP Q9GV45
F	-1	MET	-	expression tag	UNP Q9GV45
F	0	VAL	-	expression tag	UNP Q9GV45
F	4	GLU	ALA	engineered mutation	UNP Q9GV45
F	11	ARG	GLN	engineered mutation	UNP Q9GV45
F	18	LEU	GLN	engineered mutation	UNP Q9GV45
F	27	VAL	LEU	engineered mutation	UNP Q9GV45
F	33	ASN	ALA	engineered mutation	UNP Q9GV45
F	43	ARG	LYS	engineered mutation	UNP Q9GV45
F	44	ILE	VAL	engineered mutation	UNP Q9GV45
F	54	ILE	ALA	engineered mutation	UNP Q9GV45
F	68	ASP	PHE	engineered mutation	UNP Q9GV45
F	72	GLN	LEU	engineered mutation	UNP Q9GV45
F	75	LYS	MET	engineered mutation	UNP Q9GV45
F	90	VAL	ILE	engineered mutation	UNP Q9GV45
F	115	GLU	PRO	engineered mutation	UNP Q9GV45
F	124	LYS	GLN	engineered mutation	UNP Q9GV45
F	138	ILE	TYR	engineered mutation	UNP Q9GV45
F	166	ARG	ASN	engineered mutation	UNP Q9GV45
G	-11	MET	-	initiating methionine	UNP Q9GV45
G	-10	HIS	-	expression tag	UNP Q9GV45
G	-9	HIS	-	expression tag	UNP Q9GV45
G	-8	HIS	-	expression tag	UNP Q9GV45
G	-7	HIS	-	expression tag	UNP Q9GV45
G	-6	HIS	-	expression tag	UNP Q9GV45
G	-5	HIS	-	expression tag	UNP Q9GV45
G	-4	SER	-	expression tag	UNP Q9GV45
G	-3	ASP	-	expression tag	UNP Q9GV45
G	-2	ASN	-	expression tag	UNP Q9GV45
G	-1	MET	-	expression tag	UNP Q9GV45
G	0	VAL	-	expression tag	UNP Q9GV45
G	4	GLU	ALA	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
G	11	ARG	GLN	engineered mutation	UNP Q9GV45
G	18	LEU	GLN	engineered mutation	UNP Q9GV45
G	27	VAL	LEU	engineered mutation	UNP Q9GV45
G	33	ASN	ALA	engineered mutation	UNP Q9GV45
G	43	ARG	LYS	engineered mutation	UNP Q9GV45
G	44	ILE	VAL	engineered mutation	UNP Q9GV45
G	54	ILE	ALA	engineered mutation	UNP Q9GV45
G	68	ASP	PHE	engineered mutation	UNP Q9GV45
G	72	GLN	LEU	engineered mutation	UNP Q9GV45
G	75	LYS	MET	engineered mutation	UNP Q9GV45
G	90	VAL	ILE	engineered mutation	UNP Q9GV45
G	115	GLU	PRO	engineered mutation	UNP Q9GV45
G	124	LYS	GLN	engineered mutation	UNP Q9GV45
G	138	ILE	TYR	engineered mutation	UNP Q9GV45
G	166	ARG	ASN	engineered mutation	UNP Q9GV45
H	-11	MET	-	initiating methionine	UNP Q9GV45
H	-10	HIS	-	expression tag	UNP Q9GV45
H	-9	HIS	-	expression tag	UNP Q9GV45
H	-8	HIS	-	expression tag	UNP Q9GV45
H	-7	HIS	-	expression tag	UNP Q9GV45
H	-6	HIS	-	expression tag	UNP Q9GV45
H	-5	HIS	-	expression tag	UNP Q9GV45
H	-4	SER	-	expression tag	UNP Q9GV45
H	-3	ASP	-	expression tag	UNP Q9GV45
H	-2	ASN	-	expression tag	UNP Q9GV45
H	-1	MET	-	expression tag	UNP Q9GV45
H	0	VAL	-	expression tag	UNP Q9GV45
H	4	GLU	ALA	engineered mutation	UNP Q9GV45
H	11	ARG	GLN	engineered mutation	UNP Q9GV45
H	18	LEU	GLN	engineered mutation	UNP Q9GV45
H	27	VAL	LEU	engineered mutation	UNP Q9GV45
H	33	ASN	ALA	engineered mutation	UNP Q9GV45
H	43	ARG	LYS	engineered mutation	UNP Q9GV45
H	44	ILE	VAL	engineered mutation	UNP Q9GV45
H	54	ILE	ALA	engineered mutation	UNP Q9GV45
H	68	ASP	PHE	engineered mutation	UNP Q9GV45
H	72	GLN	LEU	engineered mutation	UNP Q9GV45
H	75	LYS	MET	engineered mutation	UNP Q9GV45
H	90	VAL	ILE	engineered mutation	UNP Q9GV45
H	115	GLU	PRO	engineered mutation	UNP Q9GV45
H	124	LYS	GLN	engineered mutation	UNP Q9GV45
H	138	ILE	TYR	engineered mutation	UNP Q9GV45

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| Chain	Residue	Modelled	Actual	Comment	Reference
H	166	ARG	ASN	engineered mutation	UNP Q9GV45

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).
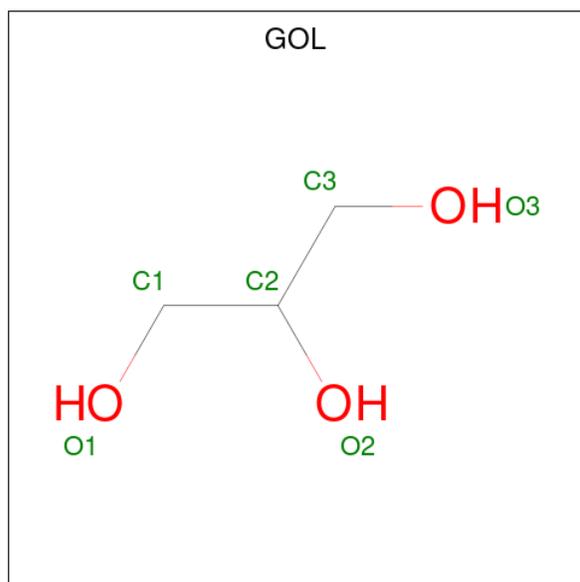
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	H	1	Total 6	C 3	O 3	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).

PG4
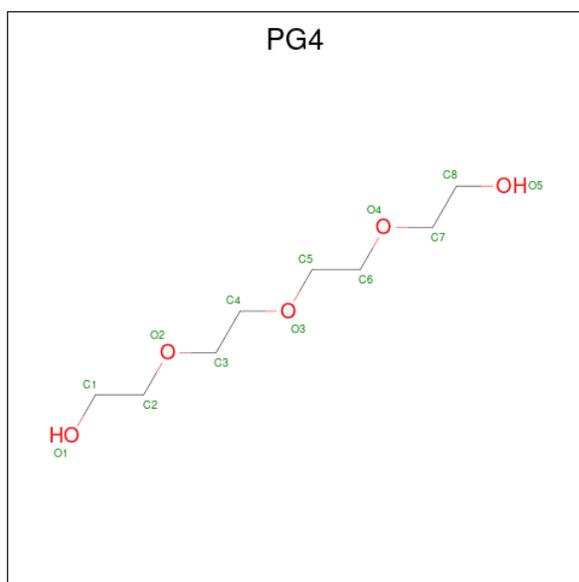
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 8	O 5	0	0
3	A	1	Total 13	C 8	O 5	0	0
3	A	1	Total 13	C 8	O 5	0	0
3	B	1	Total 13	C 8	O 5	0	0
3	C	1	Total 13	C 8	O 5	0	0
3	E	1	Total 13	C 8	O 5	0	0
3	E	1	Total 13	C 8	O 5	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).

OXY
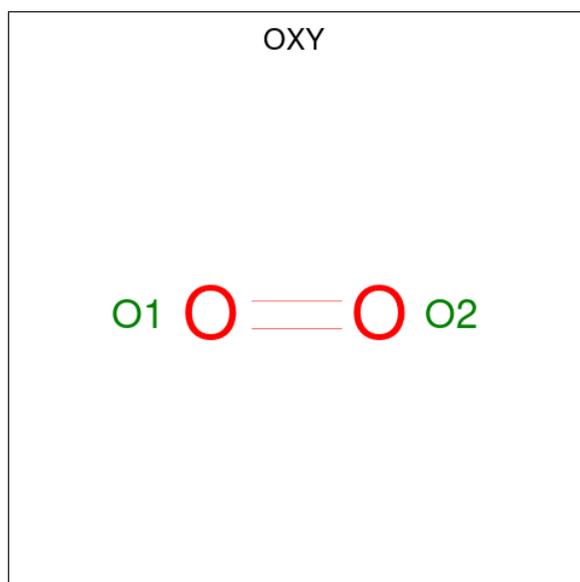
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	O 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Cl 3	0	0
5	B	3	Total 3	Cl 3	0	0
5	C	2	Total 2	Cl 2	0	0
5	D	2	Total 2	Cl 2	0	0
5	E	4	Total 4	Cl 4	0	0
5	F	2	Total 2	Cl 2	0	0
5	G	4	Total 4	Cl 4	0	0
5	H	2	Total 2	Cl 2	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).
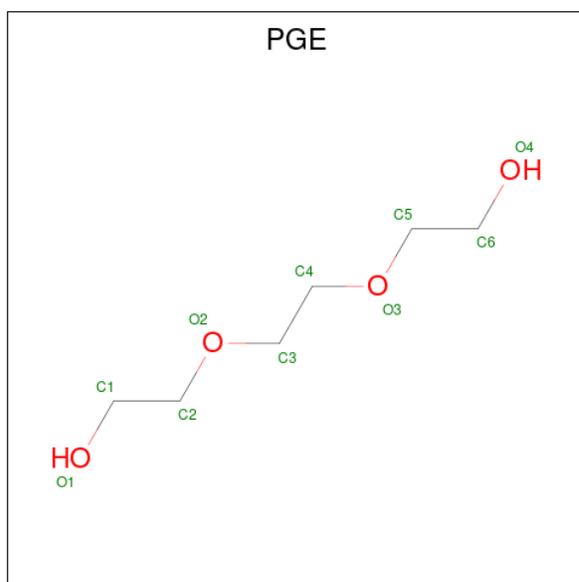
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	10	6	4	0	0

- Molecule 7 is N-(3-Benzyl-5-phenylpyrazin-2-yl)-2-(furan-2-yl)acetamide (three-letter code: NT0) (formula: $C_{23}H_{19}N_3O_2$) (labeled as "Ligand of Interest" by depositor).
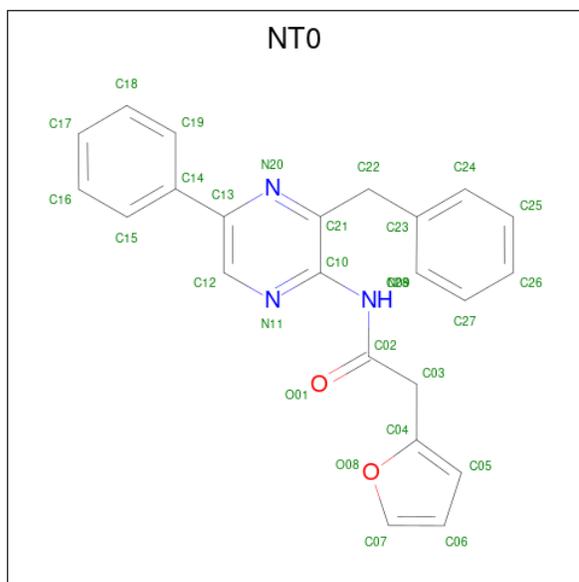
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	G	1	28	23	3	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total 79	O 79	0	0
8	B	93	Total 93	O 93	0	0
8	C	96	Total 96	O 96	0	0
8	D	86	Total 86	O 86	0	0
8	E	101	Total 101	O 101	0	0
8	F	101	Total 101	O 101	0	0
8	G	110	Total 111	O 111	0	1
8	H	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: NanoLuc luciferase

Chain A:

- Molecule 1: NanoLuc luciferase

Chain B:

- Molecule 1: NanoLuc luciferase

Chain C:

- Molecule 1: NanoLuc luciferase

Chain D:

K124 T128 I138 L142 G157 L163 C164 I167 L168 A169

• Molecule 1: NanoLuc luciferase

Chain E:

8%

62%   27%   6%

MET HIS HIS HIS HIS HIS SER ASP ASN M-1 V0 W10 Y16 D19 L22 E23 Q24 G25 G26 V27 S28 S29 L30 F31 Q32 N33 L34 S37 R43 I44 V45 I54 D55 L65 S66 G67 D68 Q69 M70 G71 Q72 I73 I76 F77 K78 V83 D84 D85 H86

K89 V90 I91 L97 D100 G101 V102 T103 I107 F110 P113 I117 A118 V119 I125 N135 K136 I137 I138 D139 E140 R141 F151 R152 V153 T154 I155 W161 R162 L163 C164 E165 R166 I167 L168 A169

• Molecule 1: NanoLuc luciferase

Chain F:

4%

77%   17%   6%

MET HIS HIS HIS HIS HIS SER ASP ASN M-1 T2 L3 E4 V7 L34 R43 I44 V45 L46 G51 L52 K53 I54 D55 I56 E63 G64 L65 S66 G67 D68 Q69 I73 E74 K75 H93 L97 G101 I107 D108 P113 V119 K124 I137

P145 D146 G147 S148 R152 A169

• Molecule 1: NanoLuc luciferase

Chain G:

9%

73%   15%   6%   6%

MET HIS HIS HIS HIS HIS SER ASP ASN M-1 W10 L22 G26 V27 S28 S29 L30 F31 Q32 N33 L34 G35 V36 I41 D55 I56 H57 V58 I59 I60 P61 Y62 E63 G64 L65 S66 G67 D68 Q69 Q72 K75 I76 F77 K78 V79 V80 Y81 P82 V83 K89 V90

I91 L92 H93 Y94 Y109 F110 G111 R112 K136 L142 T154 V158 L163 C164 E165 R166 I167 L168 A169

• Molecule 1: NanoLuc luciferase

Chain H:

6%

76%   13%   5%

MET HIS HIS HIS HIS HIS SER ASP N-2 W10 L22 E23 Q24 G25 G26 V27 S28 S29 L30 F31 Q32 N33 L34 R43 I44 K53 I54 V58 G64 L65 S66 G67 D68 Q69 M70 G71 Q72 I73 E74 K75 V90 H93 T96 R112 K124 R141

P145 D146 G147 S148 L149 L150 V158 L163 C164 I167 L168 A169

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.91Å 87.49Å 191.76Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	47.94 – 1.69 47.94 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.94-1.69) 98.5 (47.94-1.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.135 , 0.183 0.166 , 0.219	Depositor DCC
R_{free} test set	8057 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.7	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l 0.024 for -k,-h,-l 0.057 for -h,-k,l	Xtriage
Reported twinning fraction	0.606 for H, K, L 0.214 for h,-k,-l 0.089 for K, H, -L 0.090 for -K, -H, -L	Depositor
Outliers	0 of 158493 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3129e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: PG4, OXY, NT0, PGE, GOL, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.24	4/1384 (0.3%)	1.14	7/1878 (0.4%)
1	B	0.96	1/1378 (0.1%)	1.12	2/1870 (0.1%)
1	C	0.99	2/1378 (0.1%)	1.11	2/1870 (0.1%)
1	D	0.93	0/1384	1.15	3/1878 (0.2%)
1	E	0.92	1/1378 (0.1%)	1.10	4/1870 (0.2%)
1	F	0.99	2/1389 (0.1%)	1.18	1/1884 (0.1%)
1	G	0.90	0/1384	1.12	3/1878 (0.2%)
1	H	0.96	2/1386 (0.1%)	1.13	5/1881 (0.3%)
All	All	0.99	12/11061 (0.1%)	1.13	27/15009 (0.2%)

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	1	0
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	4
1	G	0	1
All	All	1	8

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	GLU	CD-OE1	23.89	1.51	1.25
1	A	74	GLU	CD-OE2	18.78	1.46	1.25
1	A	165	GLU	CD-OE1	-6.78	1.18	1.25
1	B	66	SER	CB-OG	6.01	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	51	GLY	C-O	5.97	1.33	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	43	ARG	CG-CD-NE	8.20	129.01	111.80
1	H	43	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	E	166	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	D	93	HIS	CB-CA-C	-7.47	95.46	110.40
1	A	166	ARG	NE-CZ-NH1	-7.45	116.57	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	100	ASP	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	ASP	Peptide
1	D	66	SER	Peptide
1	E	69	GLN	Peptide
1	F	63	GLU	Peptide
1	F	66	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1355	0	1357	52	0
1	B	1349	0	1353	33	0
1	C	1349	0	1353	38	0
1	D	1355	0	1357	34	0
1	E	1349	0	1353	51	0
1	F	1357	0	1366	20	0
1	G	1355	0	1357	50	0
1	H	1357	0	1359	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	3	0
2	H	6	0	8	4	0
3	A	39	0	54	8	0
3	B	13	0	18	2	0
3	C	13	0	18	5	0
3	E	26	0	36	14	0
4	A	2	0	0	2	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	3	0
5	F	2	0	0	0	0
5	G	4	0	0	0	0
5	H	2	0	0	1	0
6	D	10	0	14	2	0
7	G	28	0	0	15	0
8	A	79	0	0	9	0
8	B	93	0	0	2	0
8	C	96	0	0	0	0
8	D	86	0	0	4	0
8	E	101	0	0	4	0
8	F	101	0	0	5	0
8	G	111	0	0	1	0
8	H	104	0	0	8	0
All	All	11762	0	11011	298	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 14.

The worst 5 of 298 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:F:34:LEU:HD11	1:F:73:ILE:HD11	1.27	1.12
1:G:91:ILE:HD11	7:G:301:NT0:C05	1.88	1.03
7:G:301:NT0:C15	5:H:202:CL:CL	2.46	1.01
1:G:41:ILE:HD13	7:G:301:NT0:C18	1.95	0.96
1:D:74:GLU:HB3	1:D:78:LYS:O	1.67	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/181 (94%)	159 (94%)	6 (4%)	5 (3%)	4	0
1	B	169/181 (93%)	159 (94%)	10 (6%)	0	100	100
1	C	169/181 (93%)	162 (96%)	7 (4%)	0	100	100
1	D	170/181 (94%)	159 (94%)	9 (5%)	2 (1%)	13	3
1	E	169/181 (93%)	159 (94%)	6 (4%)	4 (2%)	6	1
1	F	170/181 (94%)	161 (95%)	8 (5%)	1 (1%)	25	11
1	G	170/181 (94%)	163 (96%)	6 (4%)	1 (1%)	25	11
1	H	170/181 (94%)	156 (92%)	10 (6%)	4 (2%)	6	1
All	All	1357/1448 (94%)	1278 (94%)	62 (5%)	17 (1%)	12	2

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	D	29	SER
1	E	66	SER
1	E	69	GLN
1	G	66	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/158 (94%)	137 (92%)	12 (8%)	11	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	B	148/158 (94%)	142 (96%)	6 (4%)		30	12
1	C	148/158 (94%)	137 (93%)	11 (7%)		13	3
1	D	149/158 (94%)	139 (93%)	10 (7%)		16	4
1	E	148/158 (94%)	138 (93%)	10 (7%)		16	4
1	F	149/158 (94%)	144 (97%)	5 (3%)		37	18
1	G	149/158 (94%)	141 (95%)	8 (5%)		22	7
1	H	149/158 (94%)	140 (94%)	9 (6%)		19	6
All	All	1189/1264 (94%)	1118 (94%)	71 (6%)		19	6

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	78	LYS
1	G	91	ILE
1	H	53	LYS
1	C	76	ILE
1	C	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	33	ASN
1	F	69	GLN
1	H	144	ASN
1	F	144	ASN
1	G	57	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PG4	A	202	-	12,12,12	0.61	0	11,11,11	0.87	0
3	PG4	E	201	-	12,12,12	0.71	0	11,11,11	1.56	2 (18%)
3	PG4	A	203	-	12,12,12	0.64	0	11,11,11	0.98	1 (9%)
4	OXY	A	205	-	1,1,1	0.09	0	-		
2	GOL	A	201	-	5,5,5	1.00	0	5,5,5	1.34	1 (20%)
7	NT0	G	301	-	27,31,31	2.71	14 (51%)	34,41,41	3.80	14 (41%)
3	PG4	E	202	-	12,12,12	0.92	1 (8%)	11,11,11	1.16	2 (18%)
3	PG4	A	204	-	12,12,12	0.91	0	11,11,11	1.46	2 (18%)
6	PGE	D	201	-	9,9,9	0.26	0	8,8,8	0.12	0
2	GOL	H	201	-	5,5,5	0.39	0	5,5,5	1.11	0
3	PG4	B	401	-	12,12,12	0.59	0	11,11,11	1.36	2 (18%)
3	PG4	C	201	-	12,12,12	0.87	0	11,11,11	1.65	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	A	202	-	-	6/10/10/10	-
3	PG4	E	201	-	-	7/10/10/10	-
3	PG4	A	203	-	-	3/10/10/10	-
2	GOL	A	201	-	-	3/4/4/4	-
7	NT0	G	301	-	-	4/14/16/16	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	E	202	-	-	7/10/10/10	-
3	PG4	A	204	-	-	6/10/10/10	-
6	PGE	D	201	-	-	4/7/7/7	-
2	GOL	H	201	-	-	2/4/4/4	-
3	PG4	B	401	-	-	6/10/10/10	-
3	PG4	C	201	-	-	5/10/10/10	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	301	NT0	C03-C04	-6.11	1.46	1.51
7	G	301	NT0	C10-N11	-5.48	1.26	1.35
7	G	301	NT0	C14-C13	4.19	1.55	1.48
7	G	301	NT0	C02-N09	4.16	1.44	1.35
7	G	301	NT0	C21-N20	-3.78	1.27	1.34

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	301	NT0	C21-C10-N09	9.03	130.81	118.40
7	G	301	NT0	C03-C02-N09	8.11	131.53	114.77
7	G	301	NT0	C21-C10-N11	-7.52	115.23	122.25
7	G	301	NT0	C13-N20-C21	7.41	124.78	118.35
7	G	301	NT0	C23-C22-C21	6.71	129.62	112.40

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GOL	C1-C2-C3-O3
2	H	201	GOL	C1-C2-C3-O3
2	H	201	GOL	O2-C2-C3-O3
7	G	301	NT0	C10-C21-C22-C23
7	G	301	NT0	N20-C21-C22-C23

There are no ring outliers.

12 monomers are involved in 55 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	PG4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201	PG4	9	0
3	A	203	PG4	1	0
4	A	205	OXY	2	0
2	A	201	GOL	3	0
7	G	301	NT0	15	0
3	E	202	PG4	5	0
3	A	204	PG4	7	0
6	D	201	PGE	2	0
2	H	201	GOL	4	0
3	B	401	PG4	2	0
3	C	201	PG4	5	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.


Ligand PG4 A 202

Bond lengths — Bond angles — Torsions — Rings

Ligand PG4 E 201

Bond lengths — Bond angles — Torsions — Rings

Ligand PG4 A 203

Bond lengths

Bond angles

Torsions

Rings

Ligand OXY A 205

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand NT0 G 301

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 E 202

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 204

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 C 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	171/181 (94%)	0.42	10 (5%)	23	25	20, 37, 56, 93	0
1	B	171/181 (94%)	0.27	8 (4%)	31	35	19, 31, 52, 70	0
1	C	171/181 (94%)	0.14	2 (1%)	79	82	18, 31, 49, 96	0
1	D	171/181 (94%)	0.38	16 (9%)	8	9	17, 30, 57, 127	0
1	E	171/181 (94%)	0.45	14 (8%)	11	13	19, 33, 59, 126	0
1	F	171/181 (94%)	0.11	7 (4%)	37	41	18, 29, 46, 78	0
1	G	171/181 (94%)	0.29	16 (9%)	8	9	17, 28, 55, 97	0
1	H	172/181 (95%)	0.28	10 (5%)	23	25	17, 30, 53, 88	0
All	All	1369/1448 (94%)	0.29	83 (6%)	21	23	17, 31, 55, 127	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	65	LEU	12.3
1	H	67	GLY	7.6
1	D	76	ILE	6.7
1	D	33	ASN	6.4
1	E	32	GLN	6.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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($Å^2$)	Q<0.9
2	GOL	H	201	6/6	0.67	0.24	30,36,42,62	0
3	PG4	B	401	13/13	0.81	0.15	36,40,46,47	0
3	PG4	A	204	13/13	0.82	0.15	34,42,51,52	0
7	NT0	G	301	28/28	0.82	0.18	24,35,50,54	0
3	PG4	A	203	13/13	0.84	0.16	41,45,53,56	0
2	GOL	A	201	6/6	0.86	0.17	33,43,45,49	0
3	PG4	E	201	13/13	0.87	0.15	28,40,58,59	0
3	PG4	A	202	13/13	0.91	0.11	34,47,66,70	0
6	PGE	D	201	10/10	0.92	0.09	43,48,54,54	0
3	PG4	E	202	13/13	0.92	0.20	26,29,31,33	0
3	PG4	C	201	13/13	0.94	0.10	32,43,49,57	0
4	OXY	A	205	2/2	0.94	0.10	32,32,32,41	0
5	CL	G	303	1/1	0.97	0.05	33,33,33,33	0
5	CL	F	202	1/1	0.98	0.05	33,33,33,33	0
5	CL	B	404	1/1	0.98	0.06	34,34,34,34	0
5	CL	G	304	1/1	0.98	0.06	32,32,32,32	0
5	CL	E	206	1/1	0.98	0.10	30,30,30,30	0
5	CL	F	201	1/1	0.98	0.06	31,31,31,31	0
5	CL	E	205	1/1	0.99	0.03	46,46,46,46	0
5	CL	A	207	1/1	0.99	0.05	32,32,32,32	0
5	CL	A	208	1/1	0.99	0.04	32,32,32,32	0
5	CL	A	206	1/1	0.99	0.04	31,31,31,31	0
5	CL	G	302	1/1	0.99	0.06	26,26,26,26	0
5	CL	D	202	1/1	0.99	0.04	26,26,26,26	0
5	CL	D	203	1/1	0.99	0.06	26,26,26,26	0
5	CL	G	305	1/1	0.99	0.08	28,28,28,28	0
5	CL	H	202	1/1	0.99	0.05	29,29,29,29	0
5	CL	H	203	1/1	0.99	0.05	34,34,34,34	0
5	CL	E	203	1/1	0.99	0.14	22,22,22,22	0
5	CL	E	204	1/1	0.99	0.04	34,34,34,34	0
5	CL	B	403	1/1	1.00	0.06	32,32,32,32	0
5	CL	B	402	1/1	1.00	0.13	22,22,22,22	1
5	CL	C	202	1/1	1.00	0.10	21,21,21,21	1
5	CL	C	203	1/1	1.00	0.03	31,31,31,31	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 GOL 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)
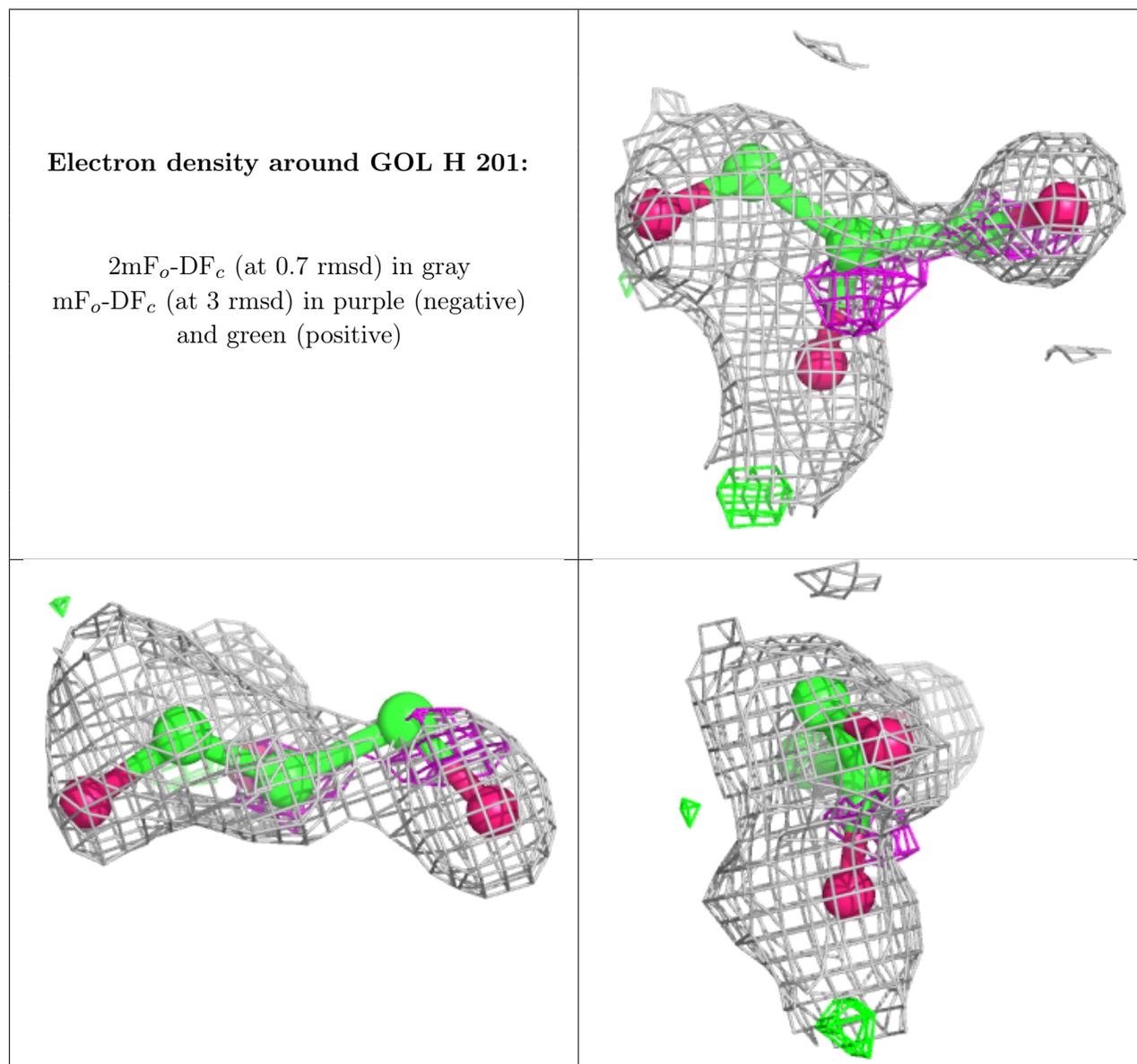
Electron density around PG4 B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
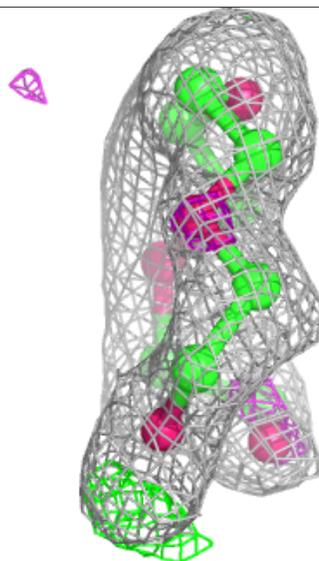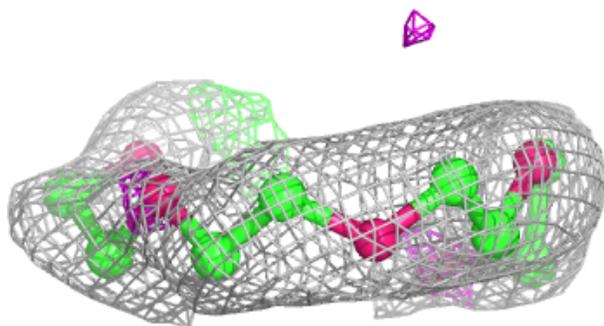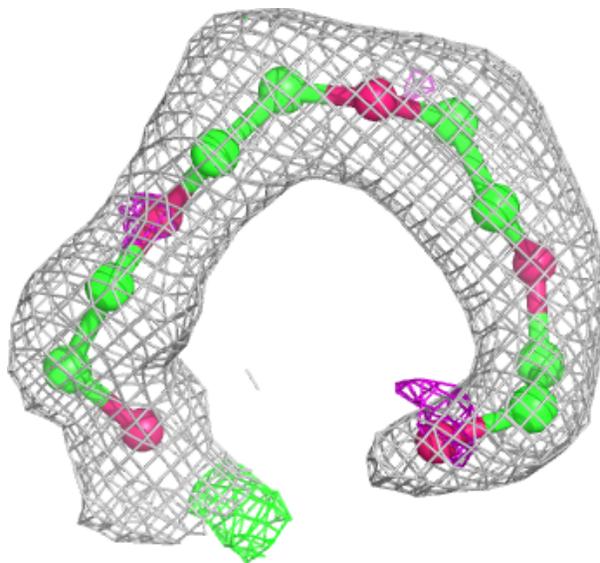
Electron density around PG4 A 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
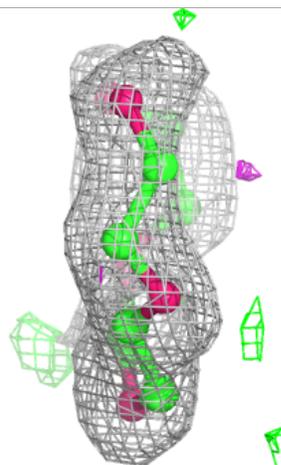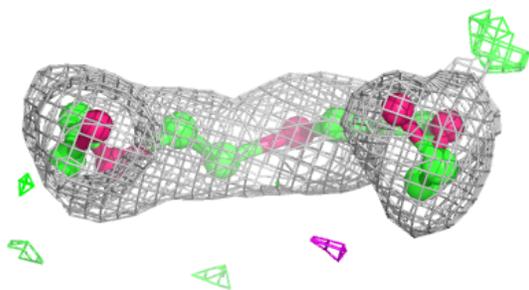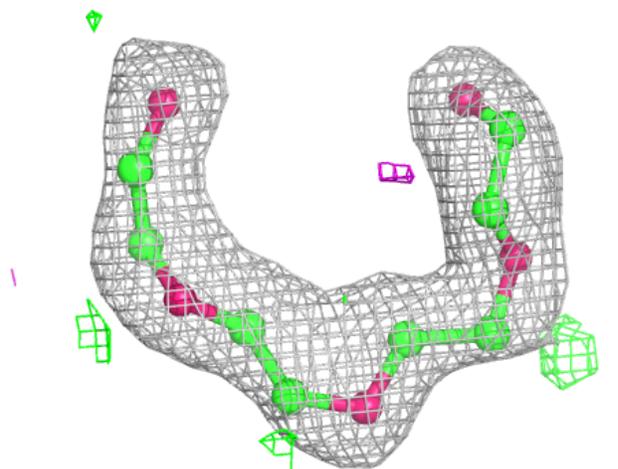
Electron density around NT0 G 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
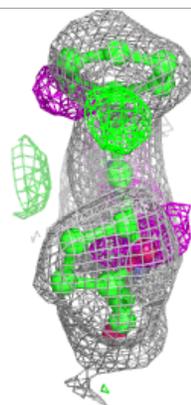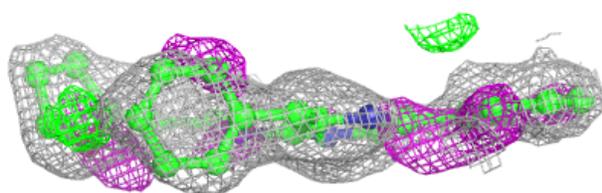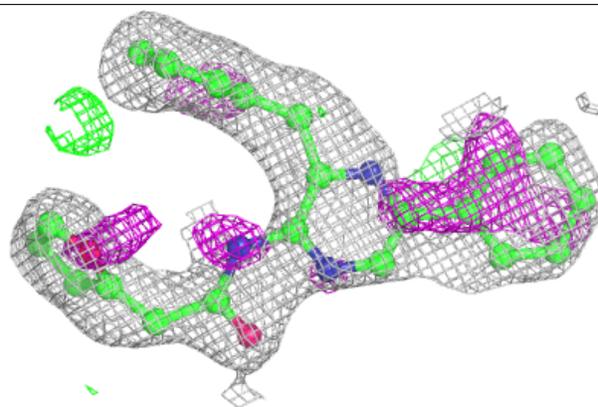
Electron density around PG4 A 203:

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

Electron density around GOL A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
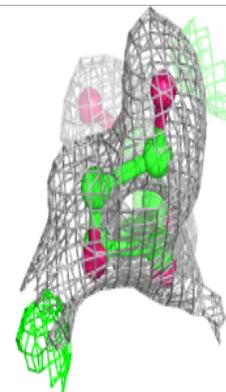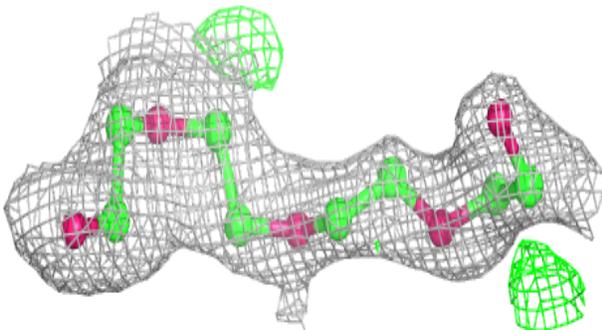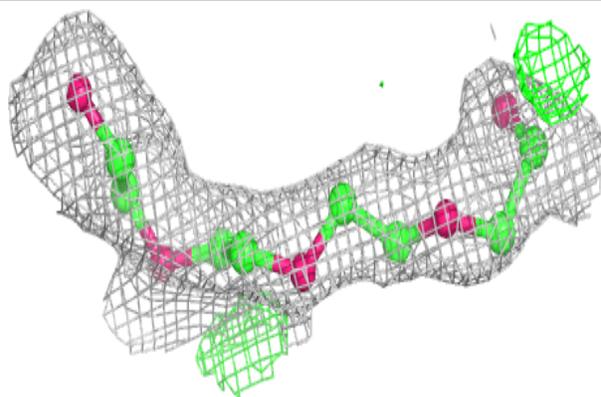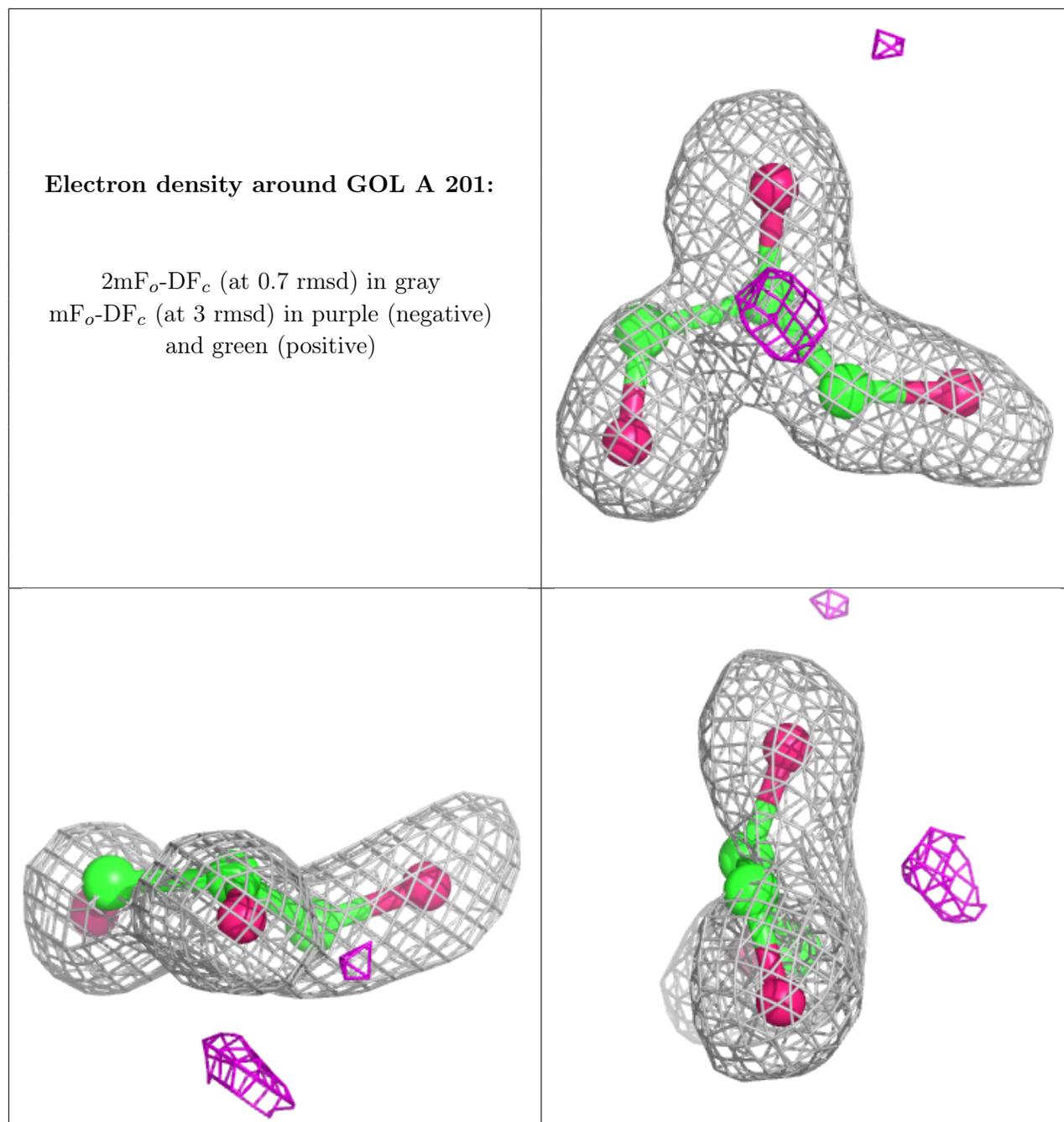
Electron density around PG4 E 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
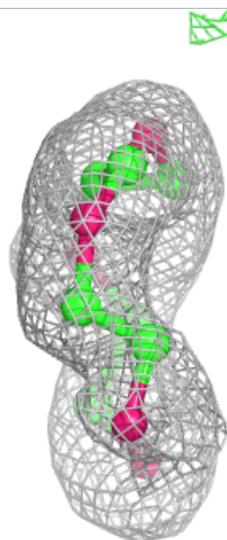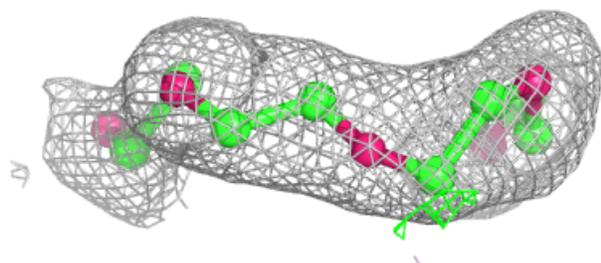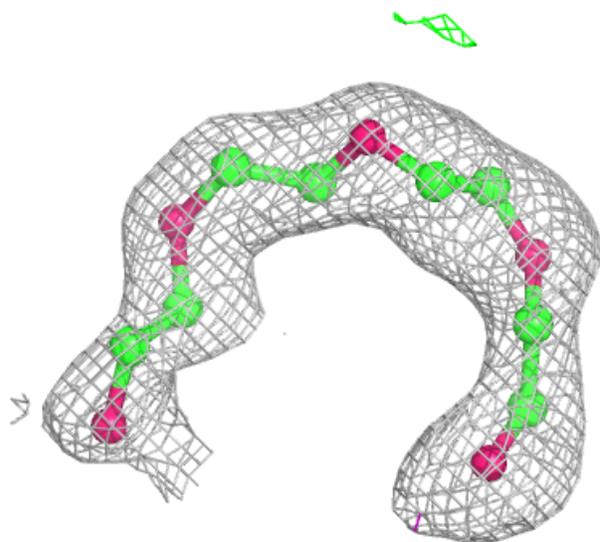
Electron density around PG4 A 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
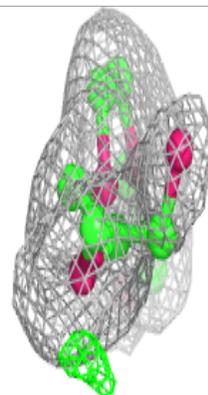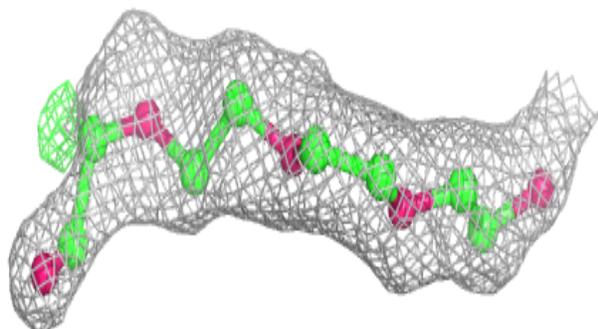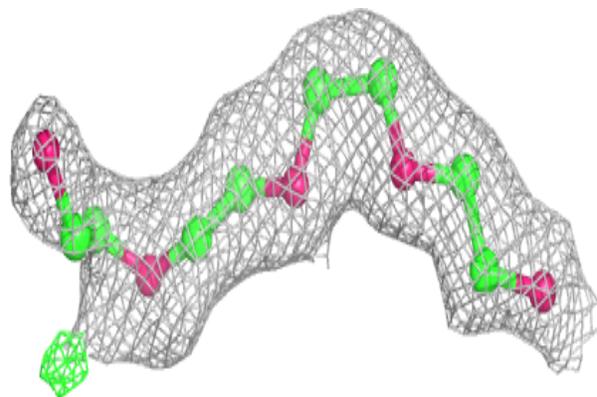
Electron density around PGE D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
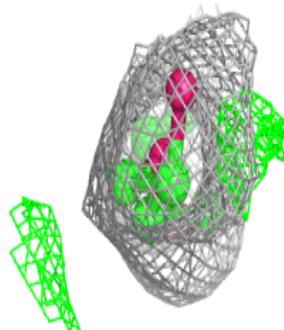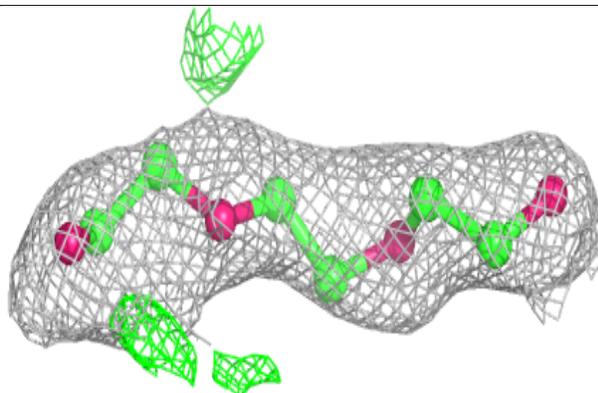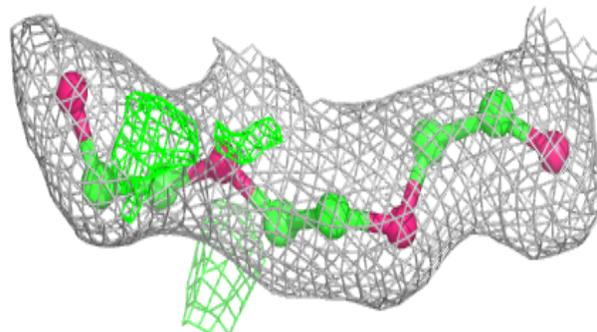
Electron density around PG4 E 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
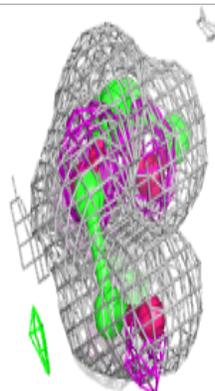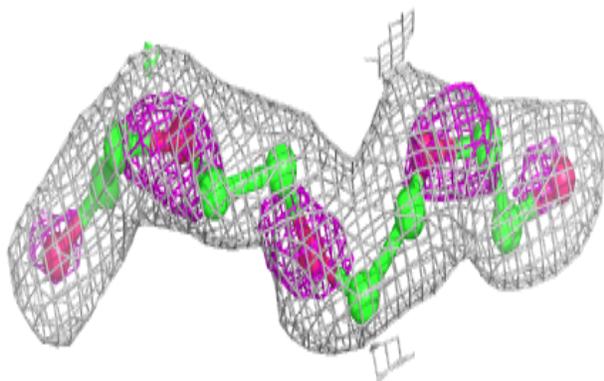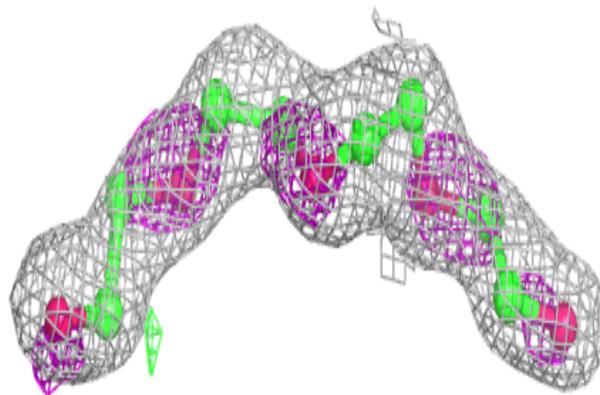
Electron density around PG4 C 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
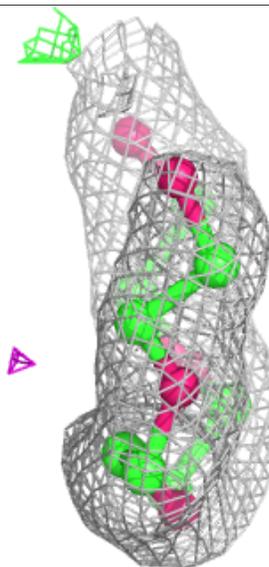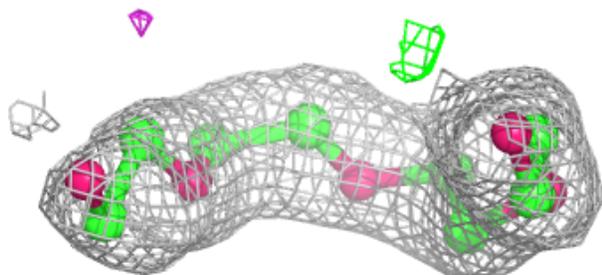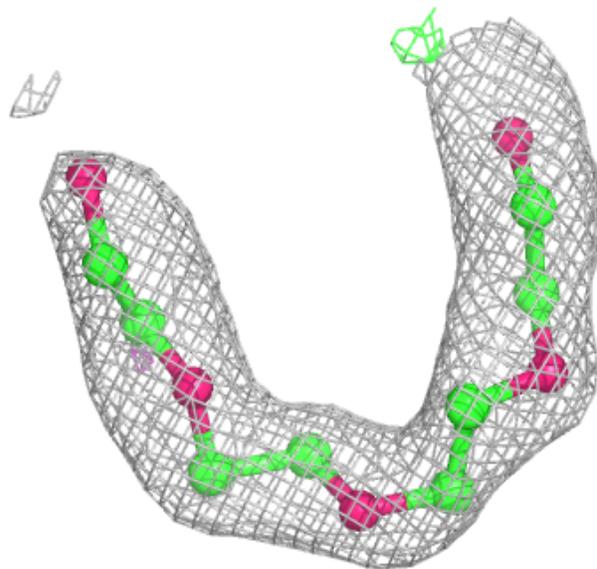
Electron density around OXY A 205:

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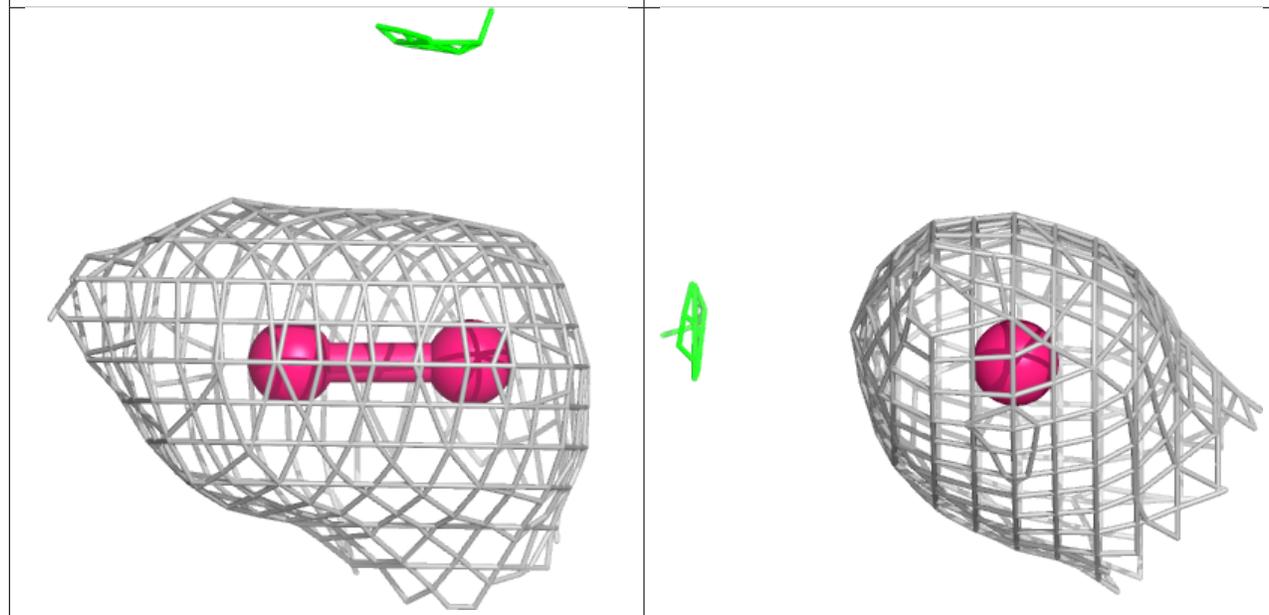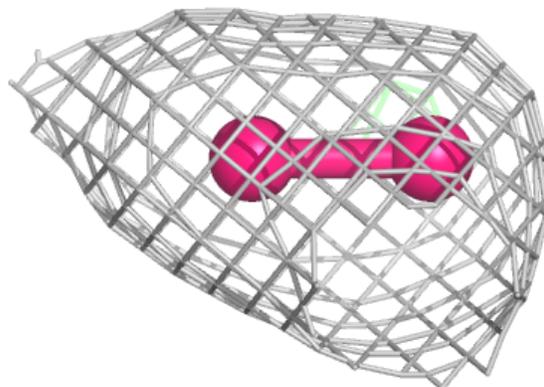
Electron density around CL G 303:

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

Electron density around CL F 202:

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

Electron density around CL B 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
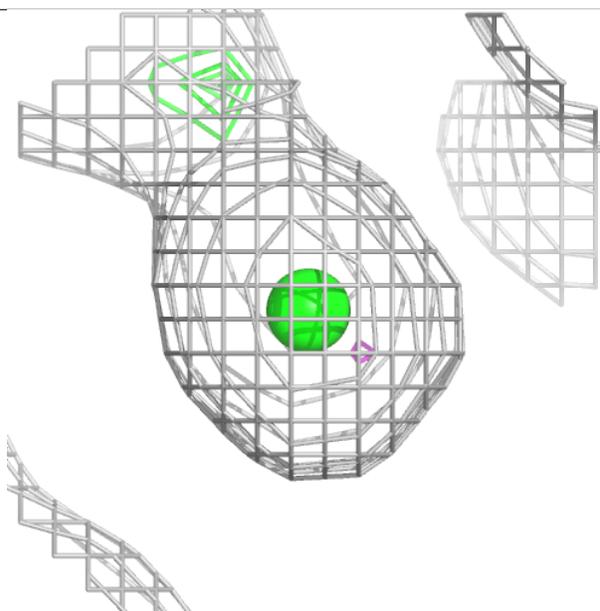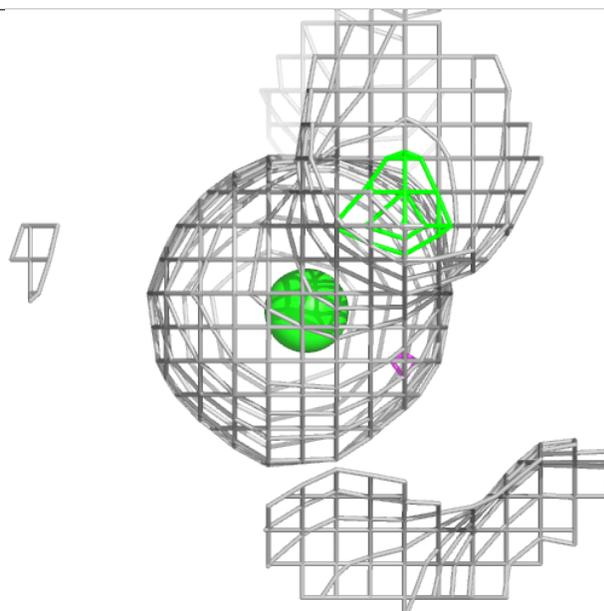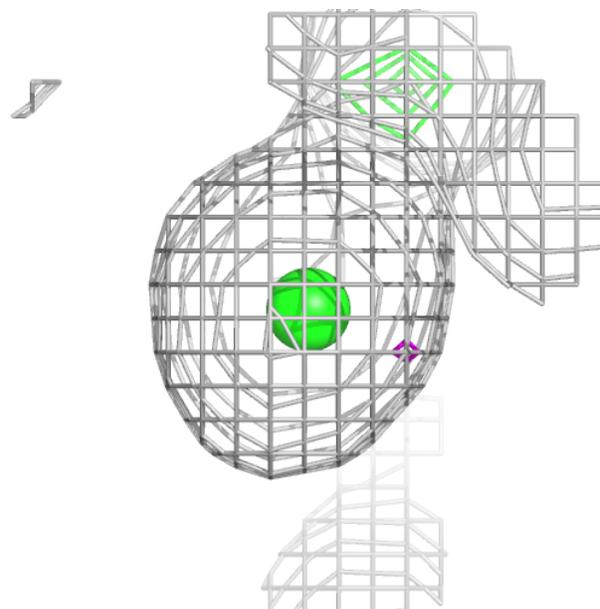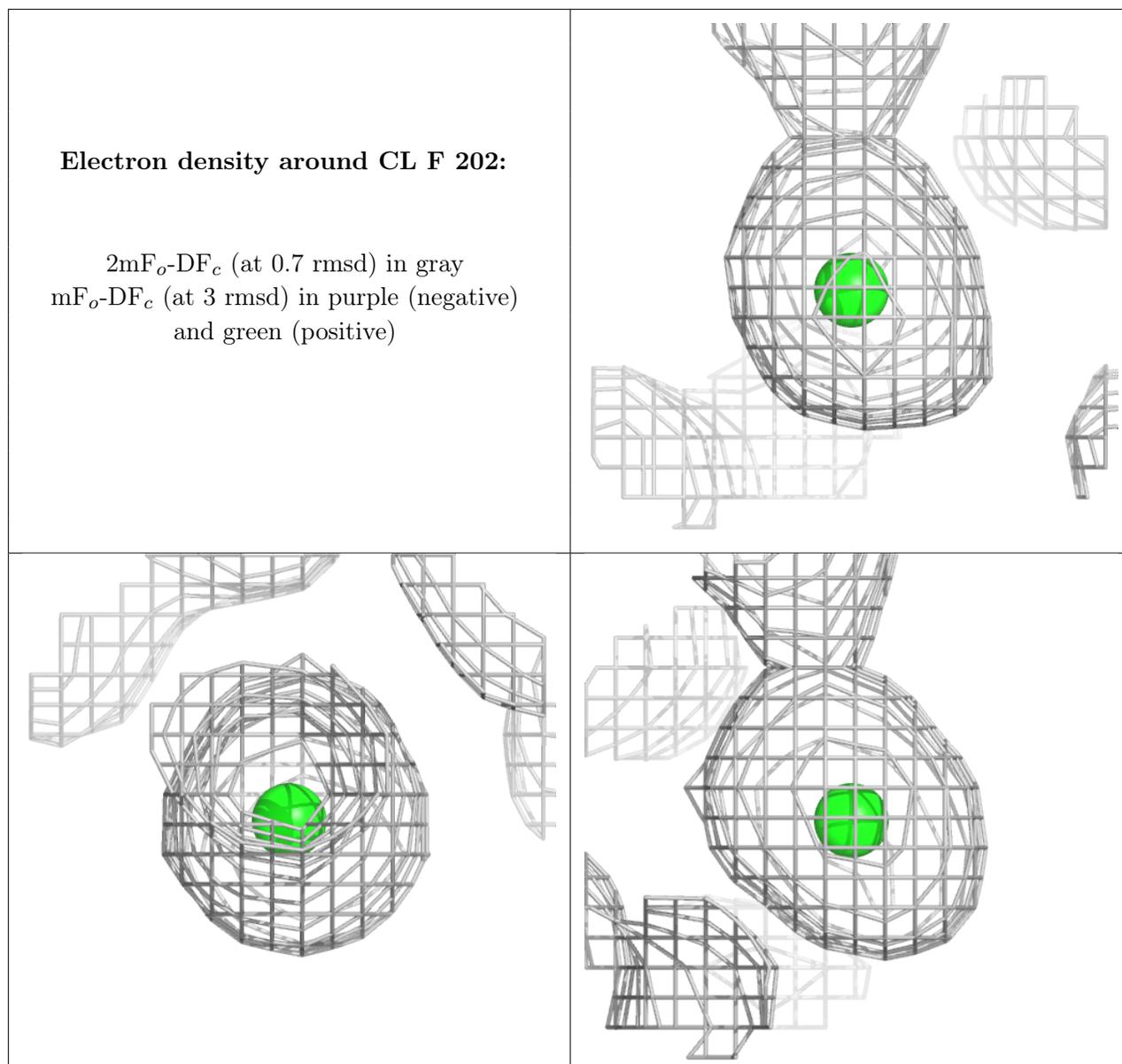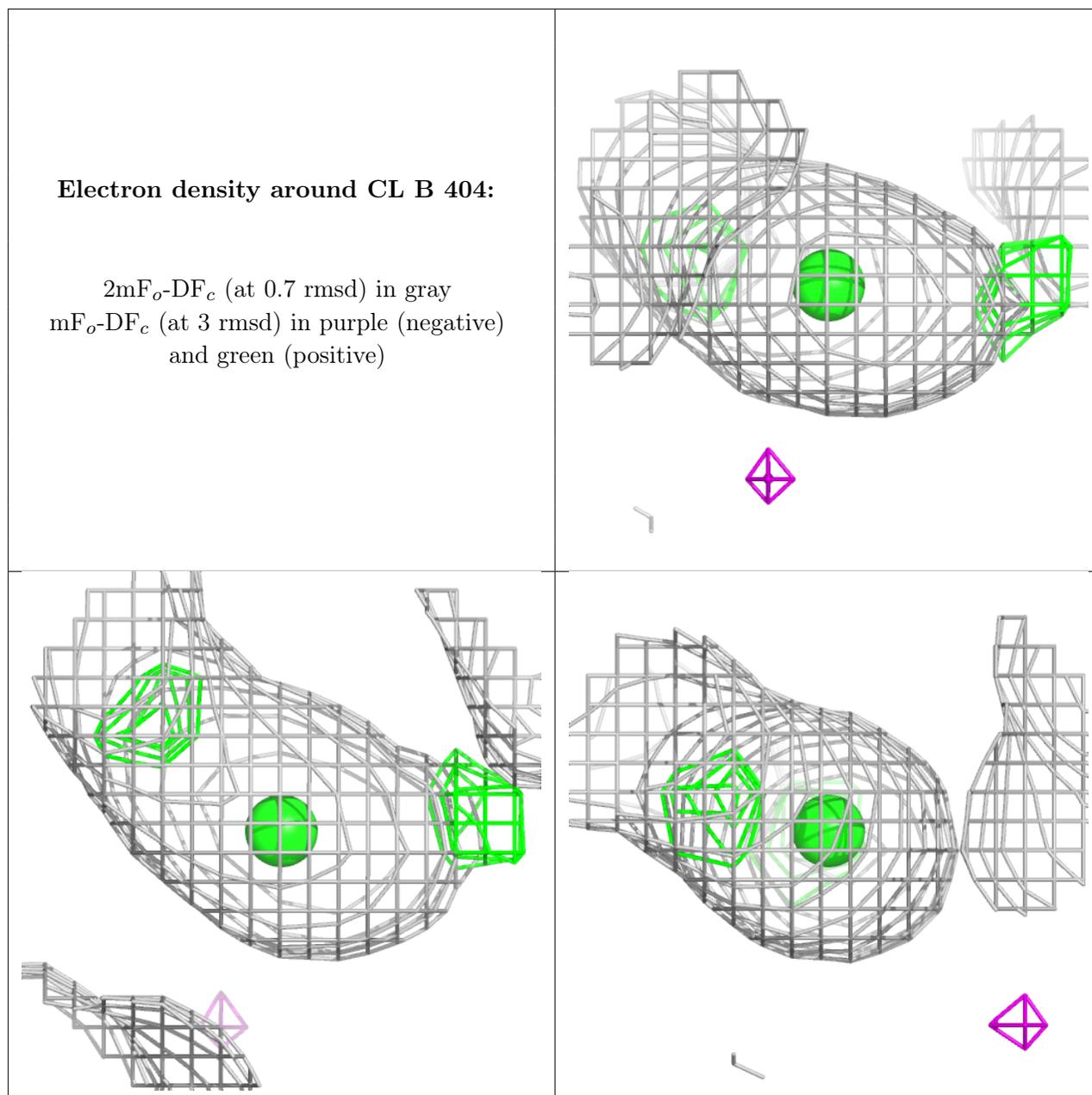
Electron density around CL G 304:

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

Electron density around CL E 206:

$2mF_o$-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:

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

Electron density around CL E 205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
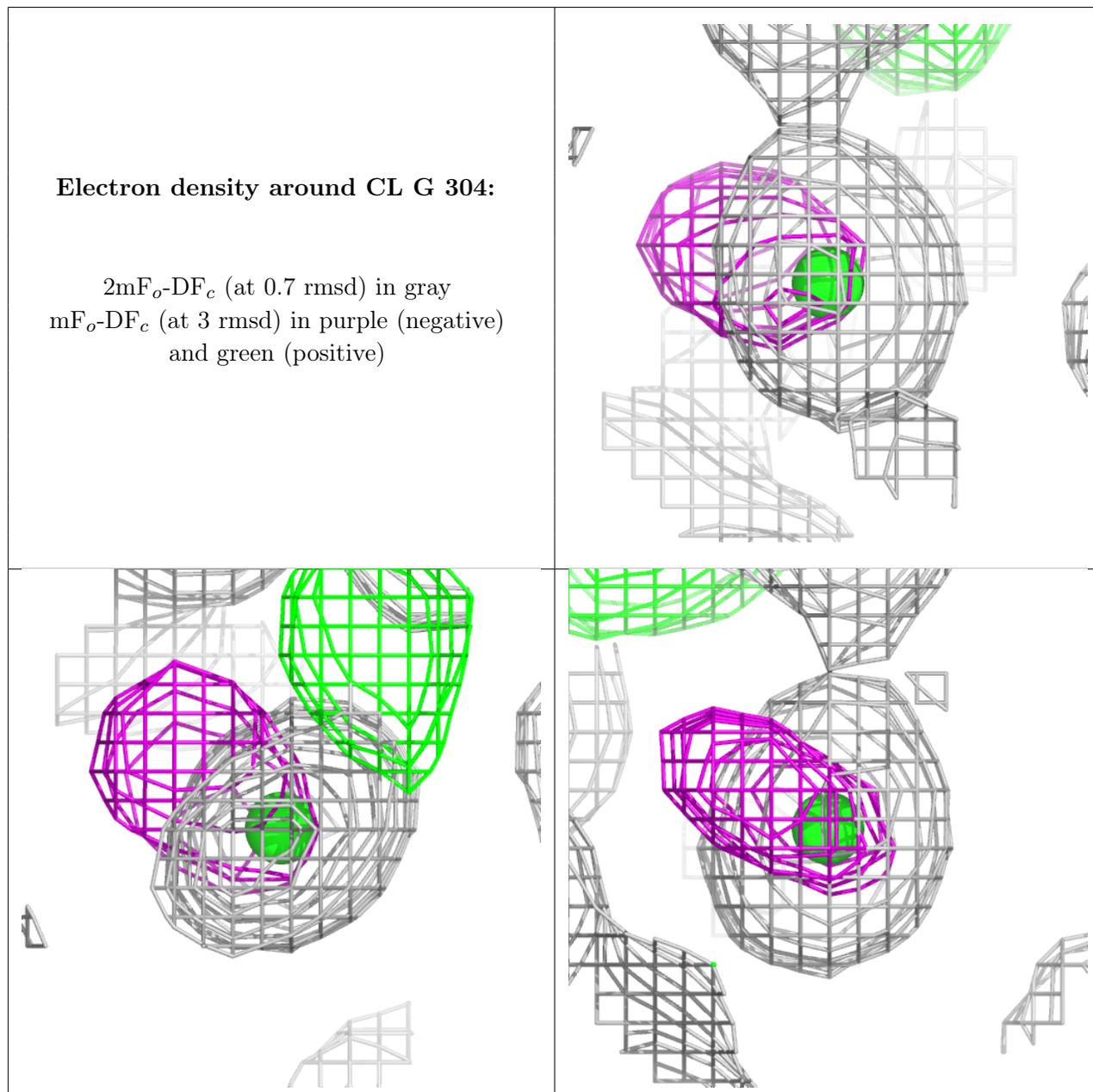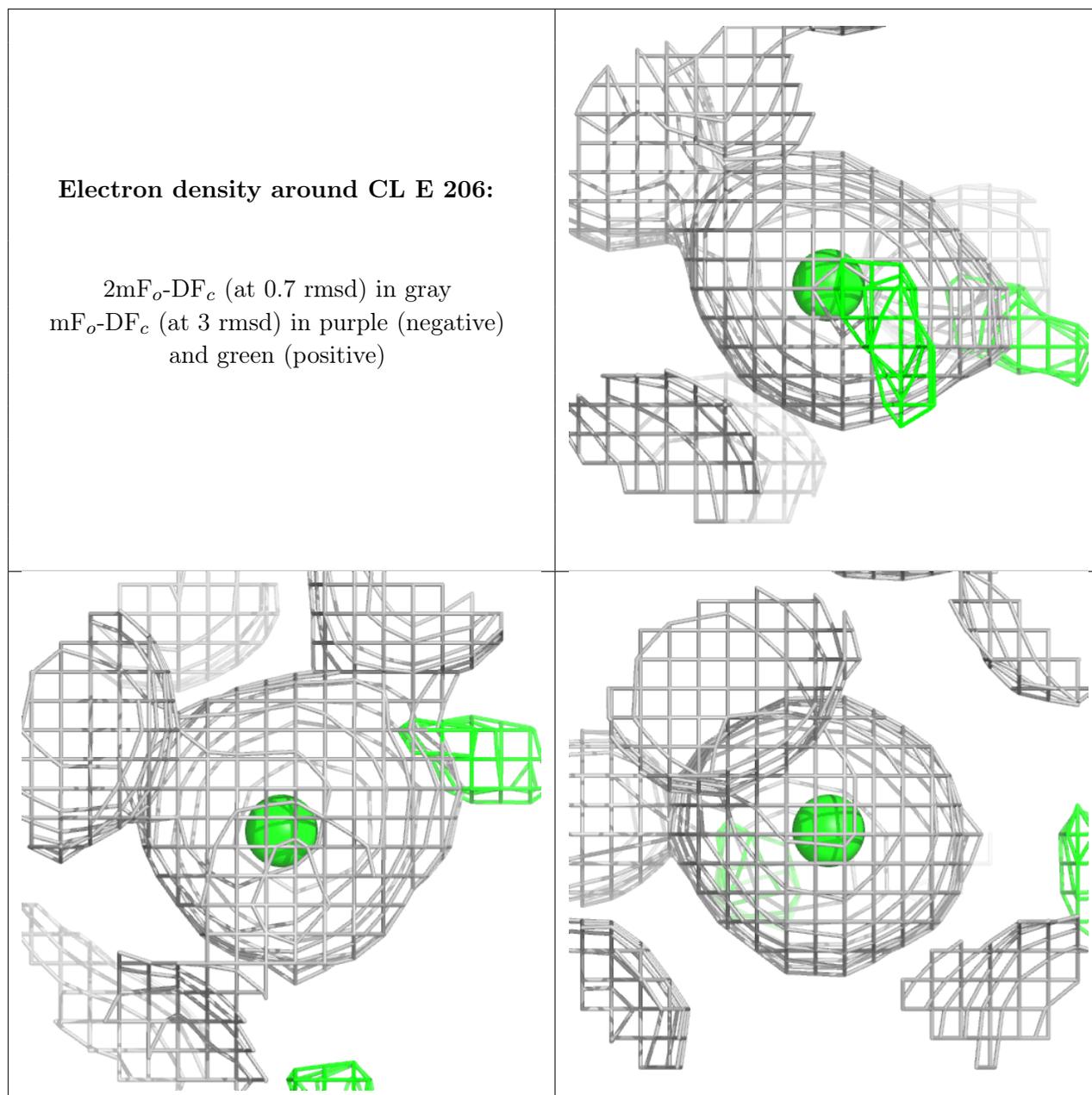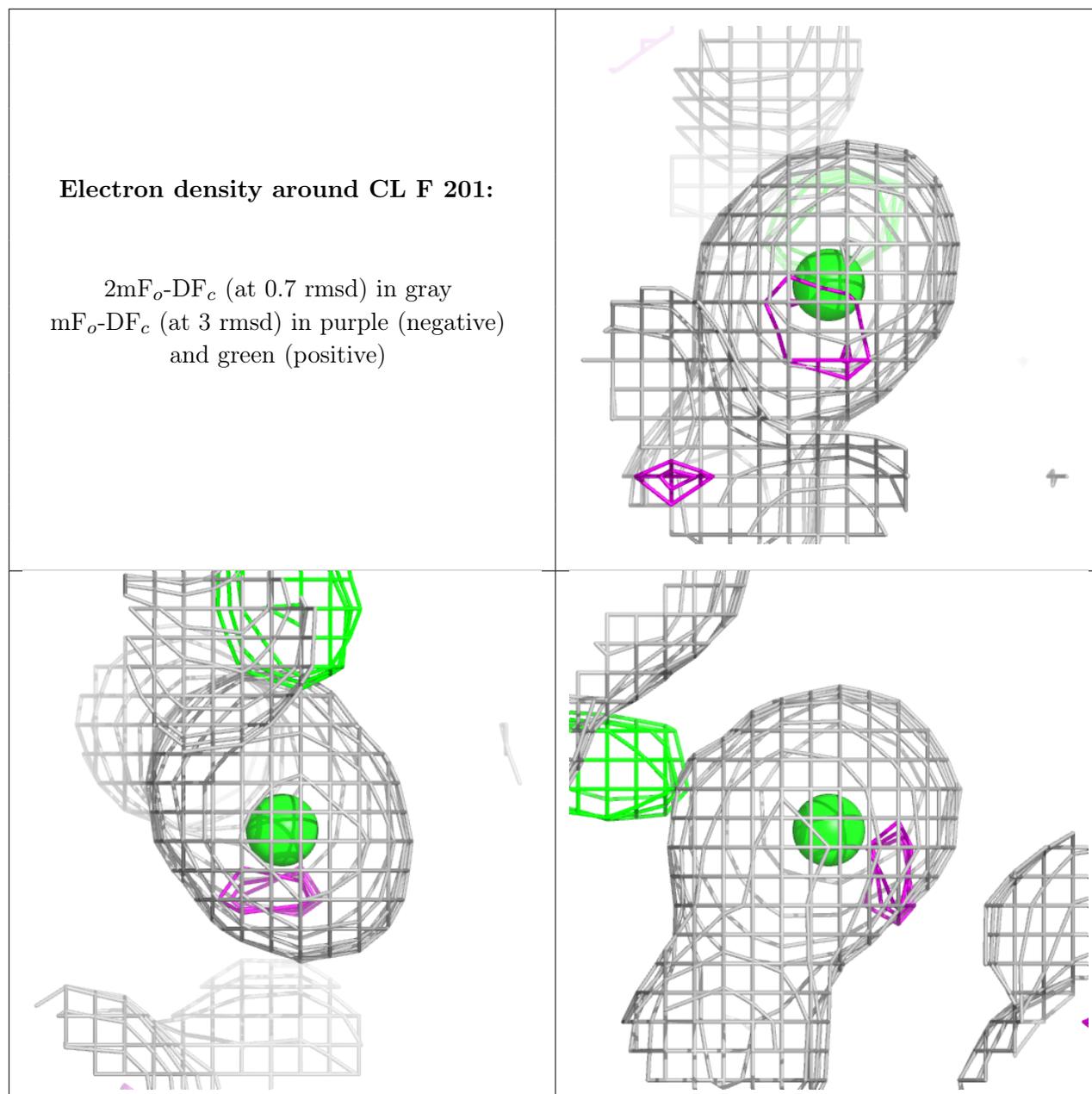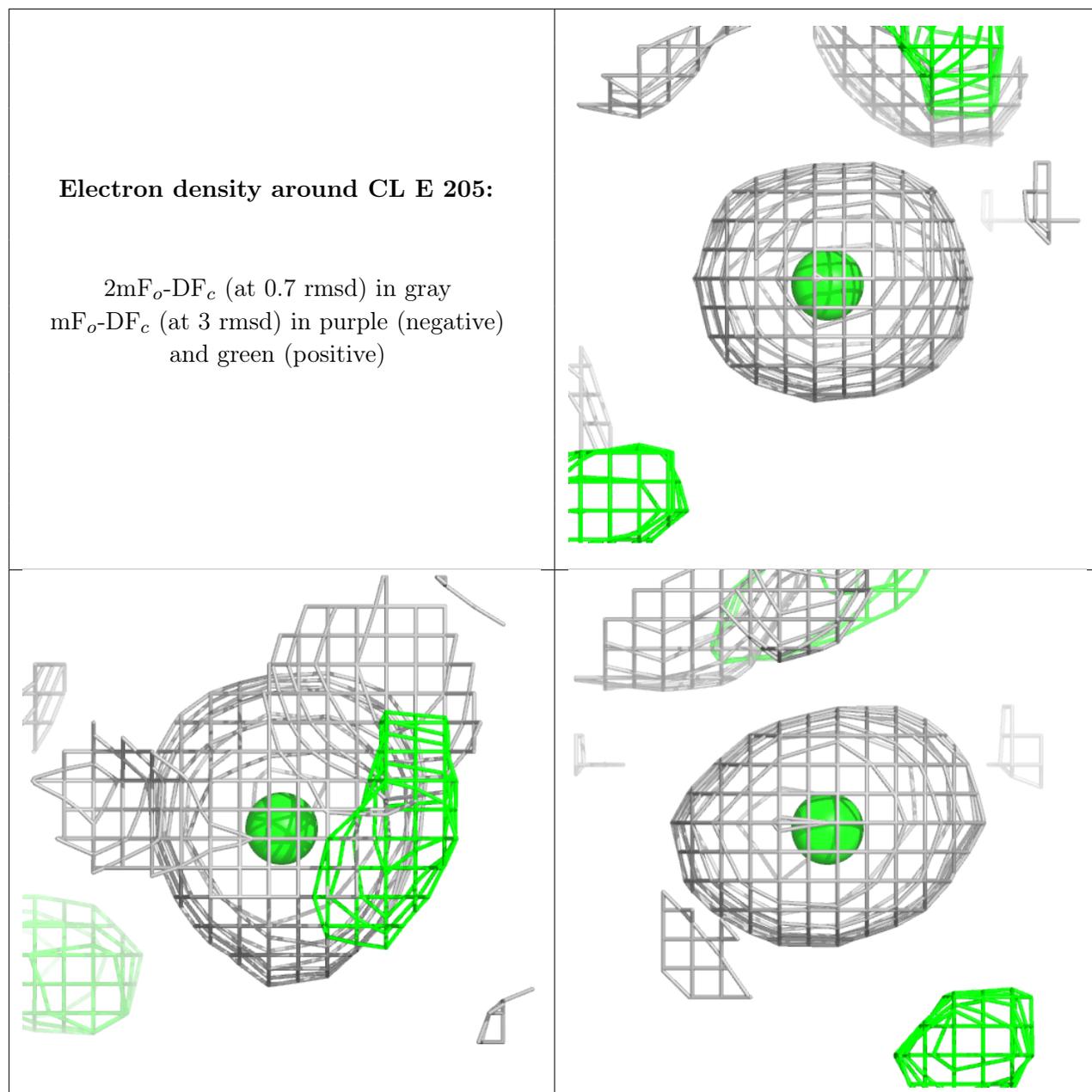
Electron density around CL A 207:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
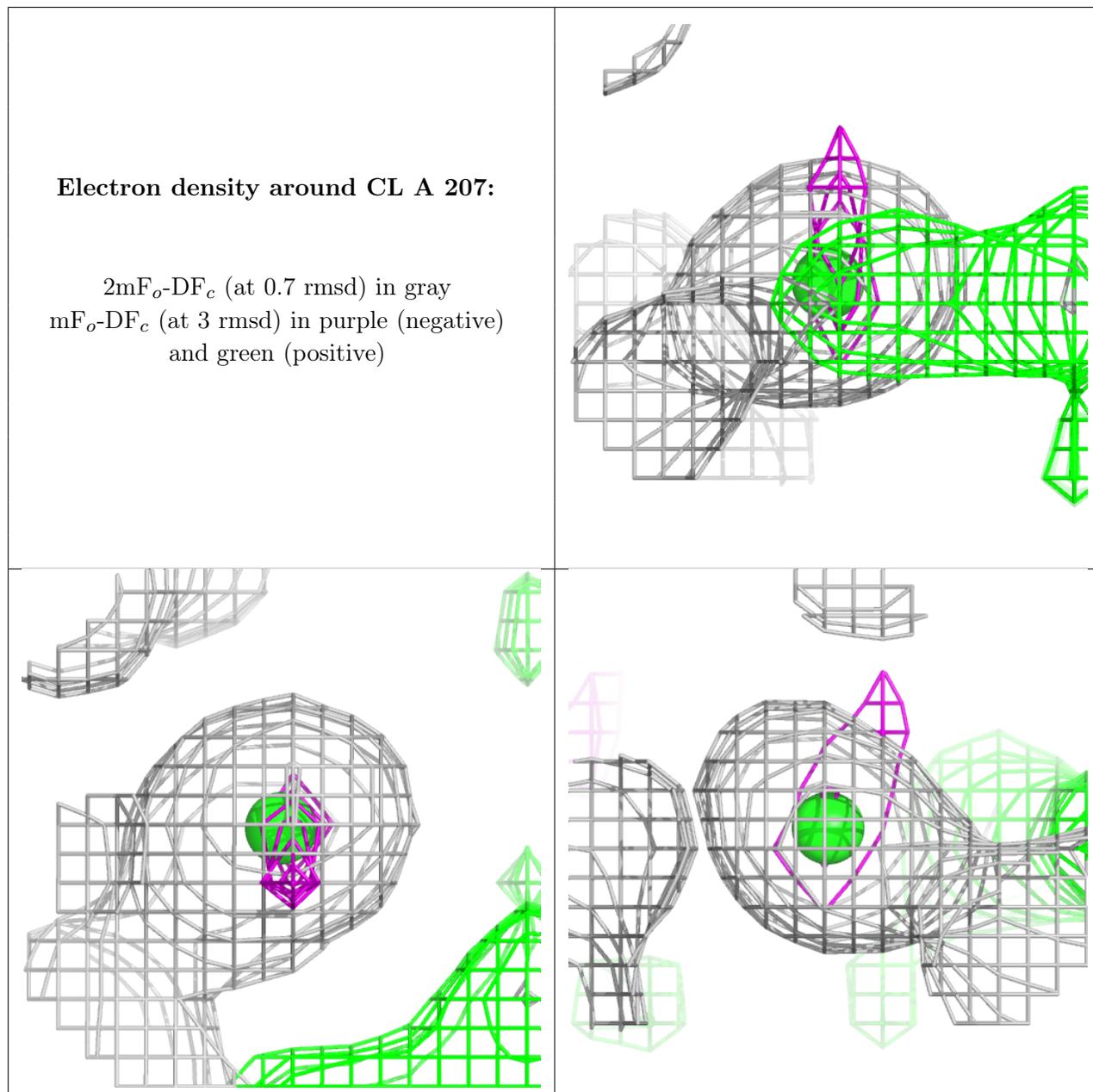
Electron density around CL A 208:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
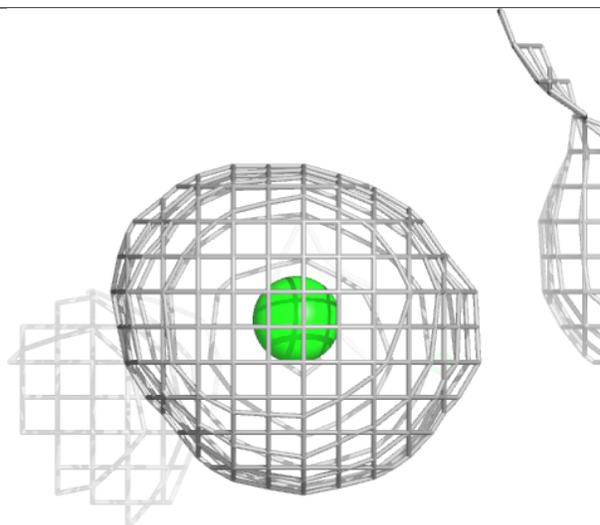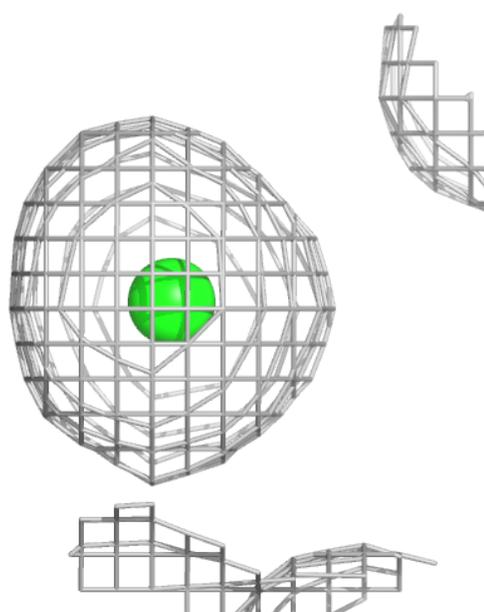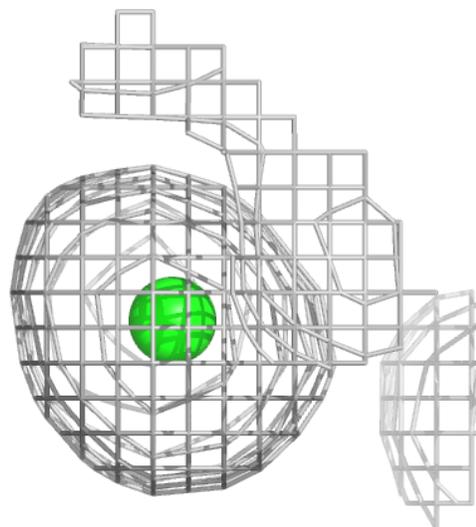
Electron density around CL A 206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
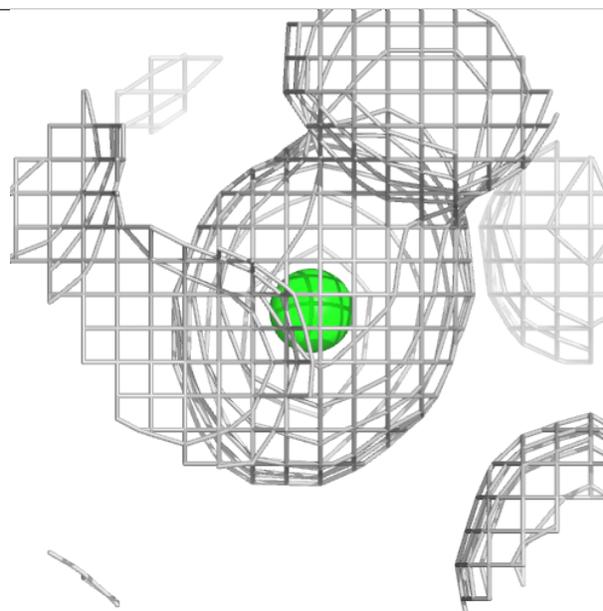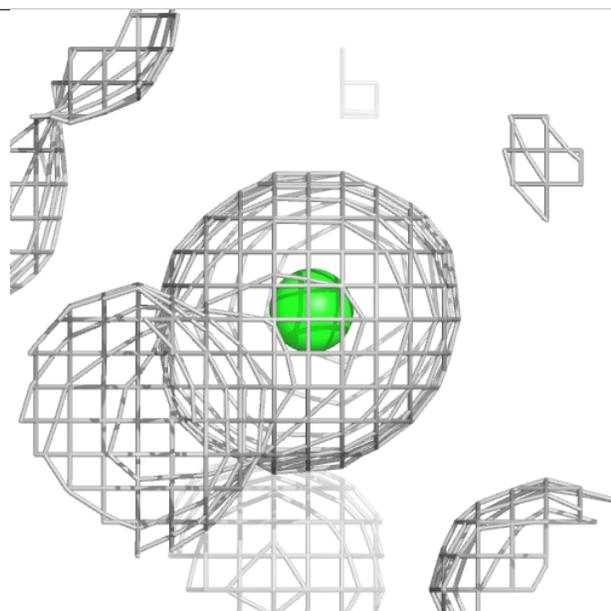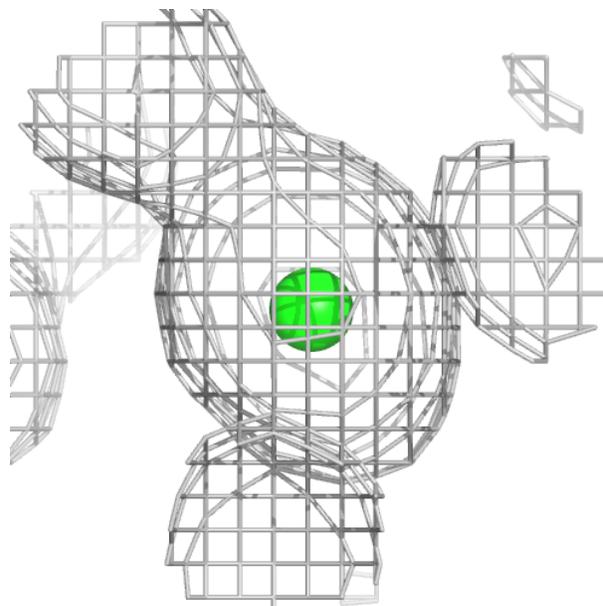
Electron density around CL G 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
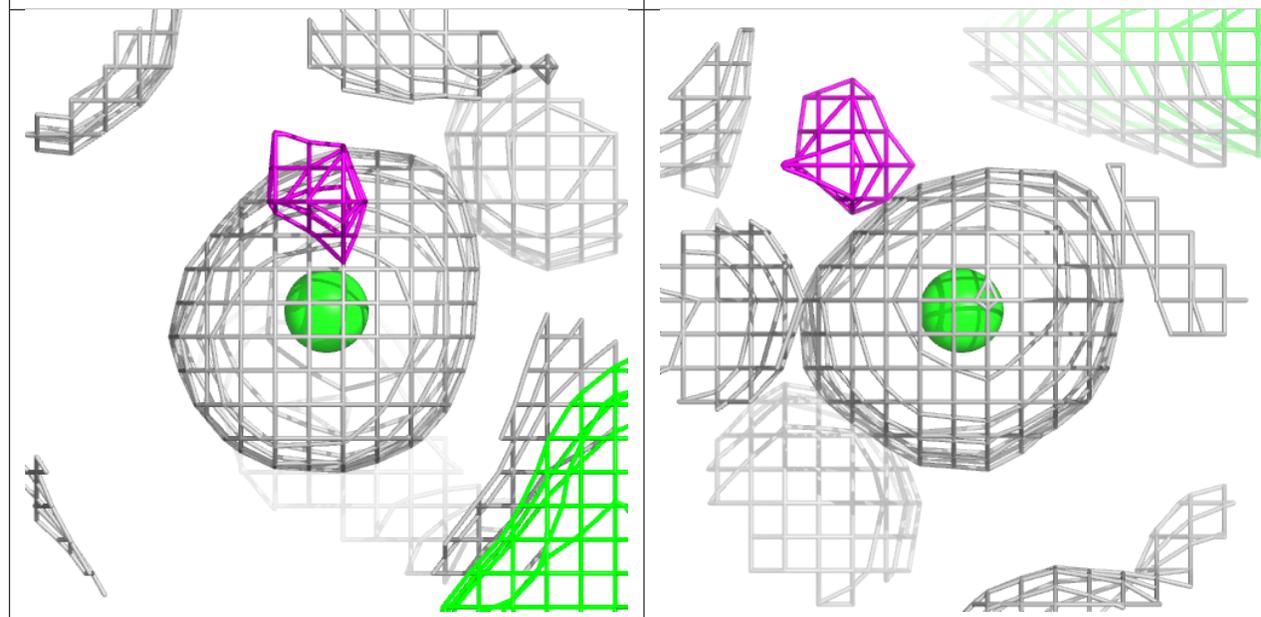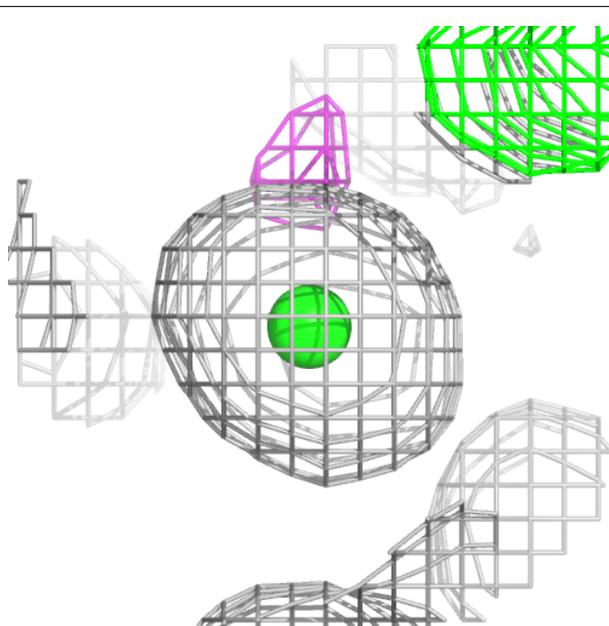
Electron density around CL D 202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
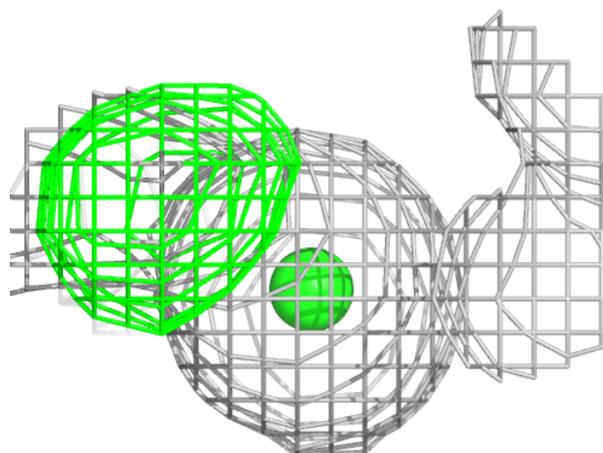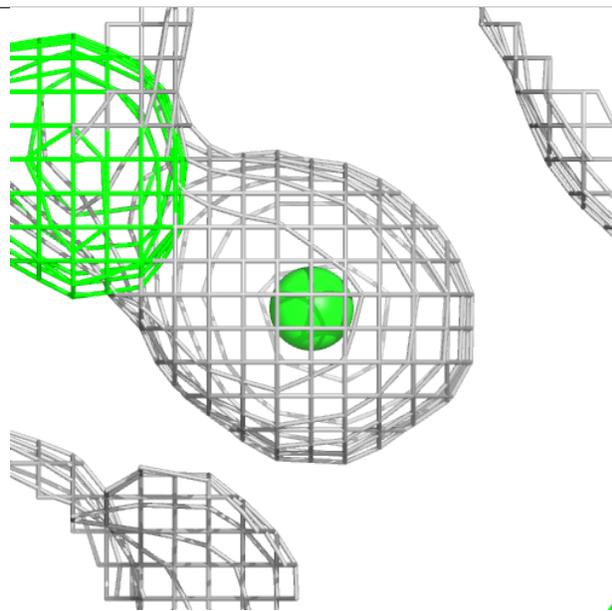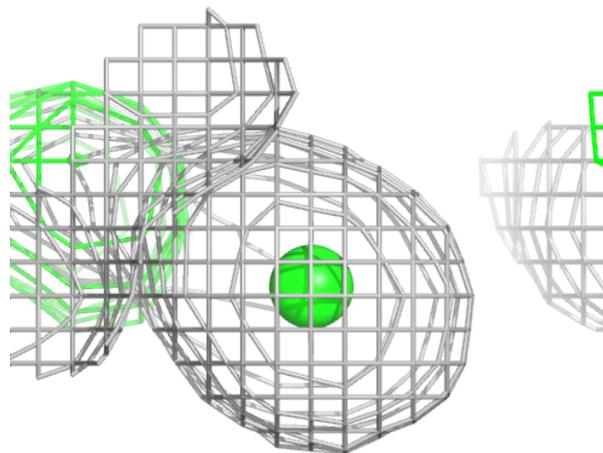
Electron density around CL D 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
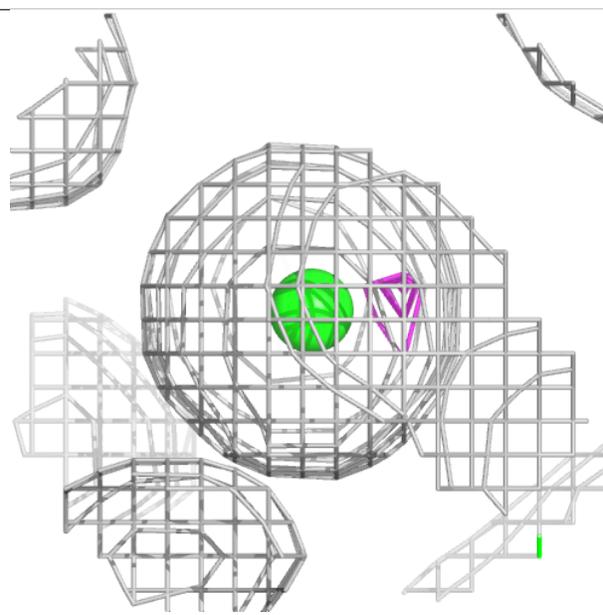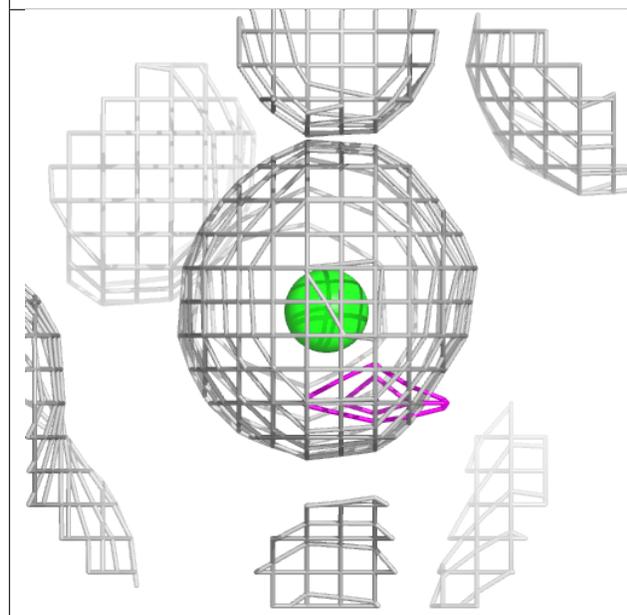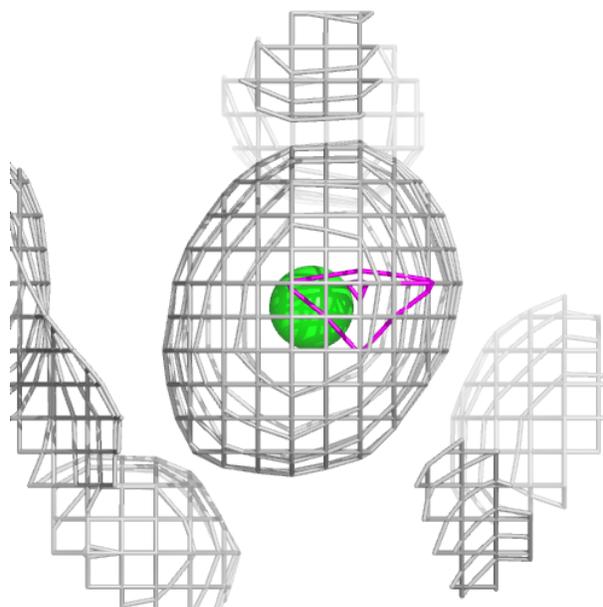
Electron density around CL G 305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
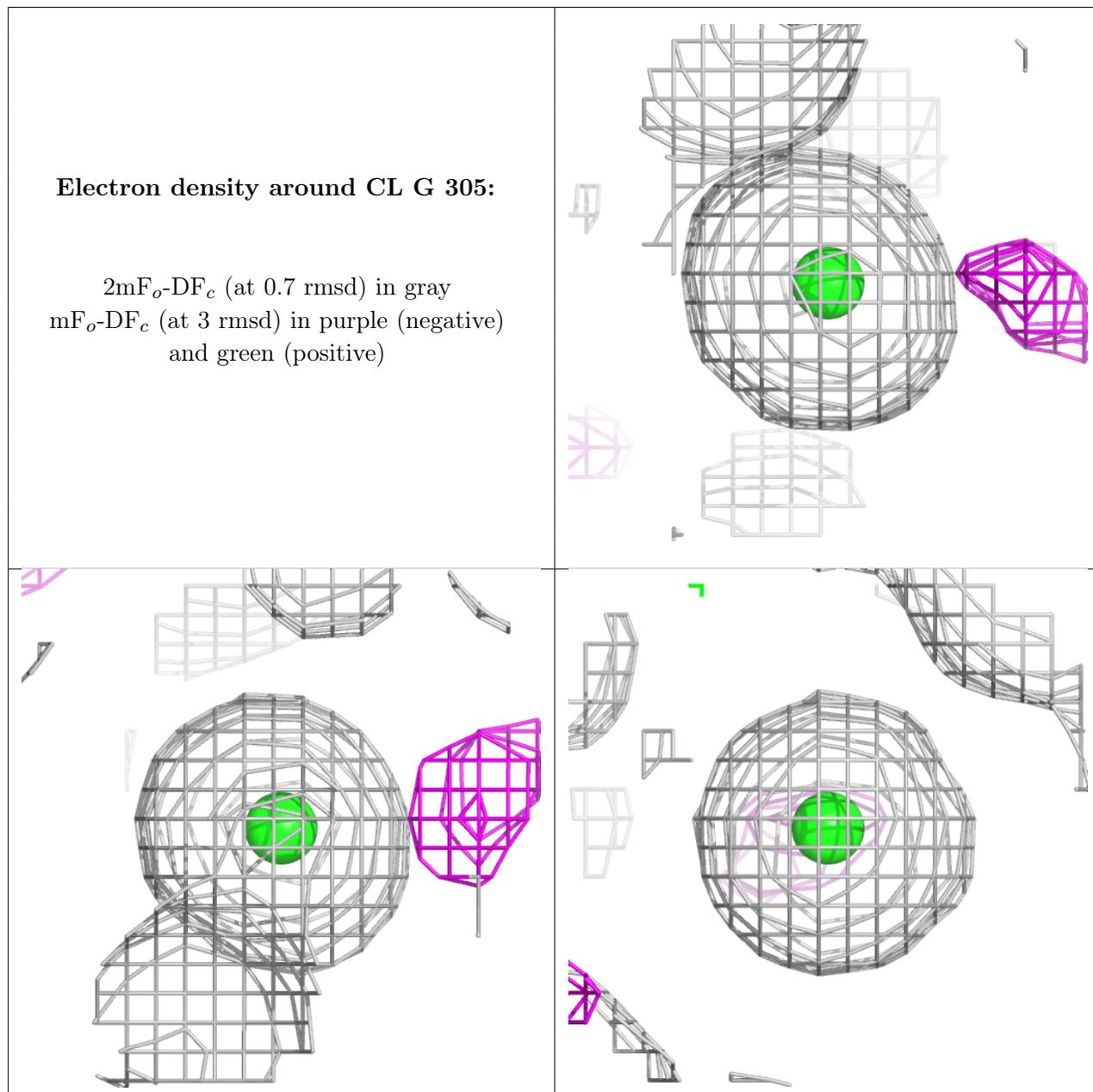
Electron density around CL H 202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
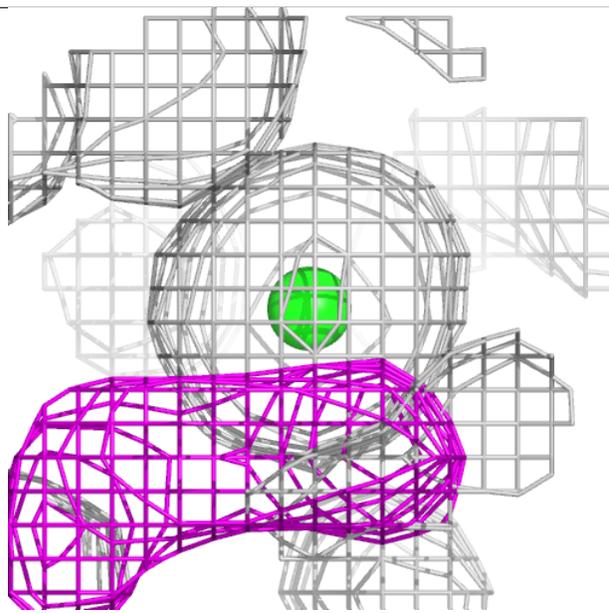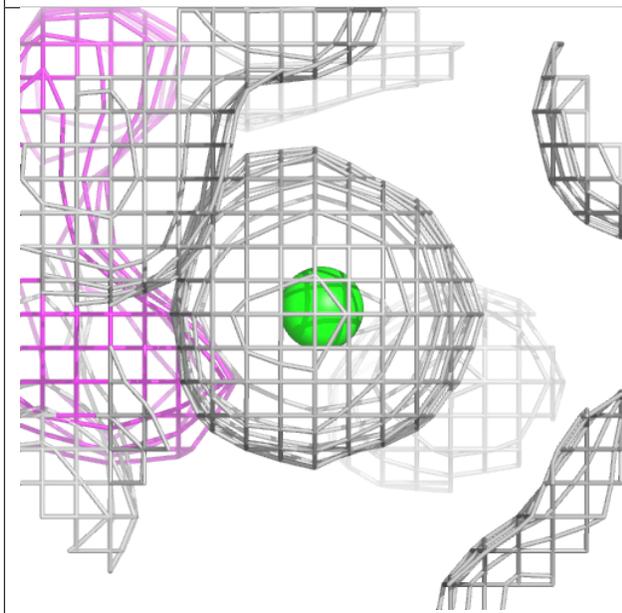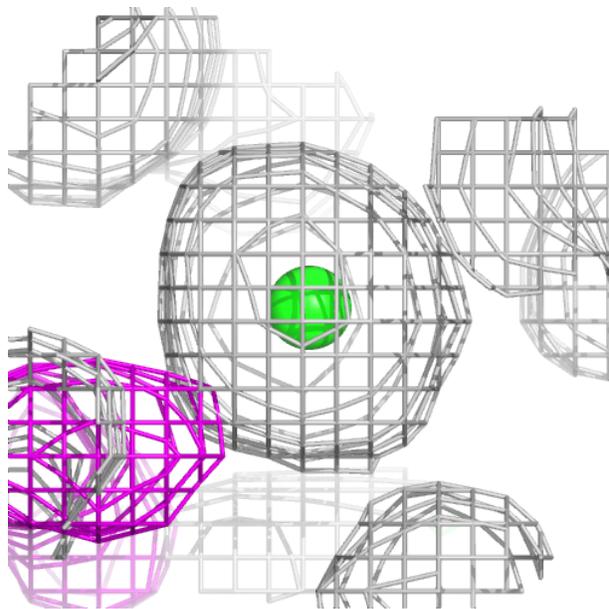
Electron density around CL H 203:

$2mF_o$-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 E 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
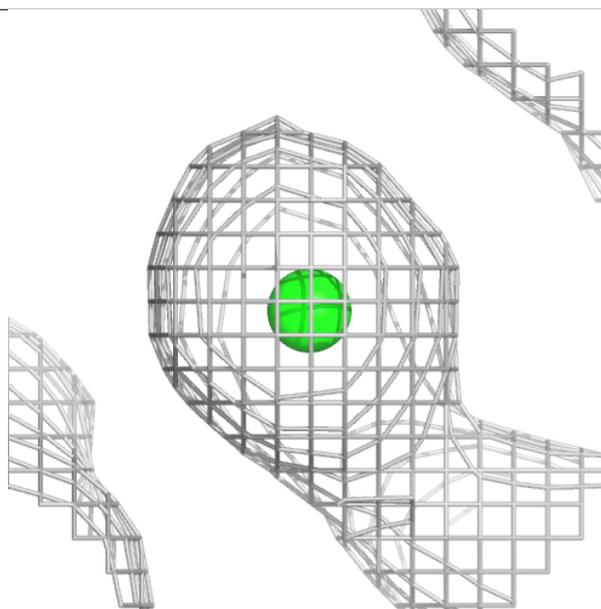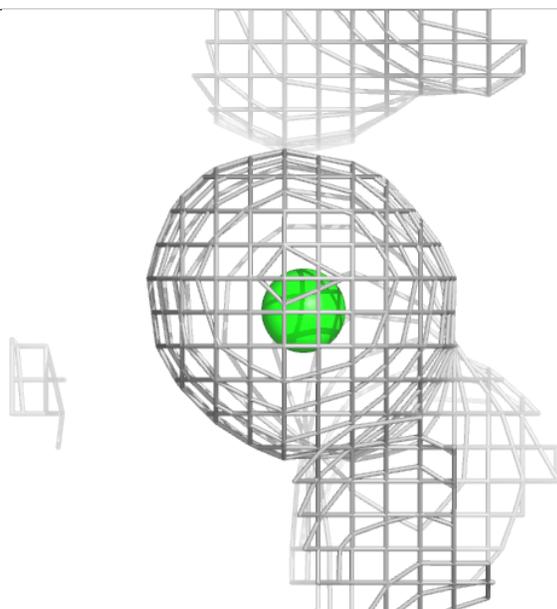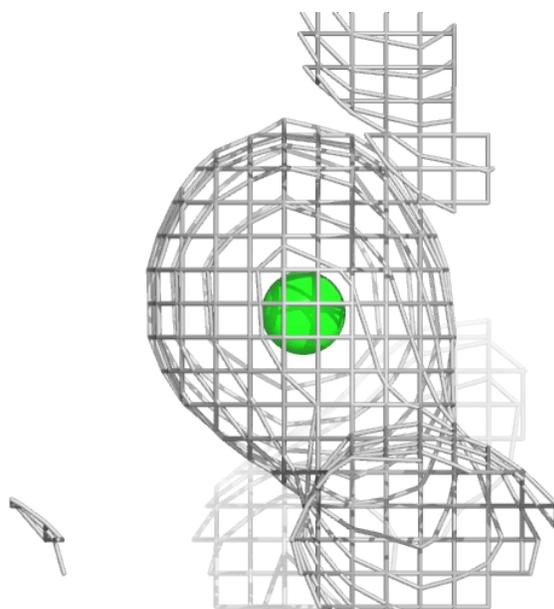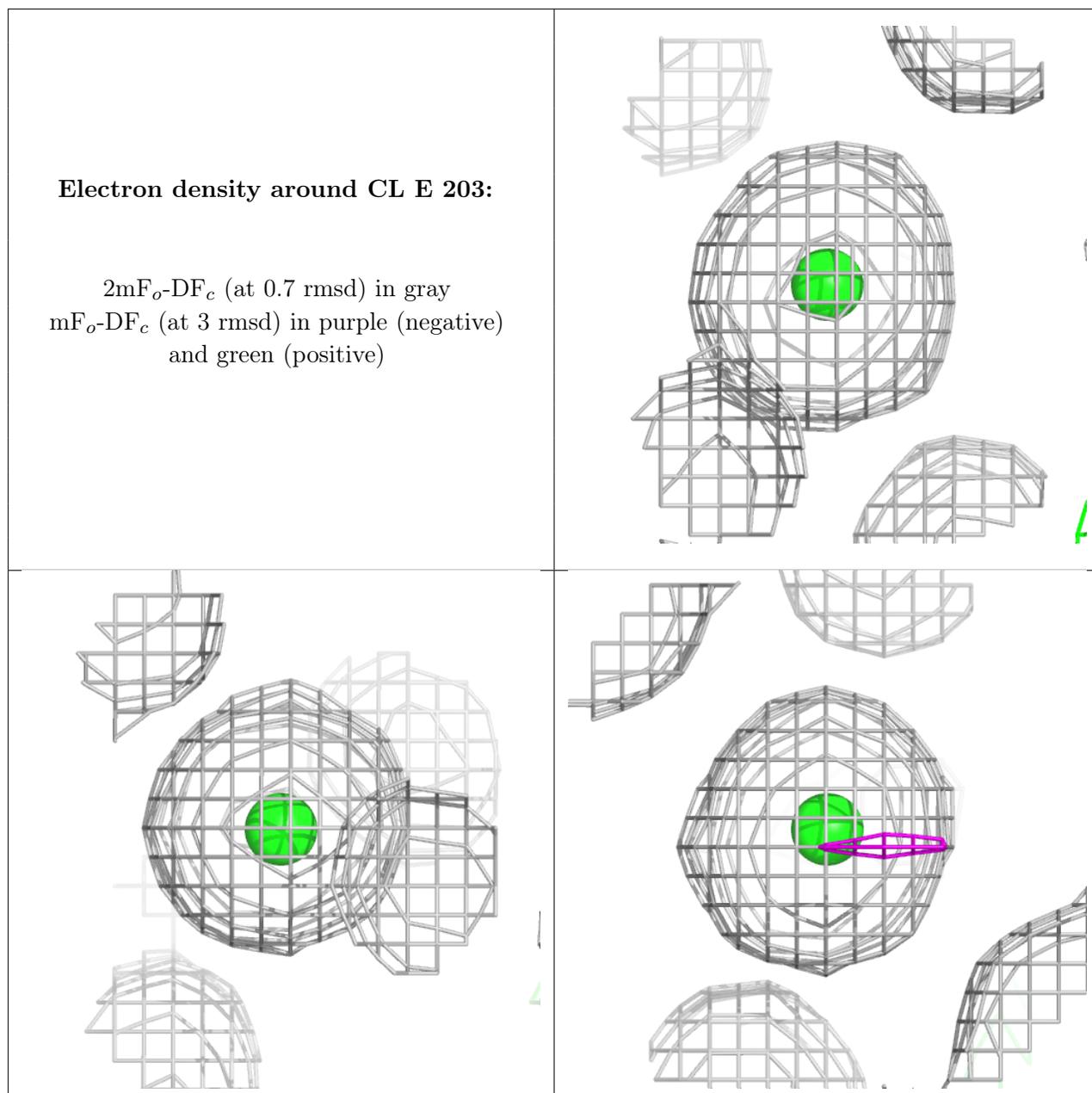
Electron density around CL E 204:

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

Electron density around CL B 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
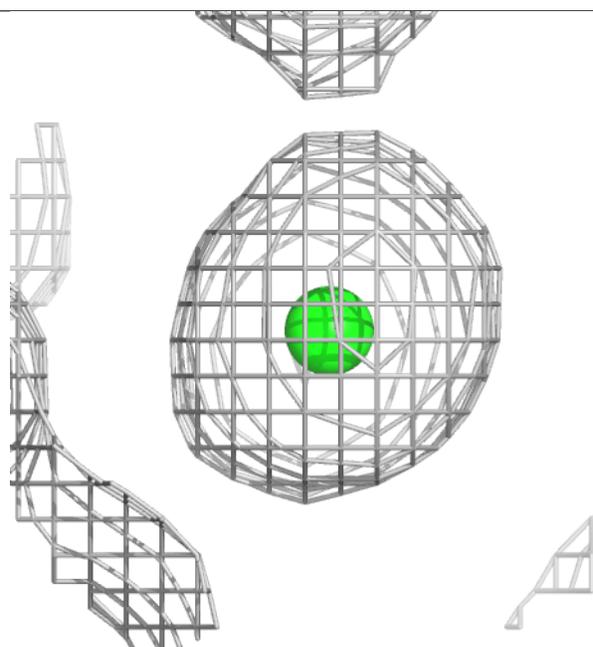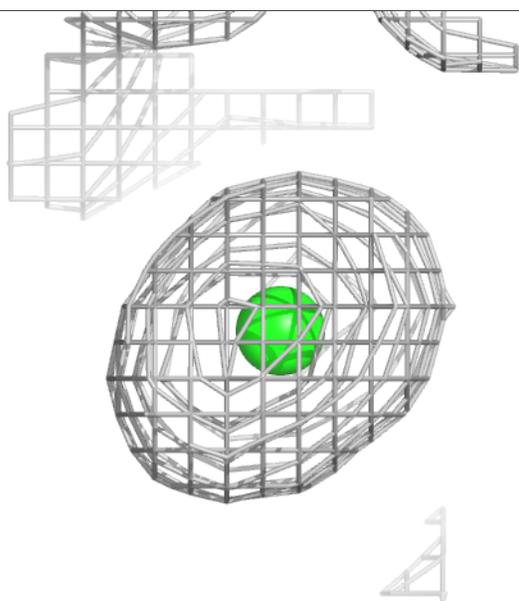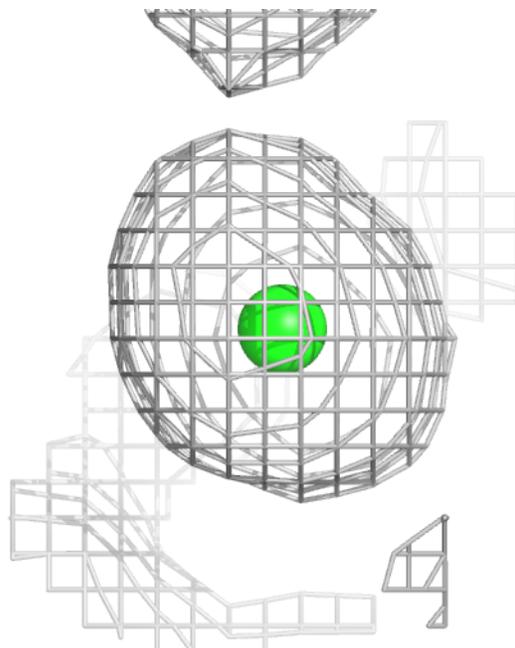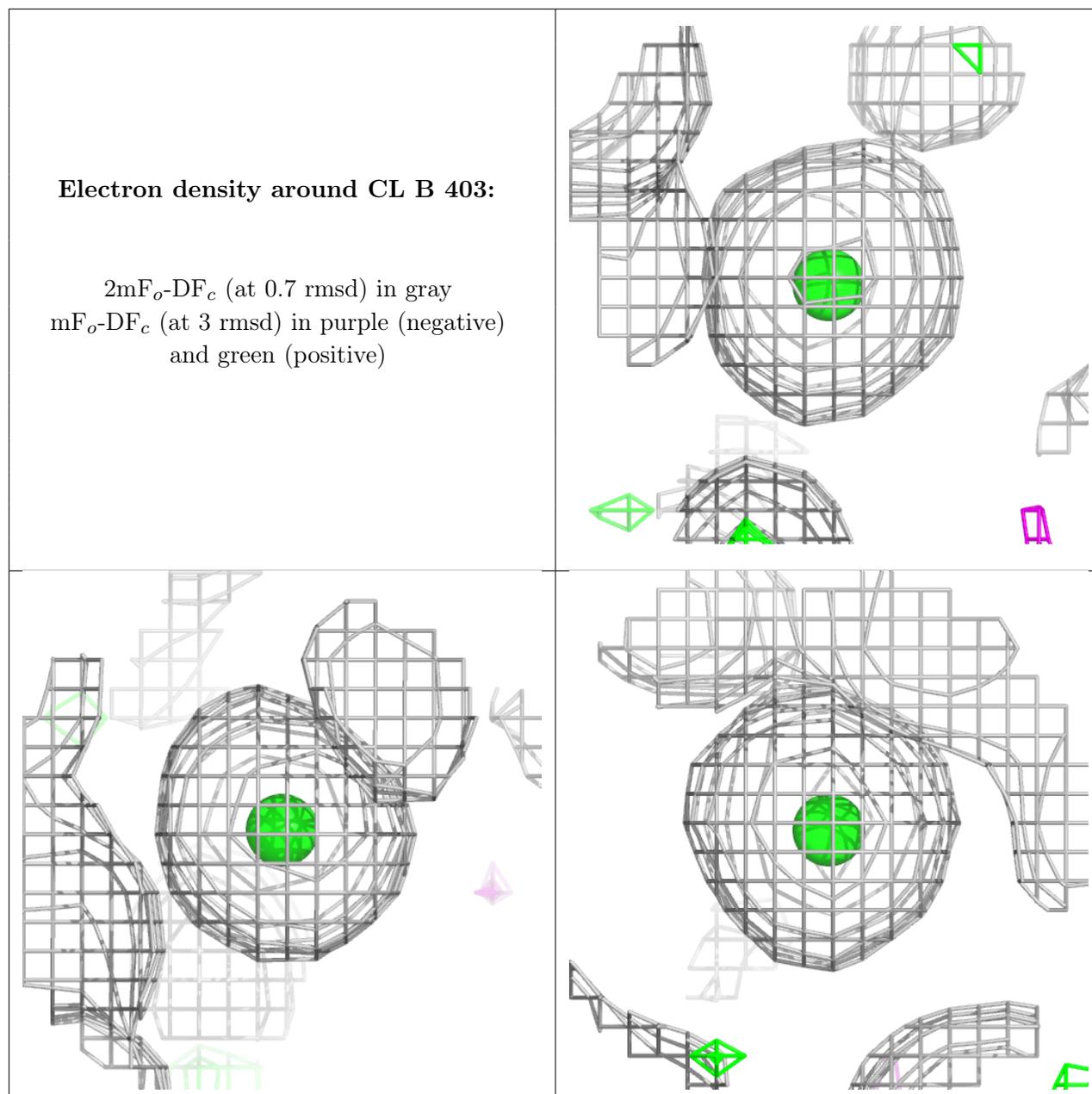
Electron density around CL B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
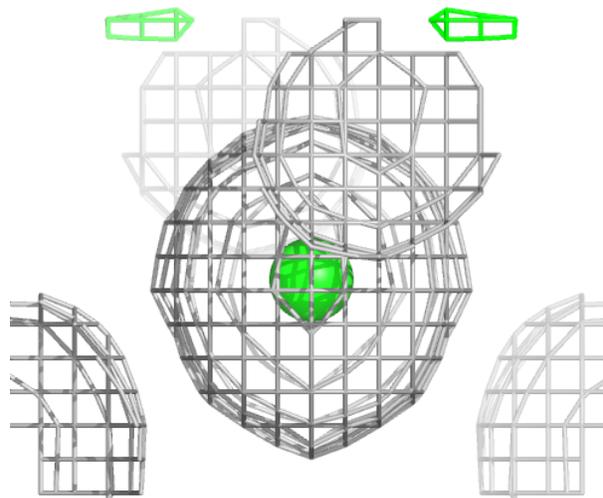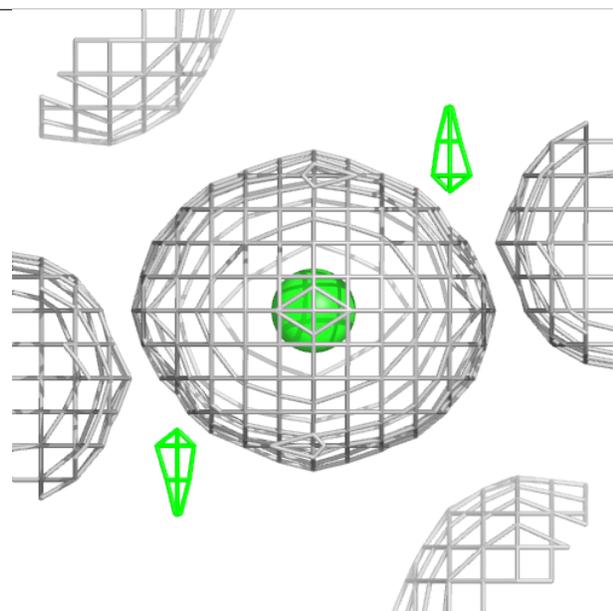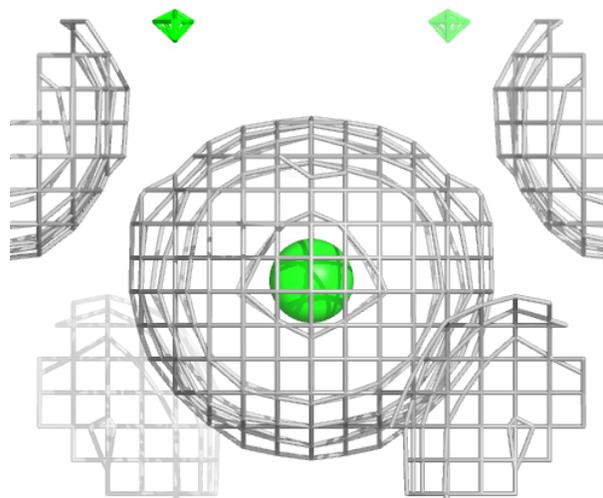
Electron density around CL C 202:

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

Electron density around CL C 203:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.