wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2026 – 01:39 pm BST

PDB ID	:	29TW / pdb_000029tw
Title	:	Crystal structure of a galactose oxidase 14G3 variant from Pseudoarthrobacter siccitolerans
Authors	:	Frazao, T.; Borges, P.T.; Martins, L.
Deposited on	:	2026-04-08
Resolution	:	2.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

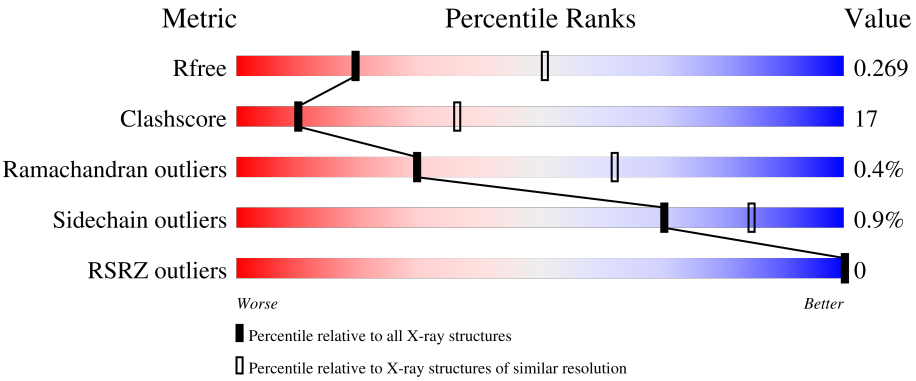
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	635	67% 29%
1	B	635	67% 30%
1	C	635	63% 33%
1	D	635	66% 30%
1	E	635	68% 28%

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Mol	Chain	Length	Quality of chain
1	F	635	65% 32%
1	G	635	68% 29%
1	H	635	70% 26%
1	I	635	65% 31%
1	J	635	69% 27%
1	K	635	67% 28%
1	L	635	64% 32%
1	M	635	63% 33%
1	N	635	66% 31%
1	O	635	65% 30%
1	P	635	66% 29%

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	J	801	-	X	-	-
2	GOL	L	802	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 71772 atoms, of which 72 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 Galactose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4497	2793	796	889	19			
1	B	620	Total	C	N	O	S	0	0	0
			4515	2804	800	891	20			
1	C	618	Total	C	N	O	S	0	0	0
			4497	2793	796	889	19			
1	D	612	Total	C	N	O	S	0	0	0
			4456	2768	790	879	19			
1	E	616	Total	C	N	O	S	0	0	0
			4484	2785	795	884	20			
1	F	620	Total	C	N	O	S	0	0	0
			4515	2804	800	891	20			
1	G	618	Total	C	N	O	S	0	0	0
			4497	2793	796	889	19			
1	H	610	Total	C	N	O	S	0	0	0
			4444	2762	787	876	19			
1	I	619	Total	C	N	O	S	0	0	0
			4505	2798	797	890	20			
1	J	611	Total	C	N	O	S	0	0	0
			4451	2766	788	878	19			
1	K	611	Total	C	N	O	S	0	0	0
			4450	2765	788	878	19			
1	L	612	Total	C	N	O	S	0	0	0
			4455	2768	789	879	19			
1	M	612	Total	C	N	O	S	0	0	0
			4455	2768	789	879	19			
1	N	619	Total	C	N	O	S	0	0	0
			4505	2798	797	890	20			
1	O	610	Total	C	N	O	S	0	0	0
			4444	2762	787	876	19			
1	P	609	Total	C	N	O	S	0	0	0
			4440	2760	786	875	19			

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	HIS	-	expression tag	UNP A0A024GZ97
A	127	HIS	-	expression tag	UNP A0A024GZ97
A	128	HIS	-	expression tag	UNP A0A024GZ97
A	129	HIS	-	expression tag	UNP A0A024GZ97
A	130	HIS	-	expression tag	UNP A0A024GZ97
A	131	HIS	-	expression tag	UNP A0A024GZ97
A	132	SER	-	expression tag	UNP A0A024GZ97
A	133	SER	-	expression tag	UNP A0A024GZ97
A	134	GLY	-	expression tag	UNP A0A024GZ97
A	135	LEU	-	expression tag	UNP A0A024GZ97
A	136	VAL	-	expression tag	UNP A0A024GZ97
A	137	PRO	-	expression tag	UNP A0A024GZ97
A	138	ARG	-	expression tag	UNP A0A024GZ97
A	139	GLY	-	expression tag	UNP A0A024GZ97
A	140	SER	-	expression tag	UNP A0A024GZ97
A	141	HIS	-	expression tag	UNP A0A024GZ97
A	142	MET	-	expression tag	UNP A0A024GZ97
A	247	THR	ASN	conflict	UNP A0A024GZ97
A	381	LYS	GLU	conflict	UNP A0A024GZ97
A	461	SER	PHE	conflict	UNP A0A024GZ97
A	485	LYS	GLU	conflict	UNP A0A024GZ97
A	511	SER	ASN	conflict	UNP A0A024GZ97
B	126	HIS	-	expression tag	UNP A0A024GZ97
B	127	HIS	-	expression tag	UNP A0A024GZ97
B	128	HIS	-	expression tag	UNP A0A024GZ97
B	129	HIS	-	expression tag	UNP A0A024GZ97
B	130	HIS	-	expression tag	UNP A0A024GZ97
B	131	HIS	-	expression tag	UNP A0A024GZ97
B	132	SER	-	expression tag	UNP A0A024GZ97
B	133	SER	-	expression tag	UNP A0A024GZ97
B	134	GLY	-	expression tag	UNP A0A024GZ97
B	135	LEU	-	expression tag	UNP A0A024GZ97
B	136	VAL	-	expression tag	UNP A0A024GZ97
B	137	PRO	-	expression tag	UNP A0A024GZ97
B	138	ARG	-	expression tag	UNP A0A024GZ97
B	139	GLY	-	expression tag	UNP A0A024GZ97
B	140	SER	-	expression tag	UNP A0A024GZ97
B	141	HIS	-	expression tag	UNP A0A024GZ97
B	142	MET	-	expression tag	UNP A0A024GZ97
B	247	THR	ASN	conflict	UNP A0A024GZ97
B	381	LYS	GLU	conflict	UNP A0A024GZ97
B	461	SER	PHE	conflict	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
B	485	LYS	GLU	conflict	UNP A0A024GZ97
B	511	SER	ASN	conflict	UNP A0A024GZ97
C	126	HIS	-	expression tag	UNP A0A024GZ97
C	127	HIS	-	expression tag	UNP A0A024GZ97
C	128	HIS	-	expression tag	UNP A0A024GZ97
C	129	HIS	-	expression tag	UNP A0A024GZ97
C	130	HIS	-	expression tag	UNP A0A024GZ97
C	131	HIS	-	expression tag	UNP A0A024GZ97
C	132	SER	-	expression tag	UNP A0A024GZ97
C	133	SER	-	expression tag	UNP A0A024GZ97
C	134	GLY	-	expression tag	UNP A0A024GZ97
C	135	LEU	-	expression tag	UNP A0A024GZ97
C	136	VAL	-	expression tag	UNP A0A024GZ97
C	137	PRO	-	expression tag	UNP A0A024GZ97
C	138	ARG	-	expression tag	UNP A0A024GZ97
C	139	GLY	-	expression tag	UNP A0A024GZ97
C	140	SER	-	expression tag	UNP A0A024GZ97
C	141	HIS	-	expression tag	UNP A0A024GZ97
C	142	MET	-	expression tag	UNP A0A024GZ97
C	247	THR	ASN	conflict	UNP A0A024GZ97
C	381	LYS	GLU	conflict	UNP A0A024GZ97
C	461	SER	PHE	conflict	UNP A0A024GZ97
C	485	LYS	GLU	conflict	UNP A0A024GZ97
C	511	SER	ASN	conflict	UNP A0A024GZ97
D	126	HIS	-	expression tag	UNP A0A024GZ97
D	127	HIS	-	expression tag	UNP A0A024GZ97
D	128	HIS	-	expression tag	UNP A0A024GZ97
D	129	HIS	-	expression tag	UNP A0A024GZ97
D	130	HIS	-	expression tag	UNP A0A024GZ97
D	131	HIS	-	expression tag	UNP A0A024GZ97
D	132	SER	-	expression tag	UNP A0A024GZ97
D	133	SER	-	expression tag	UNP A0A024GZ97
D	134	GLY	-	expression tag	UNP A0A024GZ97
D	135	LEU	-	expression tag	UNP A0A024GZ97
D	136	VAL	-	expression tag	UNP A0A024GZ97
D	137	PRO	-	expression tag	UNP A0A024GZ97
D	138	ARG	-	expression tag	UNP A0A024GZ97
D	139	GLY	-	expression tag	UNP A0A024GZ97
D	140	SER	-	expression tag	UNP A0A024GZ97
D	141	HIS	-	expression tag	UNP A0A024GZ97
D	142	MET	-	expression tag	UNP A0A024GZ97
D	247	THR	ASN	conflict	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
D	381	LYS	GLU	conflict	UNP A0A024GZ97
D	461	SER	PHE	conflict	UNP A0A024GZ97
D	485	LYS	GLU	conflict	UNP A0A024GZ97
D	511	SER	ASN	conflict	UNP A0A024GZ97
E	126	HIS	-	expression tag	UNP A0A024GZ97
E	127	HIS	-	expression tag	UNP A0A024GZ97
E	128	HIS	-	expression tag	UNP A0A024GZ97
E	129	HIS	-	expression tag	UNP A0A024GZ97
E	130	HIS	-	expression tag	UNP A0A024GZ97
E	131	HIS	-	expression tag	UNP A0A024GZ97
E	132	SER	-	expression tag	UNP A0A024GZ97
E	133	SER	-	expression tag	UNP A0A024GZ97
E	134	GLY	-	expression tag	UNP A0A024GZ97
E	135	LEU	-	expression tag	UNP A0A024GZ97
E	136	VAL	-	expression tag	UNP A0A024GZ97
E	137	PRO	-	expression tag	UNP A0A024GZ97
E	138	ARG	-	expression tag	UNP A0A024GZ97
E	139	GLY	-	expression tag	UNP A0A024GZ97
E	140	SER	-	expression tag	UNP A0A024GZ97
E	141	HIS	-	expression tag	UNP A0A024GZ97
E	142	MET	-	expression tag	UNP A0A024GZ97
E	247	THR	ASN	conflict	UNP A0A024GZ97
E	381	LYS	GLU	conflict	UNP A0A024GZ97
E	461	SER	PHE	conflict	UNP A0A024GZ97
E	485	LYS	GLU	conflict	UNP A0A024GZ97
E	511	SER	ASN	conflict	UNP A0A024GZ97
F	126	HIS	-	expression tag	UNP A0A024GZ97
F	127	HIS	-	expression tag	UNP A0A024GZ97
F	128	HIS	-	expression tag	UNP A0A024GZ97
F	129	HIS	-	expression tag	UNP A0A024GZ97
F	130	HIS	-	expression tag	UNP A0A024GZ97
F	131	HIS	-	expression tag	UNP A0A024GZ97
F	132	SER	-	expression tag	UNP A0A024GZ97
F	133	SER	-	expression tag	UNP A0A024GZ97
F	134	GLY	-	expression tag	UNP A0A024GZ97
F	135	LEU	-	expression tag	UNP A0A024GZ97
F	136	VAL	-	expression tag	UNP A0A024GZ97
F	137	PRO	-	expression tag	UNP A0A024GZ97
F	138	ARG	-	expression tag	UNP A0A024GZ97
F	139	GLY	-	expression tag	UNP A0A024GZ97
F	140	SER	-	expression tag	UNP A0A024GZ97
F	141	HIS	-	expression tag	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
F	142	MET	-	expression tag	UNP A0A024GZ97
F	247	THR	ASN	conflict	UNP A0A024GZ97
F	381	LYS	GLU	conflict	UNP A0A024GZ97
F	461	SER	PHE	conflict	UNP A0A024GZ97
F	485	LYS	GLU	conflict	UNP A0A024GZ97
F	511	SER	ASN	conflict	UNP A0A024GZ97
G	126	HIS	-	expression tag	UNP A0A024GZ97
G	127	HIS	-	expression tag	UNP A0A024GZ97
G	128	HIS	-	expression tag	UNP A0A024GZ97
G	129	HIS	-	expression tag	UNP A0A024GZ97
G	130	HIS	-	expression tag	UNP A0A024GZ97
G	131	HIS	-	expression tag	UNP A0A024GZ97
G	132	SER	-	expression tag	UNP A0A024GZ97
G	133	SER	-	expression tag	UNP A0A024GZ97
G	134	GLY	-	expression tag	UNP A0A024GZ97
G	135	LEU	-	expression tag	UNP A0A024GZ97
G	136	VAL	-	expression tag	UNP A0A024GZ97
G	137	PRO	-	expression tag	UNP A0A024GZ97
G	138	ARG	-	expression tag	UNP A0A024GZ97
G	139	GLY	-	expression tag	UNP A0A024GZ97
G	140	SER	-	expression tag	UNP A0A024GZ97
G	141	HIS	-	expression tag	UNP A0A024GZ97
G	142	MET	-	expression tag	UNP A0A024GZ97
G	247	THR	ASN	conflict	UNP A0A024GZ97
G	381	LYS	GLU	conflict	UNP A0A024GZ97
G	461	SER	PHE	conflict	UNP A0A024GZ97
G	485	LYS	GLU	conflict	UNP A0A024GZ97
G	511	SER	ASN	conflict	UNP A0A024GZ97
H	126	HIS	-	expression tag	UNP A0A024GZ97
H	127	HIS	-	expression tag	UNP A0A024GZ97
H	128	HIS	-	expression tag	UNP A0A024GZ97
H	129	HIS	-	expression tag	UNP A0A024GZ97
H	130	HIS	-	expression tag	UNP A0A024GZ97
H	131	HIS	-	expression tag	UNP A0A024GZ97
H	132	SER	-	expression tag	UNP A0A024GZ97
H	133	SER	-	expression tag	UNP A0A024GZ97
H	134	GLY	-	expression tag	UNP A0A024GZ97
H	135	LEU	-	expression tag	UNP A0A024GZ97
H	136	VAL	-	expression tag	UNP A0A024GZ97
H	137	PRO	-	expression tag	UNP A0A024GZ97
H	138	ARG	-	expression tag	UNP A0A024GZ97
H	139	GLY	-	expression tag	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
H	140	SER	-	expression tag	UNP A0A024GZ97
H	141	HIS	-	expression tag	UNP A0A024GZ97
H	142	MET	-	expression tag	UNP A0A024GZ97
H	247	THR	ASN	conflict	UNP A0A024GZ97
H	381	LYS	GLU	conflict	UNP A0A024GZ97
H	461	SER	PHE	conflict	UNP A0A024GZ97
H	485	LYS	GLU	conflict	UNP A0A024GZ97
H	511	SER	ASN	conflict	UNP A0A024GZ97
I	126	HIS	-	expression tag	UNP A0A024GZ97
I	127	HIS	-	expression tag	UNP A0A024GZ97
I	128	HIS	-	expression tag	UNP A0A024GZ97
I	129	HIS	-	expression tag	UNP A0A024GZ97
I	130	HIS	-	expression tag	UNP A0A024GZ97
I	131	HIS	-	expression tag	UNP A0A024GZ97
I	132	SER	-	expression tag	UNP A0A024GZ97
I	133	SER	-	expression tag	UNP A0A024GZ97
I	134	GLY	-	expression tag	UNP A0A024GZ97
I	135	LEU	-	expression tag	UNP A0A024GZ97
I	136	VAL	-	expression tag	UNP A0A024GZ97
I	137	PRO	-	expression tag	UNP A0A024GZ97
I	138	ARG	-	expression tag	UNP A0A024GZ97
I	139	GLY	-	expression tag	UNP A0A024GZ97
I	140	SER	-	expression tag	UNP A0A024GZ97
I	141	HIS	-	expression tag	UNP A0A024GZ97
I	142	MET	-	expression tag	UNP A0A024GZ97
I	247	THR	ASN	conflict	UNP A0A024GZ97
I	381	LYS	GLU	conflict	UNP A0A024GZ97
I	461	SER	PHE	conflict	UNP A0A024GZ97
I	485	LYS	GLU	conflict	UNP A0A024GZ97
I	511	SER	ASN	conflict	UNP A0A024GZ97
J	126	HIS	-	expression tag	UNP A0A024GZ97
J	127	HIS	-	expression tag	UNP A0A024GZ97
J	128	HIS	-	expression tag	UNP A0A024GZ97
J	129	HIS	-	expression tag	UNP A0A024GZ97
J	130	HIS	-	expression tag	UNP A0A024GZ97
J	131	HIS	-	expression tag	UNP A0A024GZ97
J	132	SER	-	expression tag	UNP A0A024GZ97
J	133	SER	-	expression tag	UNP A0A024GZ97
J	134	GLY	-	expression tag	UNP A0A024GZ97
J	135	LEU	-	expression tag	UNP A0A024GZ97
J	136	VAL	-	expression tag	UNP A0A024GZ97
J	137	PRO	-	expression tag	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
J	138	ARG	-	expression tag	UNP A0A024GZ97
J	139	GLY	-	expression tag	UNP A0A024GZ97
J	140	SER	-	expression tag	UNP A0A024GZ97
J	141	HIS	-	expression tag	UNP A0A024GZ97
J	142	MET	-	expression tag	UNP A0A024GZ97
J	247	THR	ASN	conflict	UNP A0A024GZ97
J	381	LYS	GLU	conflict	UNP A0A024GZ97
J	461	SER	PHE	conflict	UNP A0A024GZ97
J	485	LYS	GLU	conflict	UNP A0A024GZ97
J	511	SER	ASN	conflict	UNP A0A024GZ97
K	126	HIS	-	expression tag	UNP A0A024GZ97
K	127	HIS	-	expression tag	UNP A0A024GZ97
K	128	HIS	-	expression tag	UNP A0A024GZ97
K	129	HIS	-	expression tag	UNP A0A024GZ97
K	130	HIS	-	expression tag	UNP A0A024GZ97
K	131	HIS	-	expression tag	UNP A0A024GZ97
K	132	SER	-	expression tag	UNP A0A024GZ97
K	133	SER	-	expression tag	UNP A0A024GZ97
K	134	GLY	-	expression tag	UNP A0A024GZ97
K	135	LEU	-	expression tag	UNP A0A024GZ97
K	136	VAL	-	expression tag	UNP A0A024GZ97
K	137	PRO	-	expression tag	UNP A0A024GZ97
K	138	ARG	-	expression tag	UNP A0A024GZ97
K	139	GLY	-	expression tag	UNP A0A024GZ97
K	140	SER	-	expression tag	UNP A0A024GZ97
K	141	HIS	-	expression tag	UNP A0A024GZ97
K	142	MET	-	expression tag	UNP A0A024GZ97
K	247	THR	ASN	conflict	UNP A0A024GZ97
K	381	LYS	GLU	conflict	UNP A0A024GZ97
K	461	SER	PHE	conflict	UNP A0A024GZ97
K	485	LYS	GLU	conflict	UNP A0A024GZ97
K	511	SER	ASN	conflict	UNP A0A024GZ97
L	126	HIS	-	expression tag	UNP A0A024GZ97
L	127	HIS	-	expression tag	UNP A0A024GZ97
L	128	HIS	-	expression tag	UNP A0A024GZ97
L	129	HIS	-	expression tag	UNP A0A024GZ97
L	130	HIS	-	expression tag	UNP A0A024GZ97
L	131	HIS	-	expression tag	UNP A0A024GZ97
L	132	SER	-	expression tag	UNP A0A024GZ97
L	133	SER	-	expression tag	UNP A0A024GZ97
L	134	GLY	-	expression tag	UNP A0A024GZ97
L	135	LEU	-	expression tag	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
L	136	VAL	-	expression tag	UNP A0A024GZ97
L	137	PRO	-	expression tag	UNP A0A024GZ97
L	138	ARG	-	expression tag	UNP A0A024GZ97
L	139	GLY	-	expression tag	UNP A0A024GZ97
L	140	SER	-	expression tag	UNP A0A024GZ97
L	141	HIS	-	expression tag	UNP A0A024GZ97
L	142	MET	-	expression tag	UNP A0A024GZ97
L	247	THR	ASN	conflict	UNP A0A024GZ97
L	381	LYS	GLU	conflict	UNP A0A024GZ97
L	461	SER	PHE	conflict	UNP A0A024GZ97
L	485	LYS	GLU	conflict	UNP A0A024GZ97
L	511	SER	ASN	conflict	UNP A0A024GZ97
M	126	HIS	-	expression tag	UNP A0A024GZ97
M	127	HIS	-	expression tag	UNP A0A024GZ97
M	128	HIS	-	expression tag	UNP A0A024GZ97
M	129	HIS	-	expression tag	UNP A0A024GZ97
M	130	HIS	-	expression tag	UNP A0A024GZ97
M	131	HIS	-	expression tag	UNP A0A024GZ97
M	132	SER	-	expression tag	UNP A0A024GZ97
M	133	SER	-	expression tag	UNP A0A024GZ97
M	134	GLY	-	expression tag	UNP A0A024GZ97
M	135	LEU	-	expression tag	UNP A0A024GZ97
M	136	VAL	-	expression tag	UNP A0A024GZ97
M	137	PRO	-	expression tag	UNP A0A024GZ97
M	138	ARG	-	expression tag	UNP A0A024GZ97
M	139	GLY	-	expression tag	UNP A0A024GZ97
M	140	SER	-	expression tag	UNP A0A024GZ97
M	141	HIS	-	expression tag	UNP A0A024GZ97
M	142	MET	-	expression tag	UNP A0A024GZ97
M	247	THR	ASN	conflict	UNP A0A024GZ97
M	381	LYS	GLU	conflict	UNP A0A024GZ97
M	461	SER	PHE	conflict	UNP A0A024GZ97
M	485	LYS	GLU	conflict	UNP A0A024GZ97
M	511	SER	ASN	conflict	UNP A0A024GZ97
N	126	HIS	-	expression tag	UNP A0A024GZ97
N	127	HIS	-	expression tag	UNP A0A024GZ97
N	128	HIS	-	expression tag	UNP A0A024GZ97
N	129	HIS	-	expression tag	UNP A0A024GZ97
N	130	HIS	-	expression tag	UNP A0A024GZ97
N	131	HIS	-	expression tag	UNP A0A024GZ97
N	132	SER	-	expression tag	UNP A0A024GZ97
N	133	SER	-	expression tag	UNP A0A024GZ97

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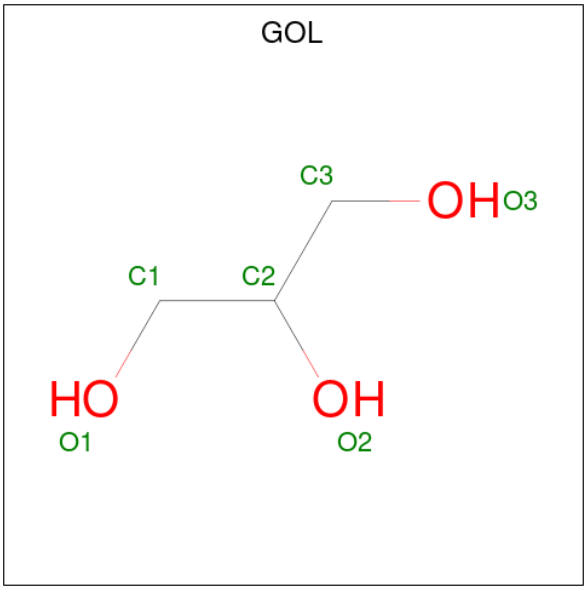
Chain	Residue	Modelled	Actual	Comment	Reference
N	134	GLY	-	expression tag	UNP A0A024GZ97
N	135	LEU	-	expression tag	UNP A0A024GZ97
N	136	VAL	-	expression tag	UNP A0A024GZ97
N	137	PRO	-	expression tag	UNP A0A024GZ97
N	138	ARG	-	expression tag	UNP A0A024GZ97
N	139	GLY	-	expression tag	UNP A0A024GZ97
N	140	SER	-	expression tag	UNP A0A024GZ97
N	141	HIS	-	expression tag	UNP A0A024GZ97
N	142	MET	-	expression tag	UNP A0A024GZ97
N	247	THR	ASN	conflict	UNP A0A024GZ97
N	381	LYS	GLU	conflict	UNP A0A024GZ97
N	461	SER	PHE	conflict	UNP A0A024GZ97
N	485	LYS	GLU	conflict	UNP A0A024GZ97
N	511	SER	ASN	conflict	UNP A0A024GZ97
O	126	HIS	-	expression tag	UNP A0A024GZ97
O	127	HIS	-	expression tag	UNP A0A024GZ97
O	128	HIS	-	expression tag	UNP A0A024GZ97
O	129	HIS	-	expression tag	UNP A0A024GZ97
O	130	HIS	-	expression tag	UNP A0A024GZ97
O	131	HIS	-	expression tag	UNP A0A024GZ97
O	132	SER	-	expression tag	UNP A0A024GZ97
O	133	SER	-	expression tag	UNP A0A024GZ97
O	134	GLY	-	expression tag	UNP A0A024GZ97
O	135	LEU	-	expression tag	UNP A0A024GZ97
O	136	VAL	-	expression tag	UNP A0A024GZ97
O	137	PRO	-	expression tag	UNP A0A024GZ97
O	138	ARG	-	expression tag	UNP A0A024GZ97
O	139	GLY	-	expression tag	UNP A0A024GZ97
O	140	SER	-	expression tag	UNP A0A024GZ97
O	141	HIS	-	expression tag	UNP A0A024GZ97
O	142	MET	-	expression tag	UNP A0A024GZ97
O	247	THR	ASN	conflict	UNP A0A024GZ97
O	381	LYS	GLU	conflict	UNP A0A024GZ97
O	461	SER	PHE	conflict	UNP A0A024GZ97
O	485	LYS	GLU	conflict	UNP A0A024GZ97
O	511	SER	ASN	conflict	UNP A0A024GZ97
P	126	HIS	-	expression tag	UNP A0A024GZ97
P	127	HIS	-	expression tag	UNP A0A024GZ97
P	128	HIS	-	expression tag	UNP A0A024GZ97
P	129	HIS	-	expression tag	UNP A0A024GZ97
P	130	HIS	-	expression tag	UNP A0A024GZ97
P	131	HIS	-	expression tag	UNP A0A024GZ97

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Chain	Residue	Modelled	Actual	Comment	Reference
P	132	SER	-	expression tag	UNP A0A024GZ97
P	133	SER	-	expression tag	UNP A0A024GZ97
P	134	GLY	-	expression tag	UNP A0A024GZ97
P	135	LEU	-	expression tag	UNP A0A024GZ97
P	136	VAL	-	expression tag	UNP A0A024GZ97
P	137	PRO	-	expression tag	UNP A0A024GZ97
P	138	ARG	-	expression tag	UNP A0A024GZ97
P	139	GLY	-	expression tag	UNP A0A024GZ97
P	140	SER	-	expression tag	UNP A0A024GZ97
P	141	HIS	-	expression tag	UNP A0A024GZ97
P	142	MET	-	expression tag	UNP A0A024GZ97
P	247	THR	ASN	conflict	UNP A0A024GZ97
P	381	LYS	GLU	conflict	UNP A0A024GZ97
P	461	SER	PHE	conflict	UNP A0A024GZ97
P	485	LYS	GLU	conflict	UNP A0A024GZ97
P	511	SER	ASN	conflict	UNP A0A024GZ97

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



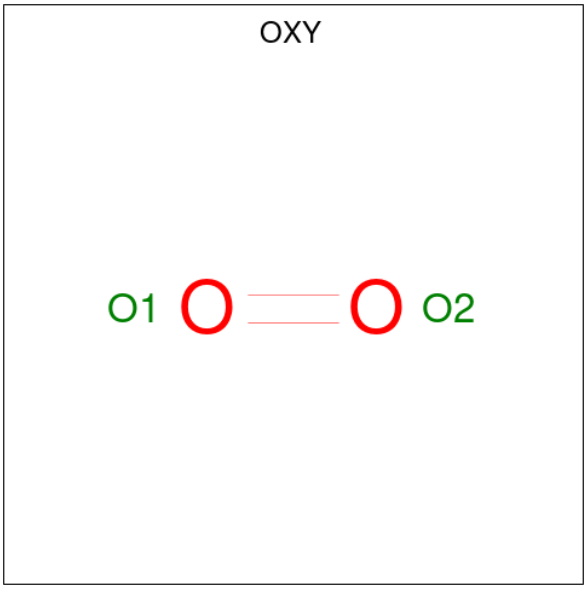
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total C H O 14 3 8 3	0	0
2	L	1	Total C H O 14 3 8 3	0	0
2	L	1	Total C H O 14 3 8 3	0	0
2	M	1	Total C H O 14 3 8 3	0	0
2	O	1	Total C H O 14 3 8 3	0	0
2	P	1	Total C H O 14 3 8 3	0	0

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	E	1	Total O 2 2	0	0
3	F	1	Total O 2 2	0	0
3	G	1	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O 2 2	0	0
3	K	1	Total O 2 2	0	0
3	M	1	Total O 2 2	0	0
3	N	1	Total O 2 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0
4	N	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 1 1	0	0
5	O	1	Total O 1 1	0	0

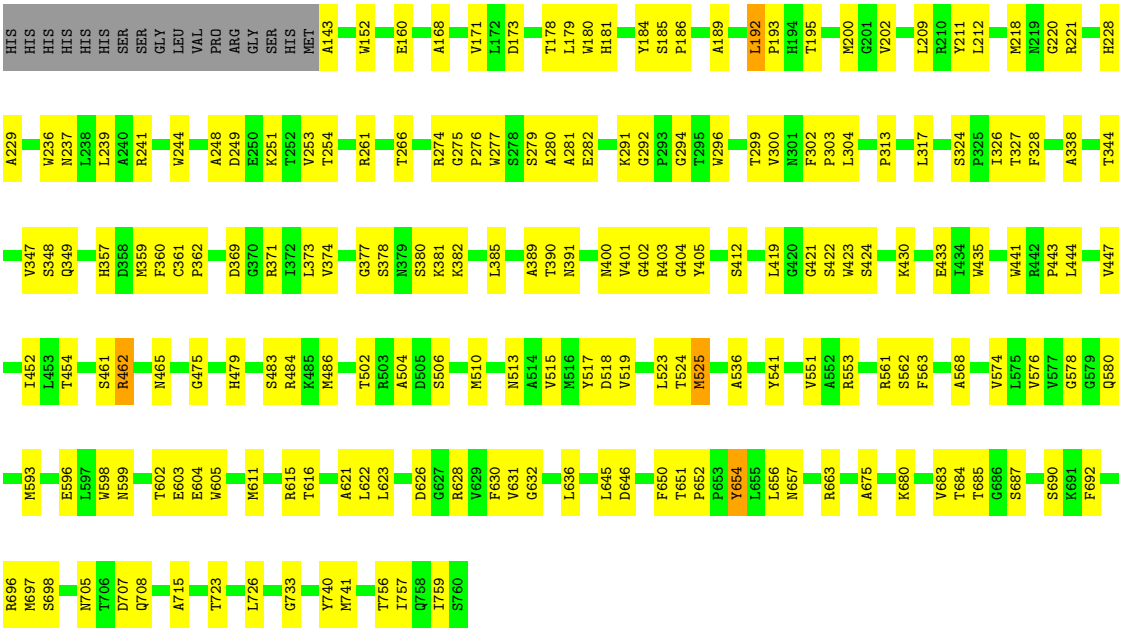
3 Residue-property plots (i)

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: Galactose oxidase

Chain A:

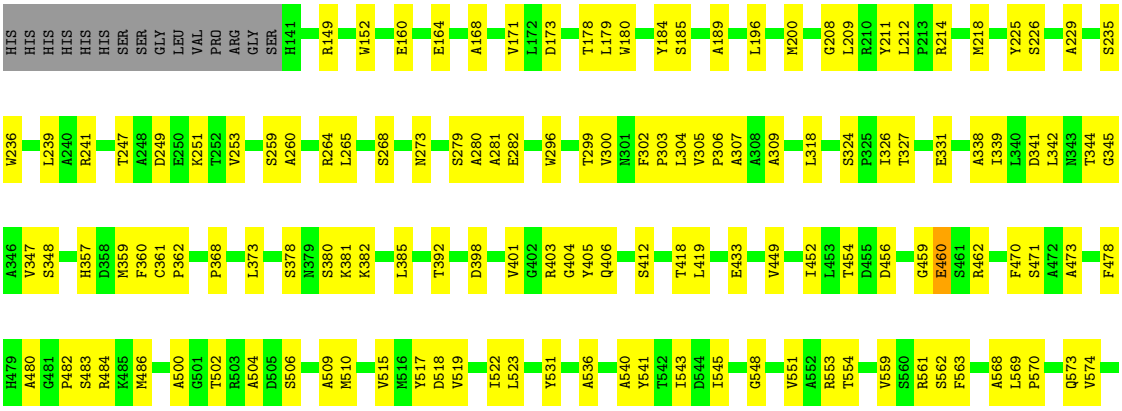


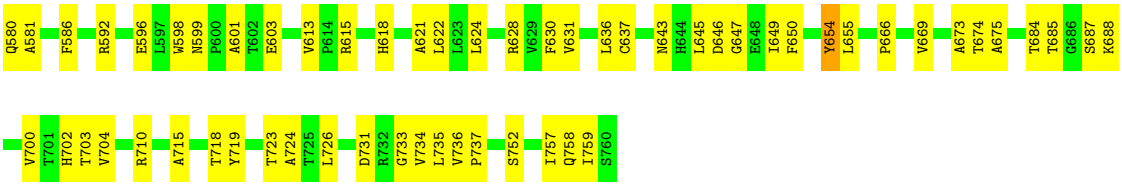


• Molecule 1: Galactose oxidase

Chain B:



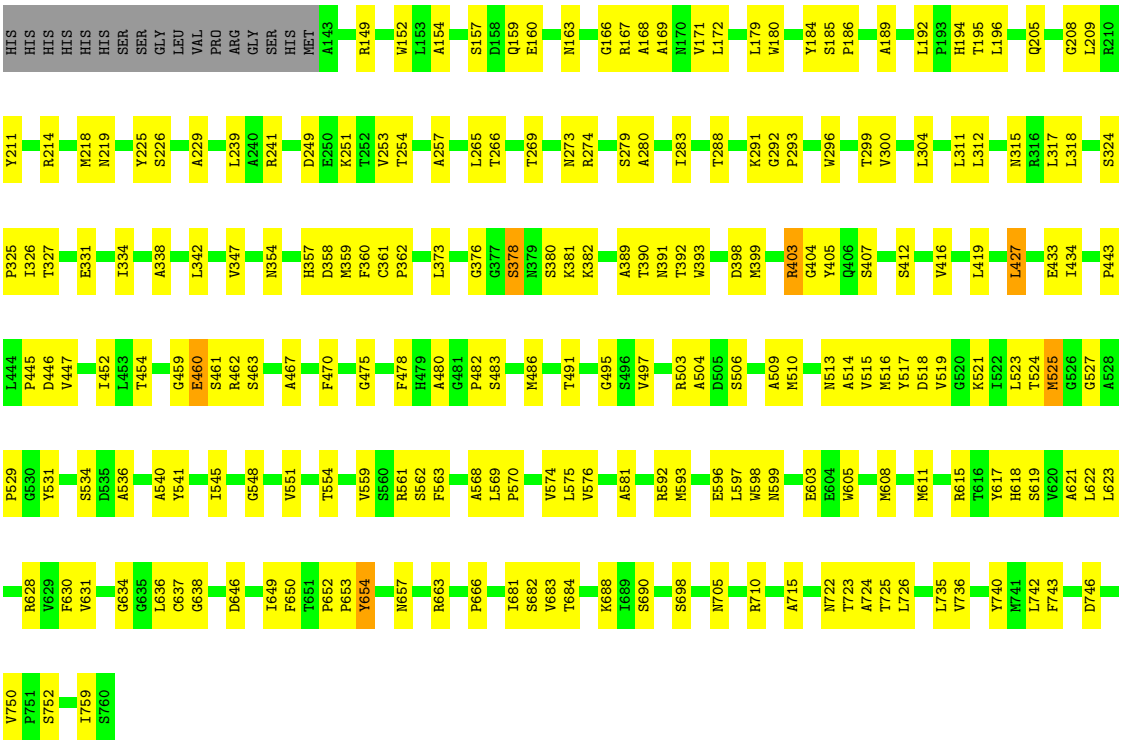




• Molecule 1: Galactose oxidase

Chain C:

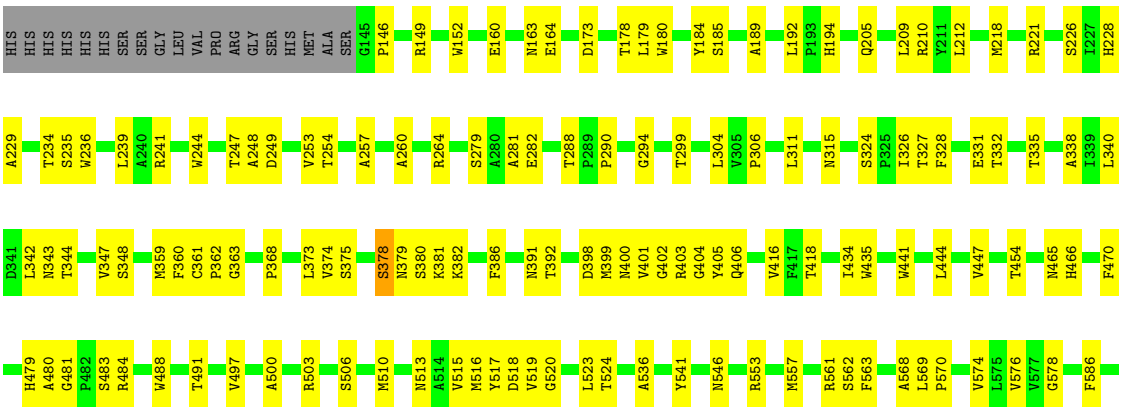


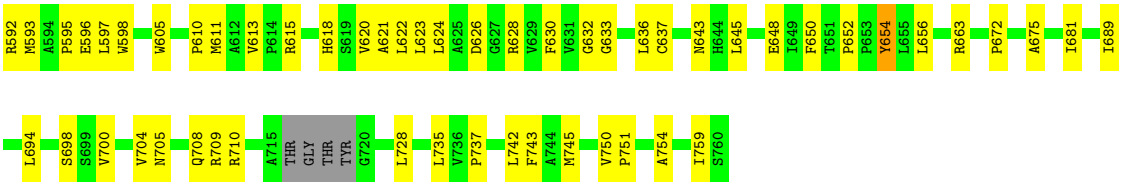


• Molecule 1: Galactose oxidase

Chain D:



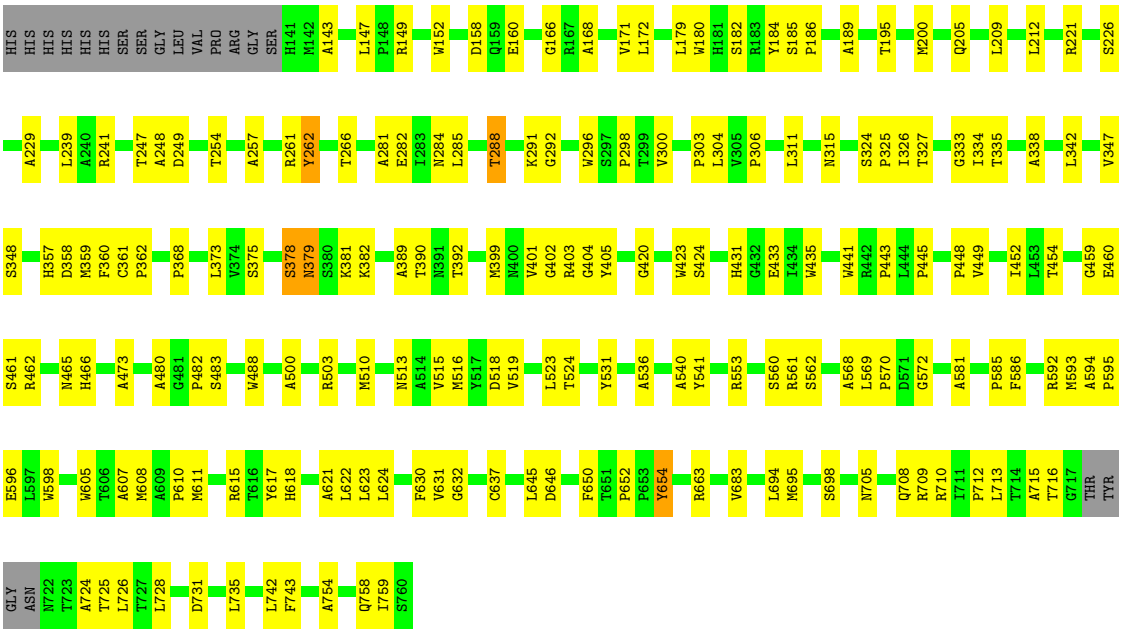




• Molecule 1: Galactose oxidase

Chain E:

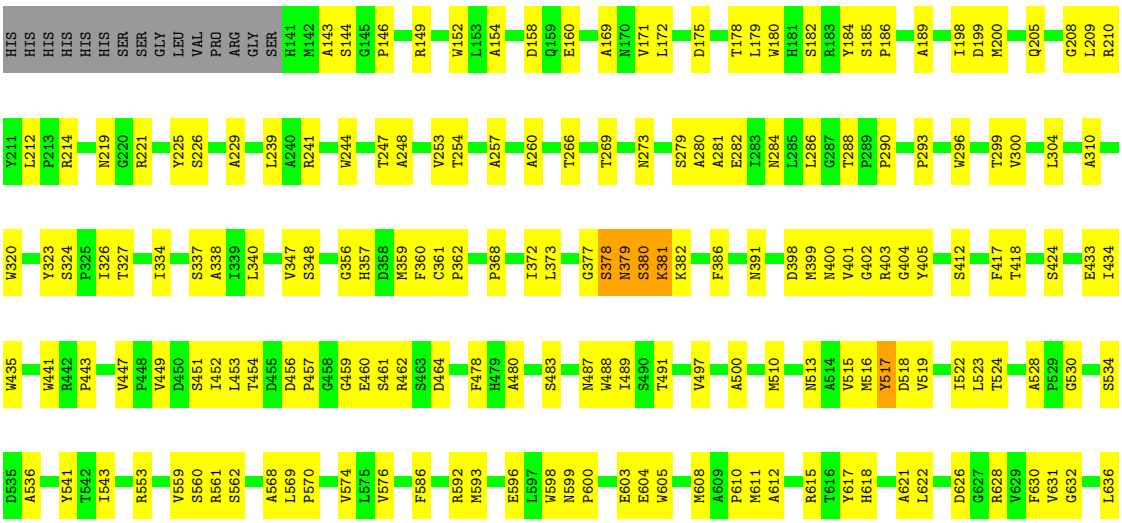




• Molecule 1: Galactose oxidase

Chain F:



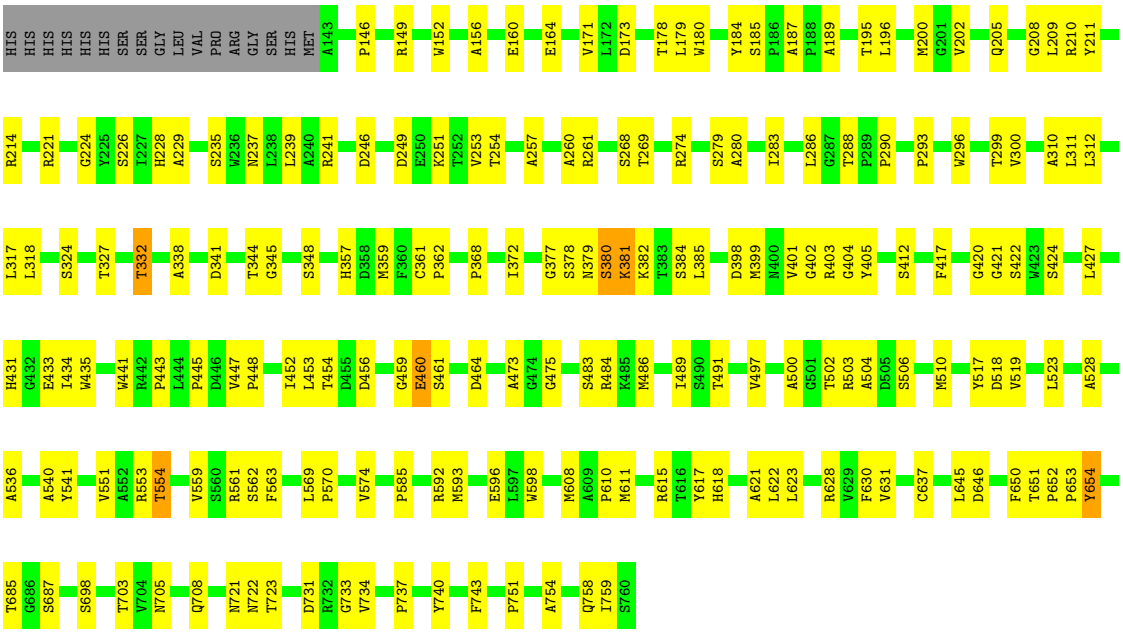




• Molecule 1: Galactose oxidase

Chain G:

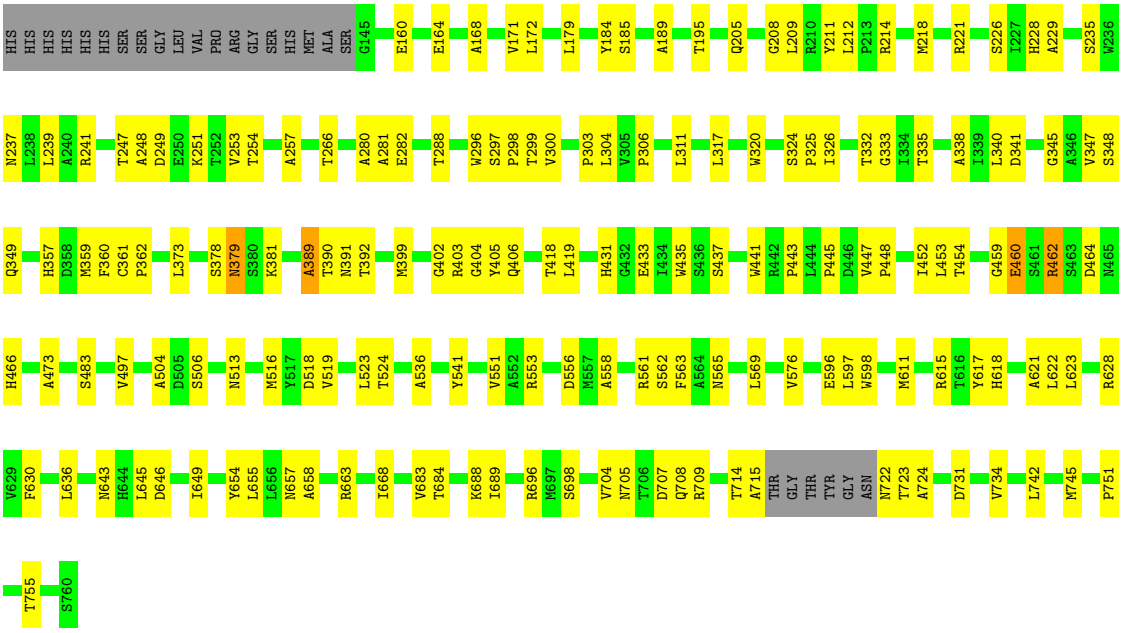




• Molecule 1: Galactose oxidase

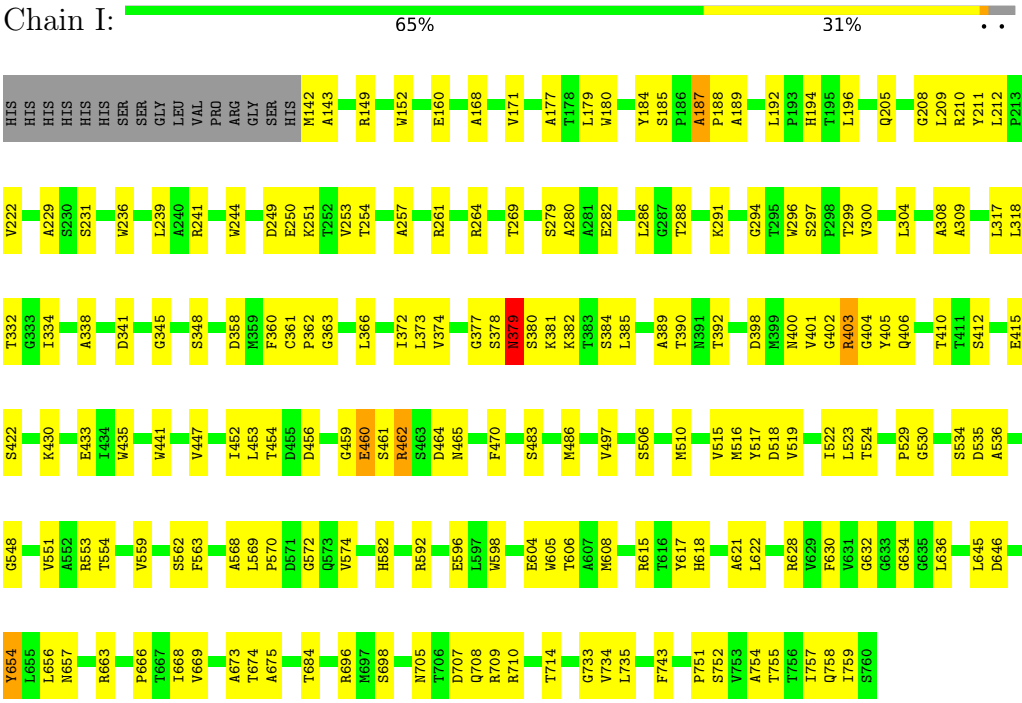
Chain H:





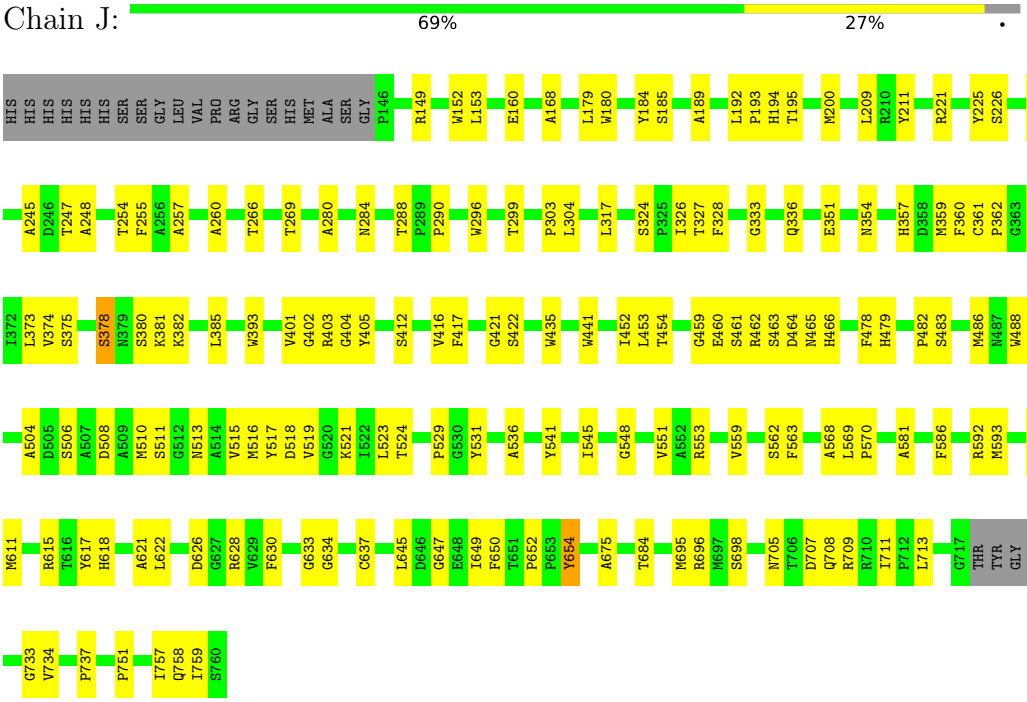
• Molecule 1: Galactose oxidase

Chain I:



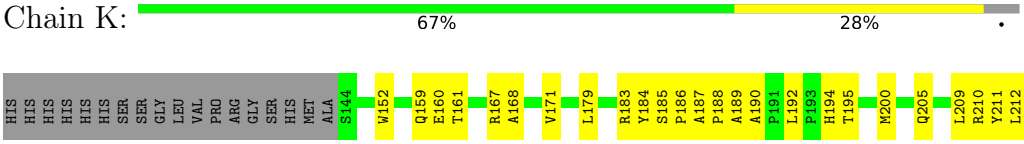
• Molecule 1: Galactose oxidase

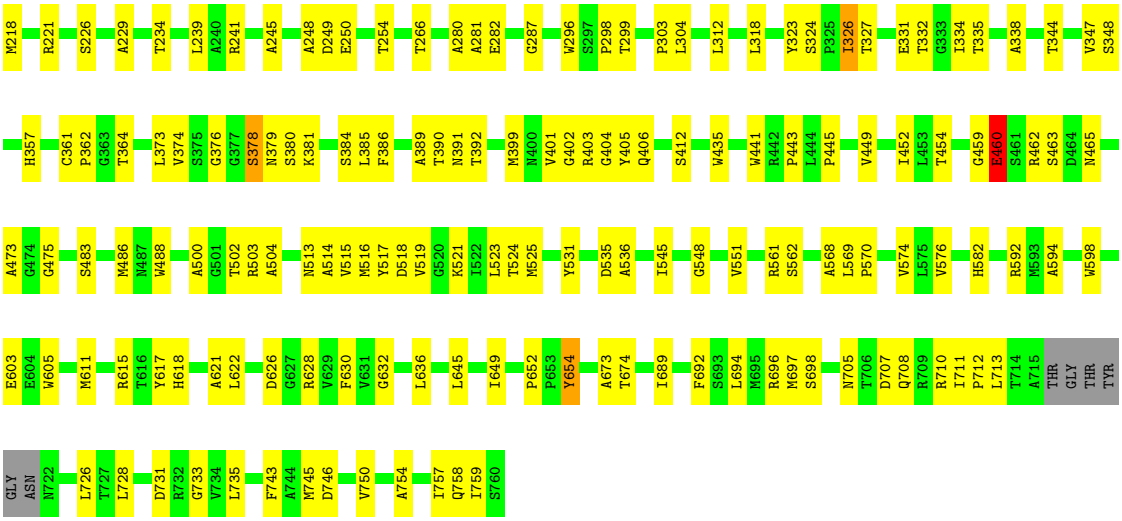
Chain J:



• Molecule 1: Galactose oxidase

Chain K:

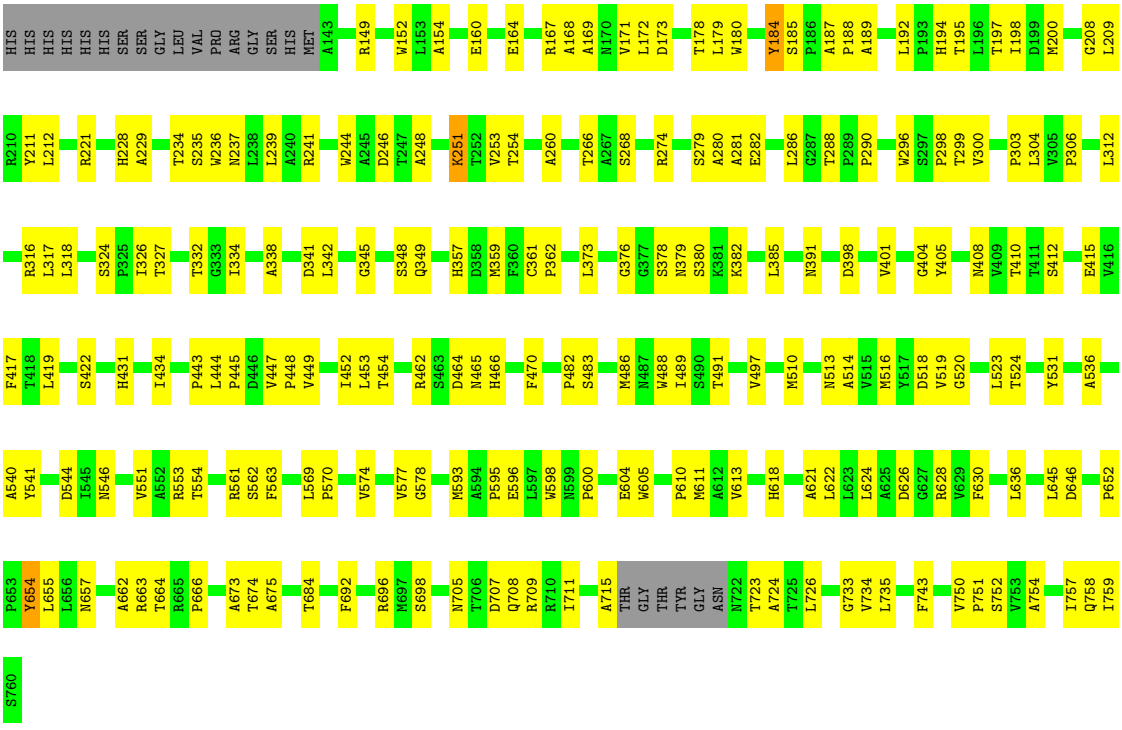




• Molecule 1: Galactose oxidase

Chain L:

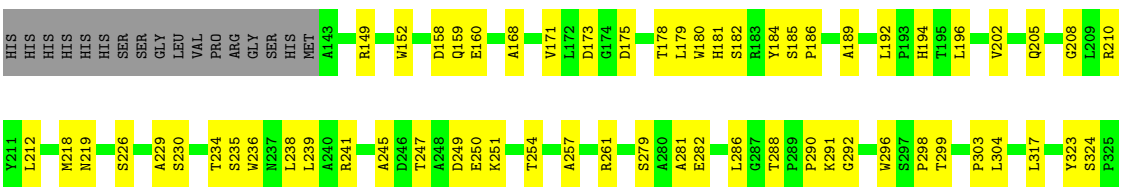


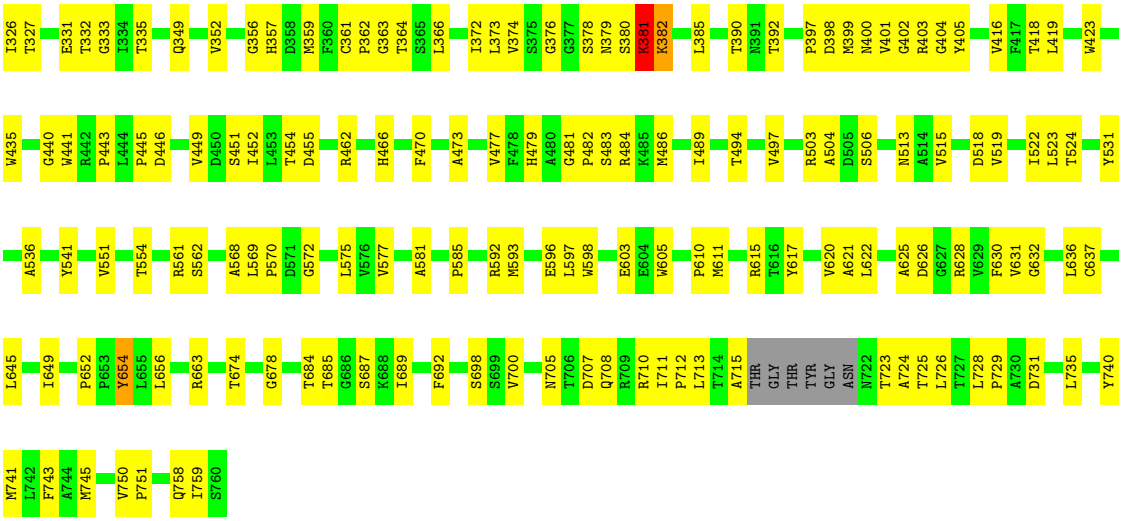


• Molecule 1: Galactose oxidase

Chain M:



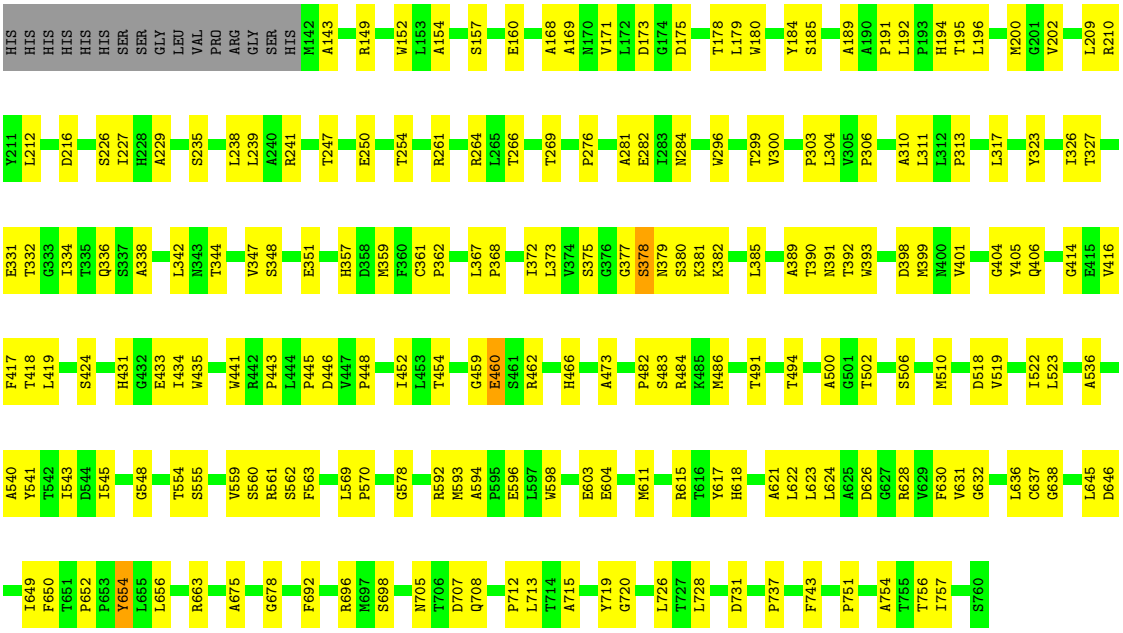




• Molecule 1: Galactose oxidase

Chain N:

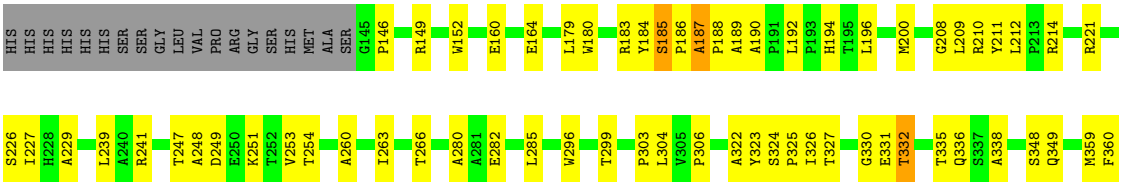


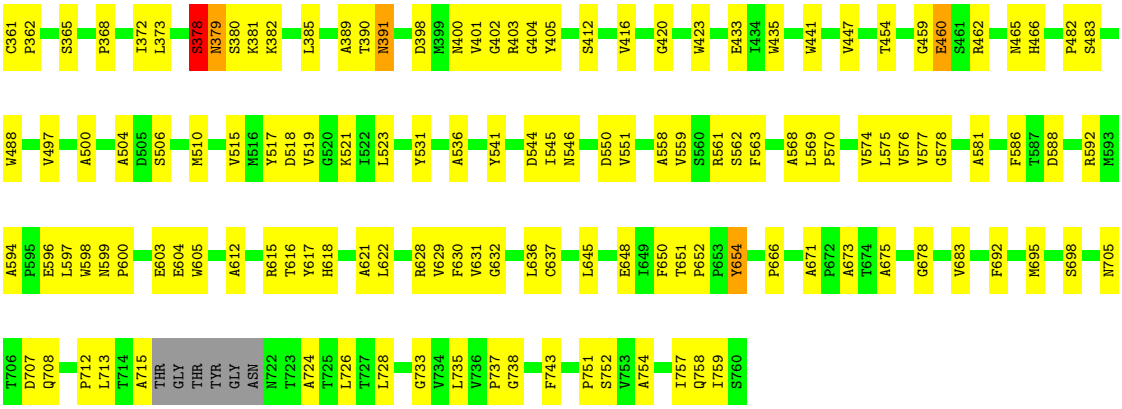


• Molecule 1: Galactose oxidase

Chain O:



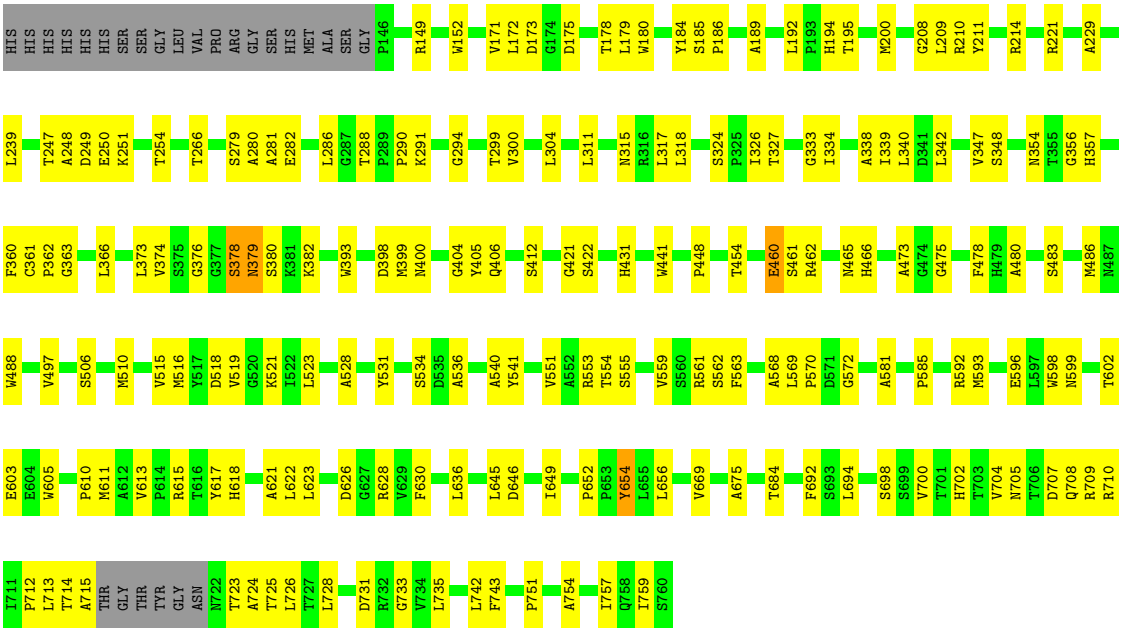




- Molecule 1: Galactose oxidase

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.52Å 472.91Å 134.85Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	77.52 – 2.98 77.52 – 2.98	Depositor EDS
% Data completeness (in resolution range)	77.2 (77.52-2.98) 77.3 (77.52-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.210 , 0.268 0.211 , 0.269	Depositor DCC
R_{free} test set	7552 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 0.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.129 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	71772	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: CA, GOL, OXY

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	0.14	0/4606	0.31	0/6304
1	B	0.11	0/4625	0.31	0/6329
1	C	0.12	0/4606	0.31	0/6304
1	D	0.13	0/4563	0.30	0/6243
1	E	0.12	0/4592	0.29	0/6282
1	F	0.11	0/4625	0.31	0/6329
1	G	0.11	0/4606	0.32	1/6304 (0.0%)
1	H	0.11	0/4551	0.29	0/6227
1	I	0.13	0/4614	0.32	0/6314
1	J	0.12	0/4558	0.29	0/6236
1	K	0.15	0/4557	0.31	0/6235
1	L	0.11	0/4562	0.32	1/6242 (0.0%)
1	M	0.12	0/4562	0.35	1/6242 (0.0%)
1	N	0.09	0/4614	0.29	0/6314
1	O	0.15	0/4551	0.33	0/6227
1	P	0.11	0/4547	0.29	0/6221
All	All	0.12	0/73339	0.31	3/100353 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	I	0	1
1	O	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	381	LYS	N-CA-C	-12.92	99.27	112.97
1	L	184	TYR	N-CA-C	-5.33	107.44	114.31
1	G	460	GLU	CB-CA-C	-5.00	110.82	116.63

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	187	ALA	Peptide
1	I	187	ALA	Peptide
1	O	185	SER	Peptide
1	O	187	ALA	Peptide

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	4497	0	4344	154	0
1	B	4515	0	4361	149	0
1	C	4497	0	4345	176	0
1	D	4456	0	4307	161	0
1	E	4484	0	4334	148	0
1	F	4515	0	4360	170	0
1	G	4497	0	4344	166	0
1	H	4444	0	4298	138	0
1	I	4505	0	4353	154	0
1	J	4451	0	4306	129	0
1	K	4450	0	4303	151	0
1	L	4455	0	4308	163	0
1	M	4455	0	4308	189	0
1	N	4505	0	4353	146	0
1	O	4444	0	4299	150	0
1	P	4440	0	4296	154	0
2	A	6	8	8	0	0
2	B	6	8	8	2	0
2	D	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	6	8	8	0	0
2	L	12	16	16	0	0
2	M	6	8	8	1	0
2	O	6	8	8	1	0
2	P	6	8	8	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	K	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	D	1	0	0	0	0
5	O	1	0	0	0	0
All	All	71700	72	69291	2429	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 17.

The worst 5 of 2429 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:H:303:PRO:HB3	1:H:349:GLN:HE21	1.10	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:229:ALA:HB2	1:M:239:LEU:HD11	1.41	1.00
1:P:229:ALA:HB2	1:P:239:LEU:HD11	1.42	0.98
1:F:715:ALA:HB1	1:F:724:ALA:HB1	1.43	0.97
1:G:293:PRO:HG2	1:G:608:MET:HA	1.48	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	616/635 (97%)	586 (95%)	29 (5%)	1 (0%)	43	73
1	B	618/635 (97%)	586 (95%)	30 (5%)	2 (0%)	36	67
1	C	616/635 (97%)	587 (95%)	27 (4%)	2 (0%)	36	67
1	D	608/635 (96%)	578 (95%)	28 (5%)	2 (0%)	36	67
1	E	612/635 (96%)	583 (95%)	26 (4%)	3 (0%)	24	58
1	F	618/635 (97%)	588 (95%)	25 (4%)	5 (1%)	16	47
1	G	616/635 (97%)	585 (95%)	27 (4%)	4 (1%)	21	53
1	H	606/635 (95%)	574 (95%)	28 (5%)	4 (1%)	18	50
1	I	617/635 (97%)	583 (94%)	31 (5%)	3 (0%)	24	58
1	J	607/635 (96%)	578 (95%)	27 (4%)	2 (0%)	36	67
1	K	607/635 (96%)	576 (95%)	29 (5%)	2 (0%)	36	67
1	L	608/635 (96%)	578 (95%)	28 (5%)	2 (0%)	36	67
1	M	608/635 (96%)	578 (95%)	30 (5%)	0	100	100
1	N	617/635 (97%)	587 (95%)	27 (4%)	3 (0%)	24	58
1	O	606/635 (95%)	576 (95%)	26 (4%)	4 (1%)	18	50
1	P	605/635 (95%)	579 (96%)	23 (4%)	3 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9785/10160 (96%)	9302 (95%)	441 (4%)	42 (0%)	30 62

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460	GLU
1	C	460	GLU
1	D	378	SER
1	D	379	ASN
1	E	460	GLU

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	470/485 (97%)	466 (99%)	4 (1%)	70 85
1	B	472/485 (97%)	467 (99%)	5 (1%)	65 82
1	C	470/485 (97%)	464 (99%)	6 (1%)	61 81
1	D	466/485 (96%)	461 (99%)	5 (1%)	65 82
1	E	469/485 (97%)	465 (99%)	4 (1%)	70 85
1	F	472/485 (97%)	469 (99%)	3 (1%)	78 88
1	G	470/485 (97%)	466 (99%)	4 (1%)	70 85
1	H	465/485 (96%)	462 (99%)	3 (1%)	78 88
1	I	471/485 (97%)	461 (98%)	10 (2%)	47 74
1	J	466/485 (96%)	465 (100%)	1 (0%)	87 92
1	K	466/485 (96%)	462 (99%)	4 (1%)	70 85
1	L	466/485 (96%)	460 (99%)	6 (1%)	61 81
1	M	466/485 (96%)	463 (99%)	3 (1%)	78 88
1	N	471/485 (97%)	468 (99%)	3 (1%)	78 88
1	O	465/485 (96%)	459 (99%)	6 (1%)	61 81
1	P	465/485 (96%)	462 (99%)	3 (1%)	78 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7490/7760 (96%)	7420 (99%)	70 (1%)	70 85

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	654	TYR
1	N	332	THR
1	O	391	ASN
1	F	379	ASN
1	E	654	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	573	GLN
1	N	336	GLN
1	L	301	ASN
1	M	273	ASN
1	N	580	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 16 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
2	GOL	D	801	-	5,5,5	1.02	0	5,5,5	1.18	1 (20%)
2	GOL	L	802	-	5,5,5	1.07	1 (20%)	5,5,5	1.21	1 (20%)
2	GOL	P	801	-	5,5,5	0.91	0	5,5,5	1.08	0
2	GOL	A	801	-	5,5,5	0.98	0	5,5,5	1.02	0
2	GOL	M	801	-	5,5,5	0.96	0	5,5,5	1.25	1 (20%)
2	GOL	J	801	-	5,5,5	1.18	1 (20%)	5,5,5	1.28	1 (20%)
3	OXY	G	801	-	1,1,1	0.14	0	-		
3	OXY	H	801	-	1,1,1	0.14	0	-		
3	OXY	K	801	-	1,1,1	0.14	0	-		
3	OXY	M	802	-	1,1,1	0.15	0	-		
2	GOL	L	801	-	5,5,5	1.11	0	5,5,5	1.39	1 (20%)
2	GOL	B	801	-	5,5,5	1.14	0	5,5,5	1.38	1 (20%)
3	OXY	A	802	-	1,1,1	0.14	0	-		
3	OXY	C	801	-	1,1,1	0.14	0	-		
3	OXY	E	801	-	1,1,1	0.14	0	-		
3	OXY	F	801	-	1,1,1	0.15	0	-		
2	GOL	O	801	-	5,5,5	0.13	0	5,5,5	0.30	0
3	OXY	N	801	-	1,1,1	0.14	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	801	-	-	2/4/4/4	-
2	GOL	L	802	-	-	4/4/4/4	-
2	GOL	P	801	-	-	2/4/4/4	-
2	GOL	A	801	-	-	3/4/4/4	-
2	GOL	M	801	-	-	2/4/4/4	-
2	GOL	J	801	-	-	4/4/4/4	-
2	GOL	L	801	-	-	2/4/4/4	-
2	GOL	B	801	-	-	0/4/4/4	-
2	GOL	O	801	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	801	GOL	O2-C2	-2.17	1.36	1.43
2	L	802	GOL	O2-C2	-2.02	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	801	GOL	C3-C2-C1	-2.73	101.11	111.70
2	B	801	GOL	C3-C2-C1	-2.63	101.47	111.70
2	J	801	GOL	C3-C2-C1	-2.54	101.84	111.70
2	M	801	GOL	C3-C2-C1	-2.44	102.22	111.70
2	L	802	GOL	C3-C2-C1	-2.21	103.12	111.70

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	D	801	GOL	O1-C1-C2-C3
2	J	801	GOL	O1-C1-C2-C3
2	J	801	GOL	C1-C2-C3-O3
2	L	801	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	801	GOL	1	0
2	B	801	GOL	2	0
2	O	801	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	618/635 (97%)	-1.77	0	100	100	13, 24, 43, 64	0
1	B	620/635 (97%)	-1.75	0	100	100	13, 27, 47, 68	0
1	C	618/635 (97%)	-1.78	0	100	100	14, 24, 40, 62	0
1	D	612/635 (96%)	-1.76	0	100	100	15, 28, 47, 71	0
1	E	616/635 (97%)	-1.75	0	100	100	14, 26, 44, 77	0
1	F	620/635 (97%)	-1.77	0	100	100	15, 26, 43, 71	0
1	G	618/635 (97%)	-1.76	0	100	100	16, 30, 48, 75	0
1	H	610/635 (96%)	-1.75	0	100	100	18, 35, 51, 74	0
1	I	619/635 (97%)	-1.73	0	100	100	17, 36, 56, 86	0
1	J	611/635 (96%)	-1.77	0	100	100	16, 28, 45, 76	0
1	K	611/635 (96%)	-1.74	0	100	100	17, 36, 59, 95	0
1	L	612/635 (96%)	-1.73	0	100	100	16, 36, 57, 86	0
1	M	612/635 (96%)	-1.73	0	100	100	17, 40, 66, 92	0
1	N	619/635 (97%)	-1.77	0	100	100	17, 29, 48, 63	0
1	O	610/635 (96%)	-1.74	0	100	100	16, 34, 50, 73	0
1	P	609/635 (95%)	-1.74	0	100	100	18, 34, 54, 72	0
All	All	9835/10160 (96%)	-1.75	0	100	100	13, 30, 52, 95	0

There are no RSRZ outliers to report.

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GOL	A	801	6/6	0.99	0.03	32,43,52,60	0
2	GOL	B	801	6/6	0.99	0.07	24,31,38,40	0
2	GOL	D	801	6/6	0.99	0.03	25,31,36,37	0
2	GOL	J	801	6/6	0.99	0.04	26,37,45,46	0
2	GOL	O	801	6/6	0.99	0.06	26,37,45,50	0
2	GOL	P	801	6/6	0.99	0.05	26,38,46,46	0
3	OXY	A	802	2/2	0.99	0.03	16,16,16,20	0
3	OXY	E	801	2/2	0.99	0.04	19,19,19,22	0
3	OXY	F	801	2/2	0.99	0.04	17,17,17,21	0
3	OXY	G	801	2/2	0.99	0.02	15,15,15,16	0
3	OXY	H	801	2/2	0.99	0.03	11,11,11,17	0
3	OXY	K	801	2/2	0.99	0.02	23,23,23,26	0
3	OXY	N	801	2/2	0.99	0.04	24,24,24,25	0
2	GOL	M	801	6/6	1.00	0.04	29,36,41,43	0
3	OXY	C	801	2/2	1.00	0.02	10,10,10,12	0
2	GOL	L	801	6/6	1.00	0.02	24,29,36,36	0
3	OXY	M	802	2/2	1.00	0.02	19,19,19,21	0
2	GOL	L	802	6/6	1.00	0.04	24,39,45,55	0
4	CA	A	803	1/1	1.00	0.01	39,39,39,39	0
4	CA	B	802	1/1	1.00	0.01	42,42,42,42	0
4	CA	C	802	1/1	1.00	0.03	87,87,87,87	0
4	CA	D	802	1/1	1.00	0.01	33,33,33,33	0
4	CA	E	802	1/1	1.00	0.01	31,31,31,31	0
4	CA	F	802	1/1	1.00	0.01	26,26,26,26	0
4	CA	G	802	1/1	1.00	0.01	26,26,26,26	0
4	CA	H	802	1/1	1.00	0.01	30,30,30,30	0
4	CA	I	801	1/1	1.00	0.01	48,48,48,48	0
4	CA	J	802	1/1	1.00	0.01	30,30,30,30	0
4	CA	K	802	1/1	1.00	0.01	39,39,39,39	0
4	CA	L	803	1/1	1.00	0.01	30,30,30,30	0
4	CA	M	803	1/1	1.00	0.01	26,26,26,26	0
4	CA	N	802	1/1	1.00	0.01	53,53,53,53	0

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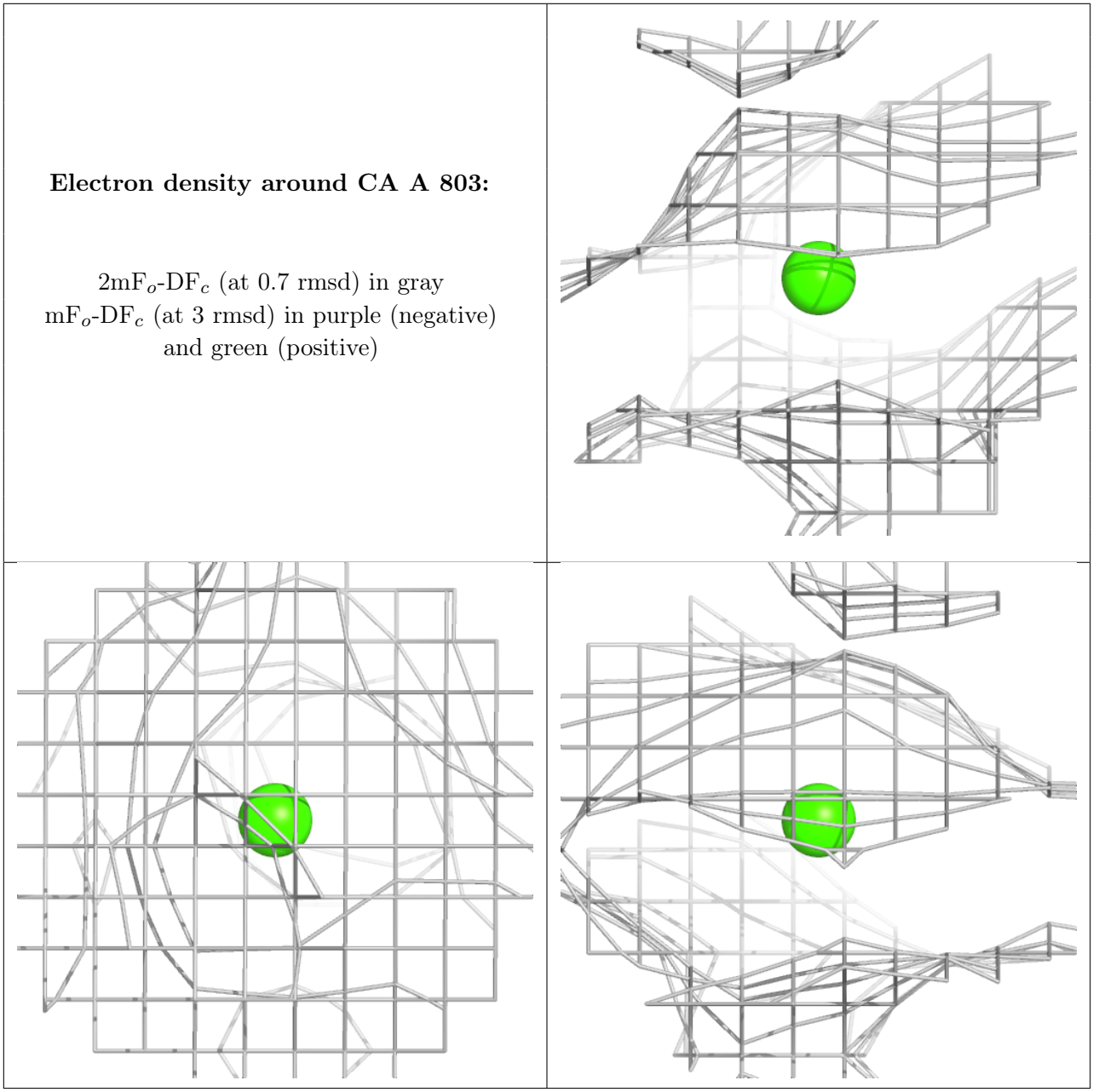
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	O	802	1/1	1.00	0.01	36,36,36,36	0
4	CA	P	802	1/1	1.00	0.01	56,56,56,56	0

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.

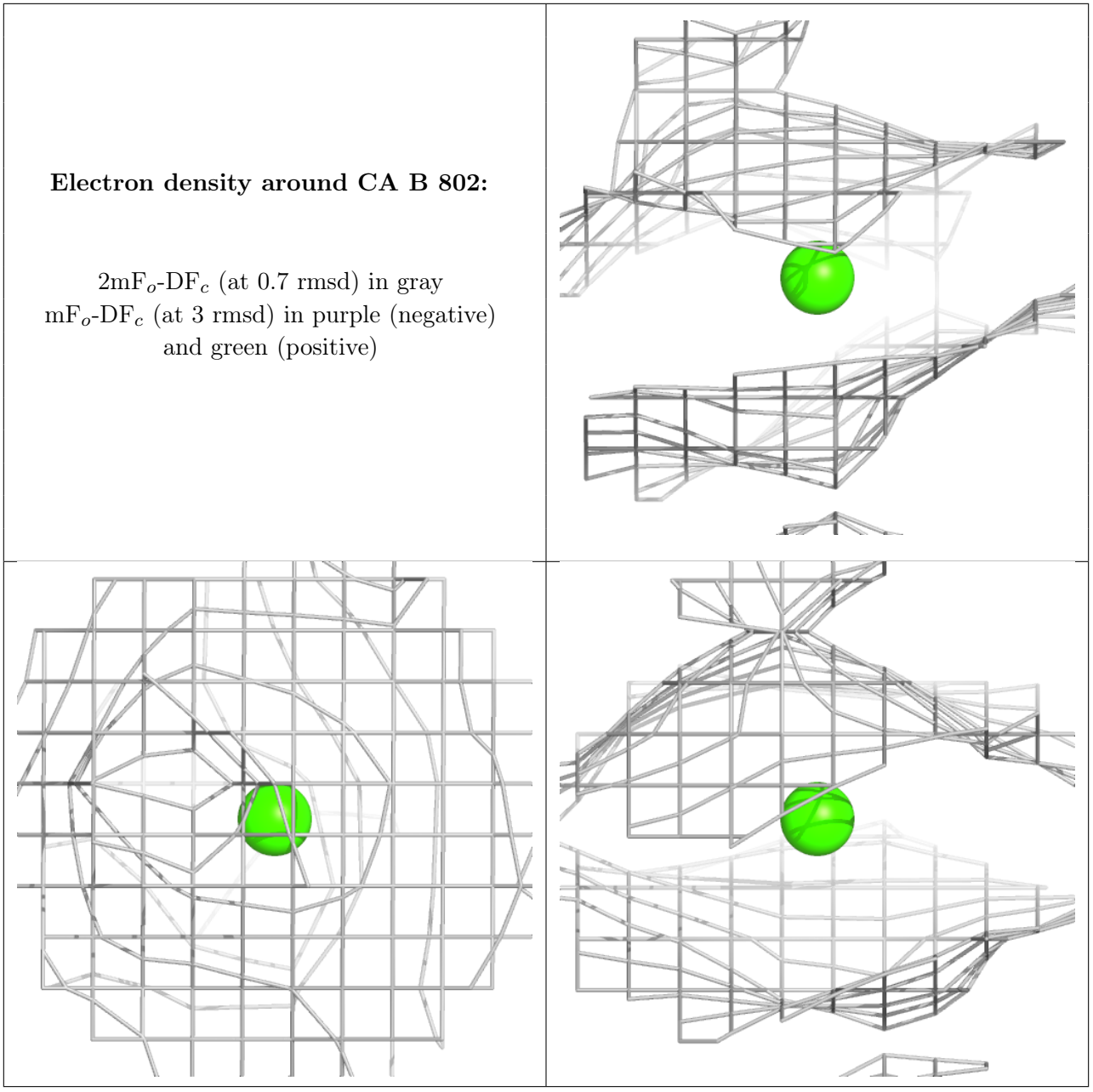
Electron density around CA A 803:

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



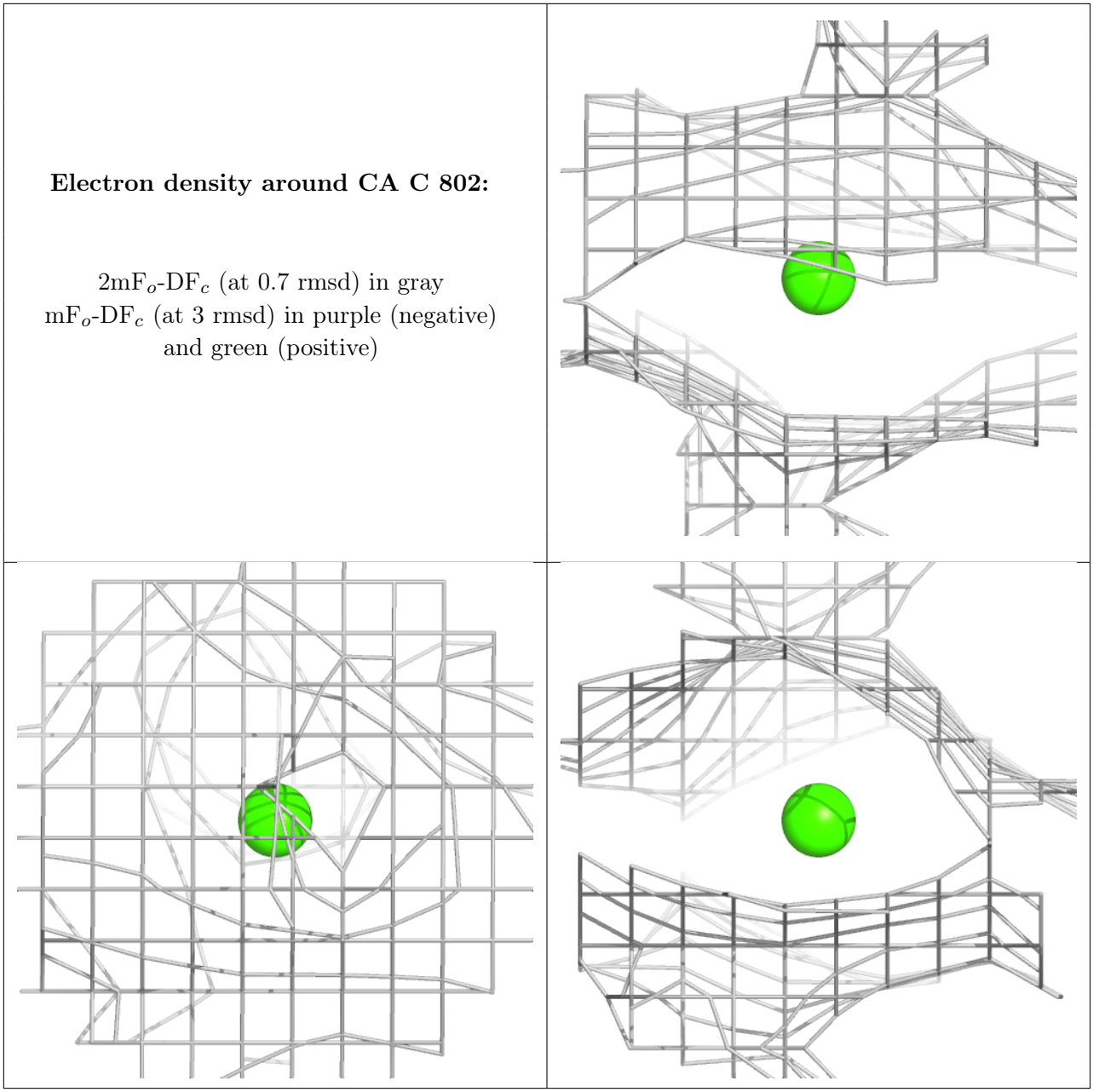
Electron density around CA B 802:

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



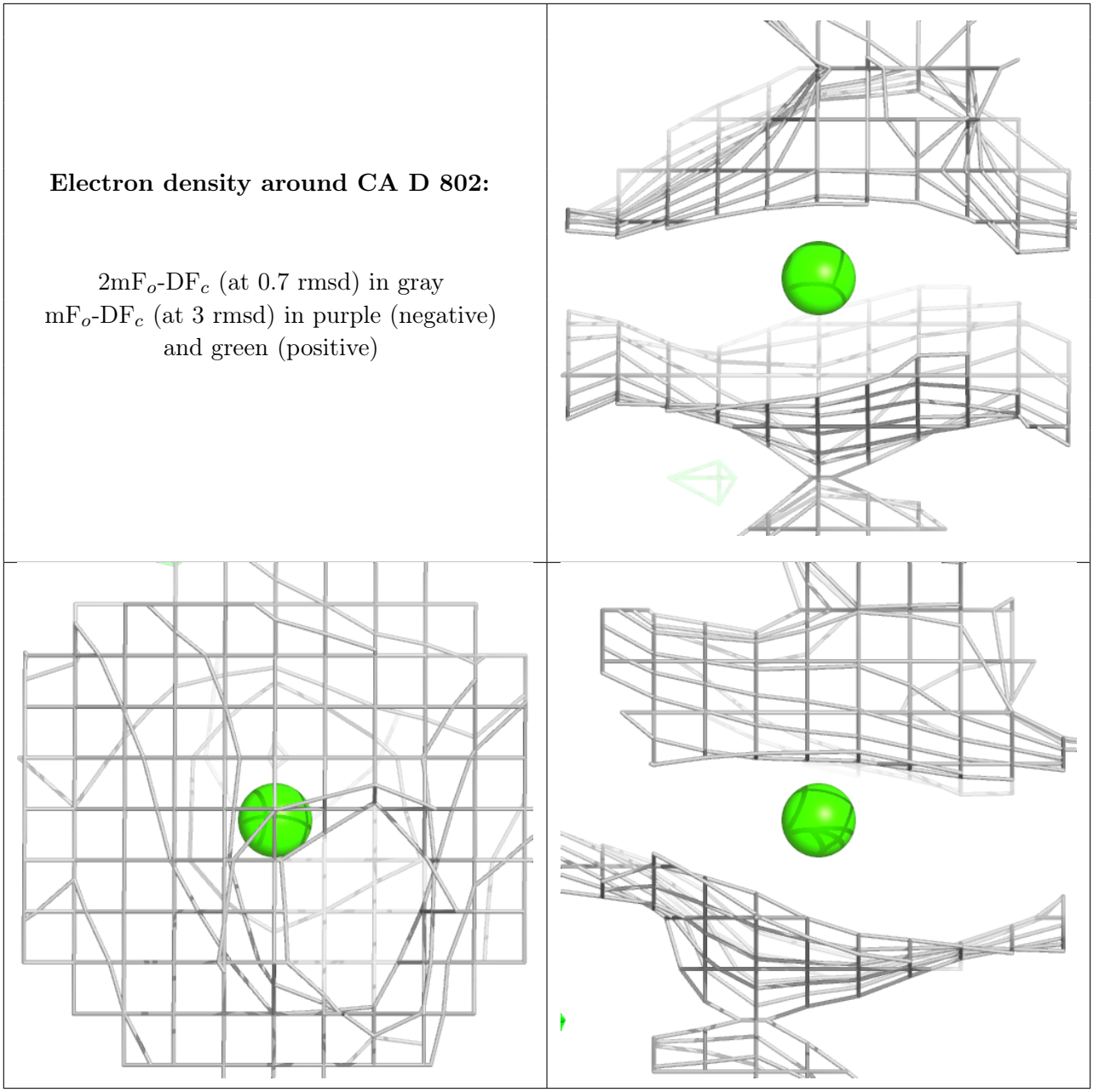
Electron density around CA C 802:

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



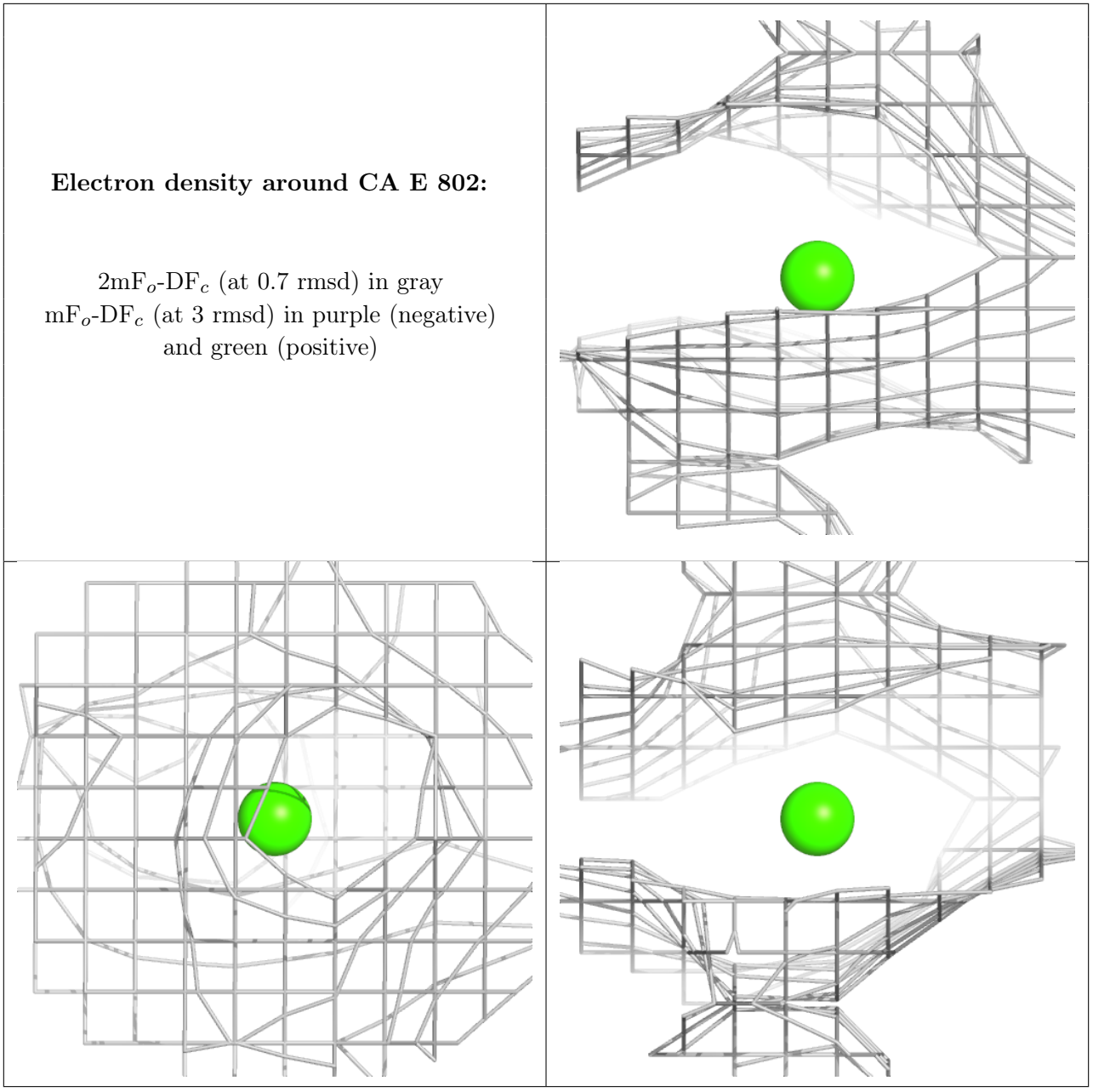
Electron density around CA D 802:

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



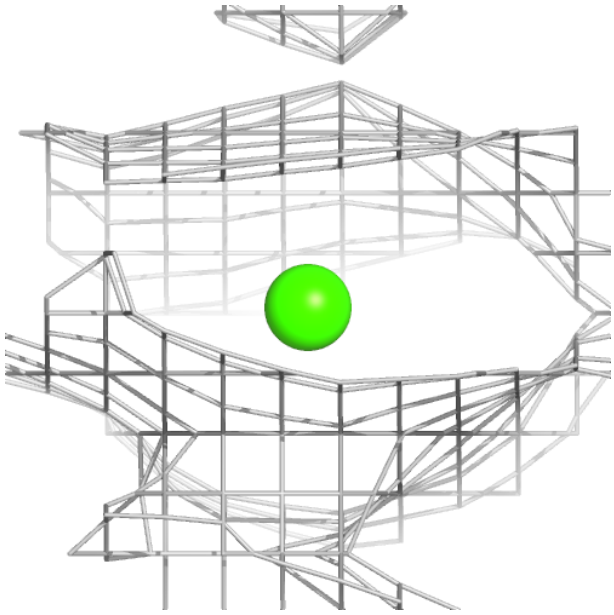
Electron density around CA E 802:

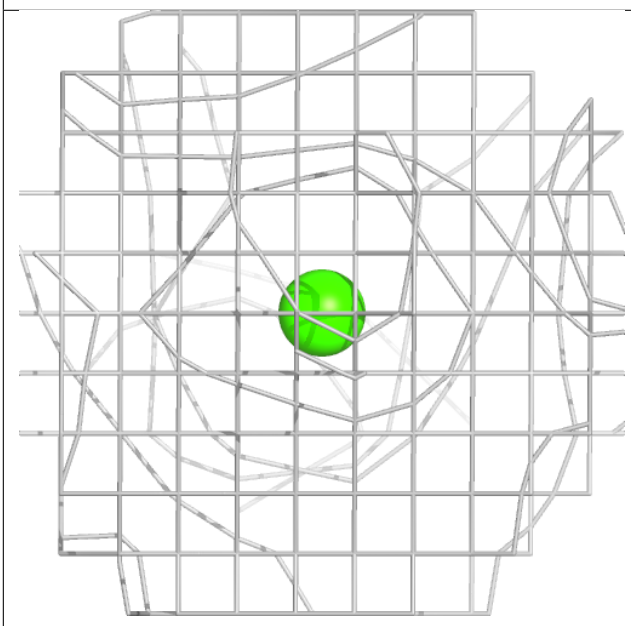
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

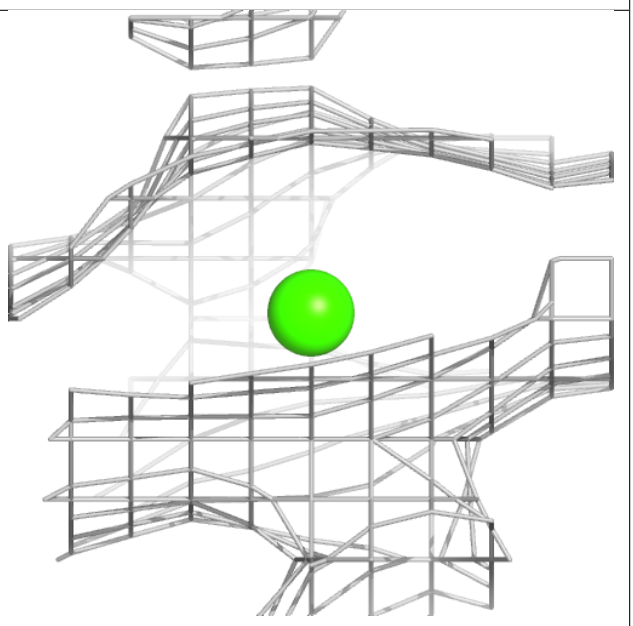


Electron density around CA F 802:

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

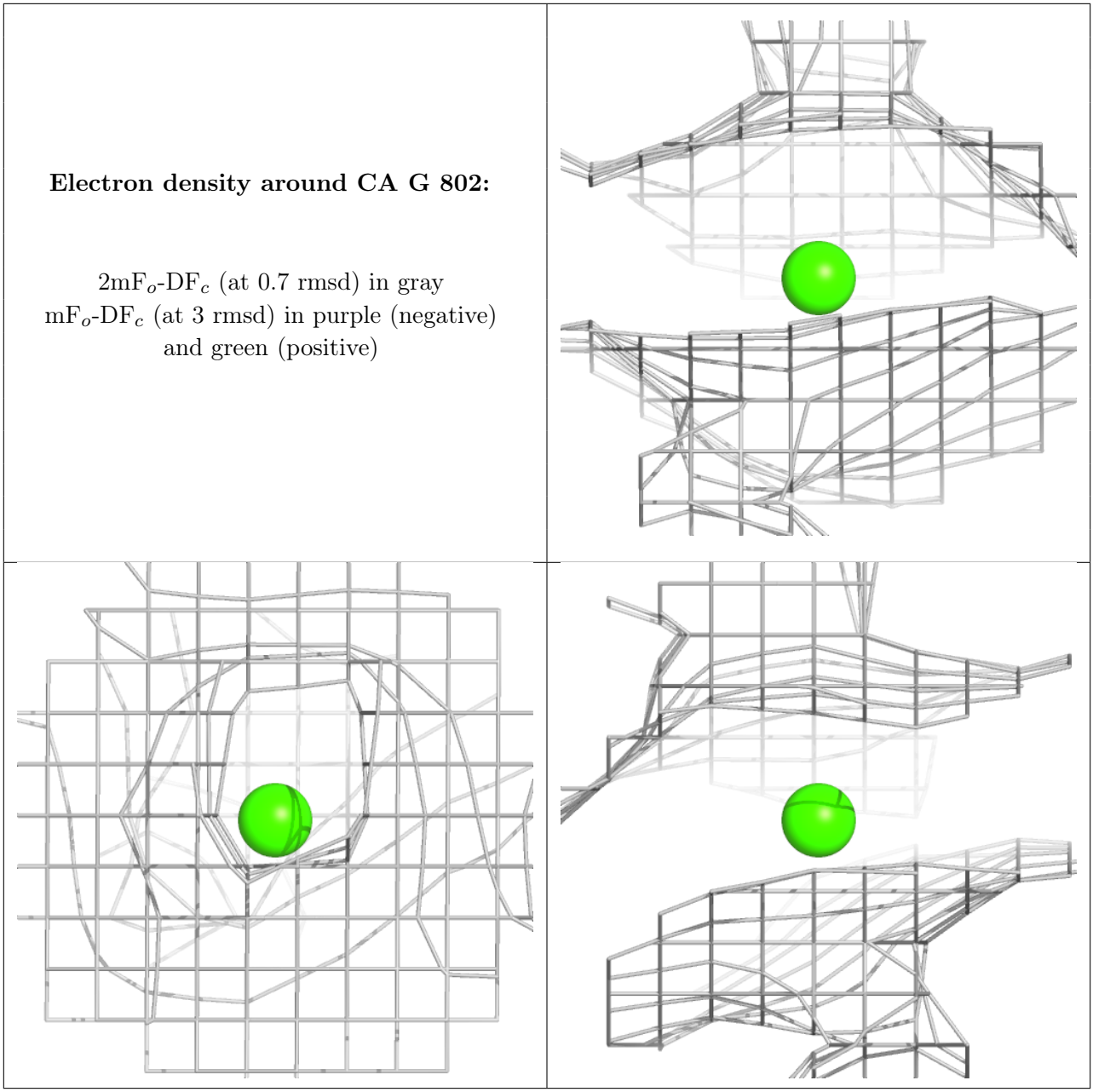






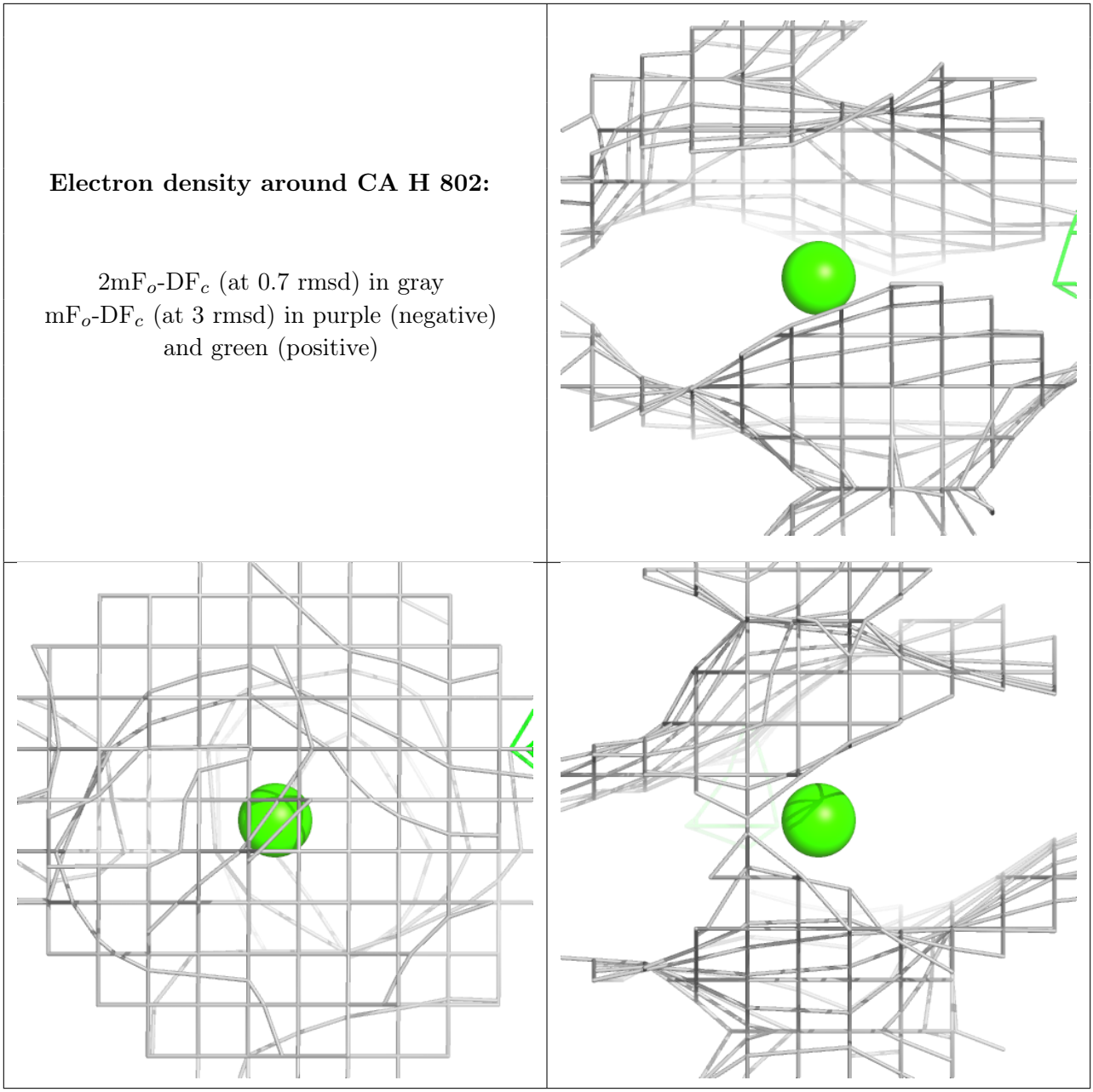
Electron density around CA G 802:

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



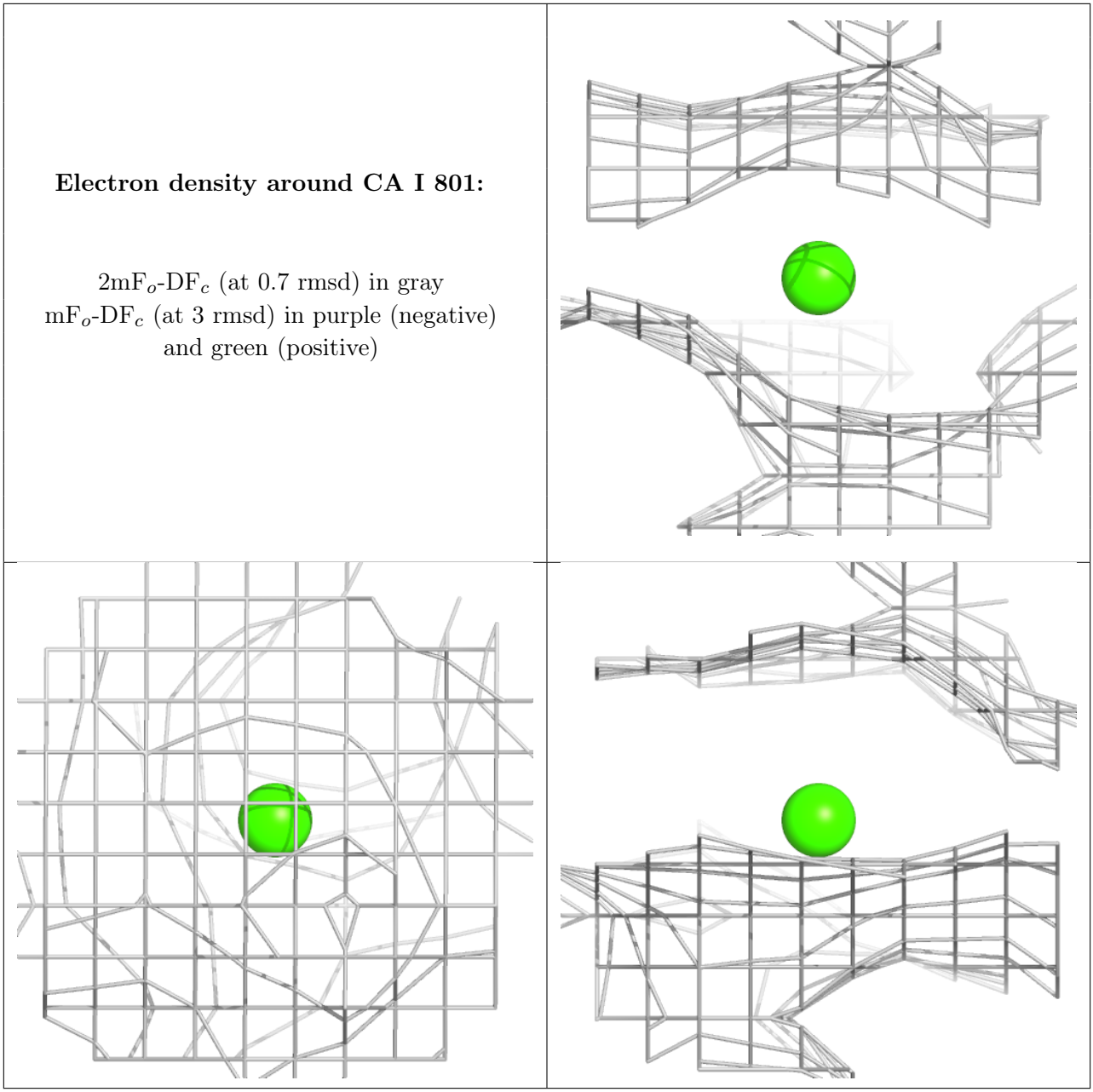
Electron density around CA H 802:

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



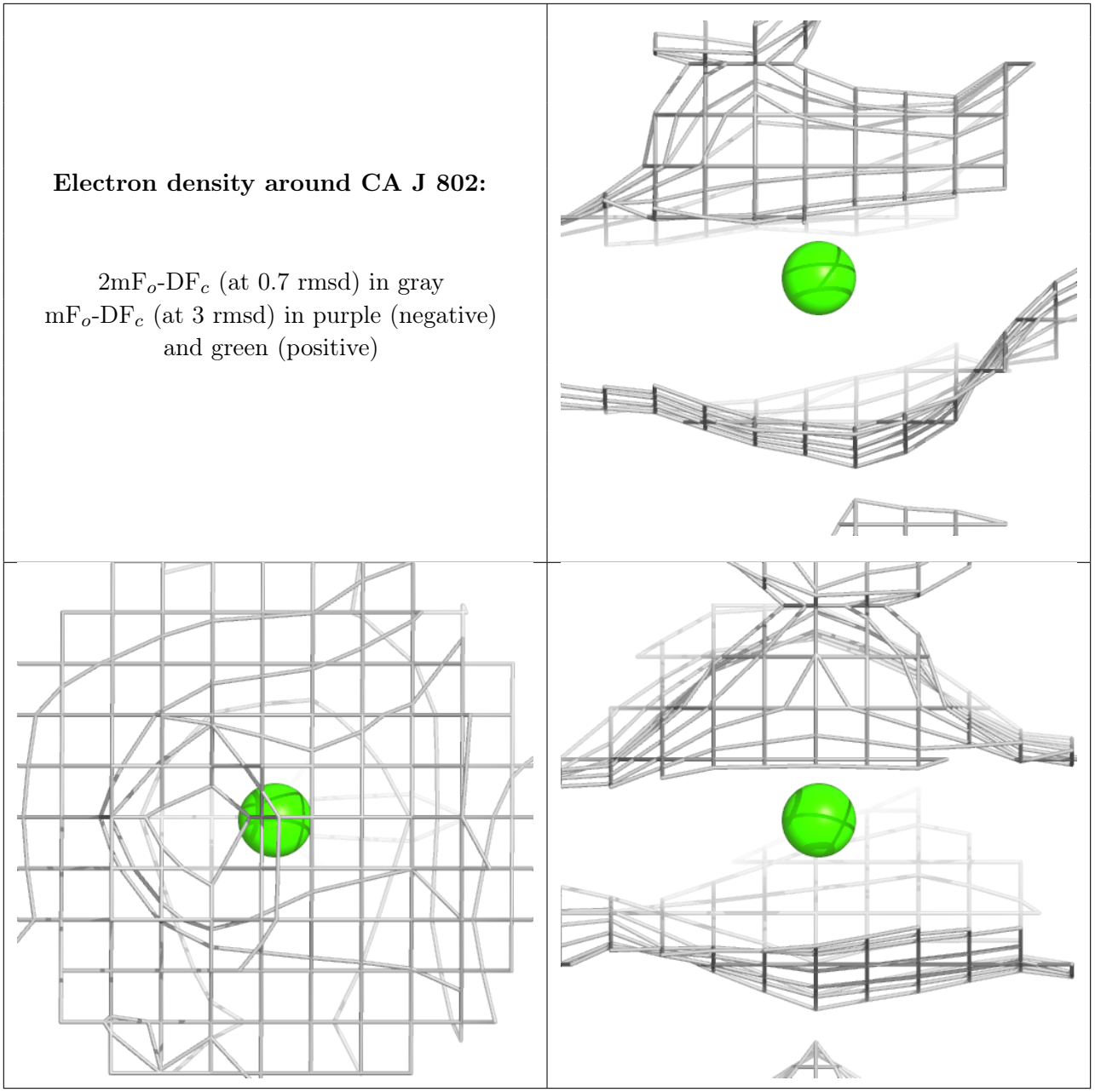
Electron density around CA I 801:

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



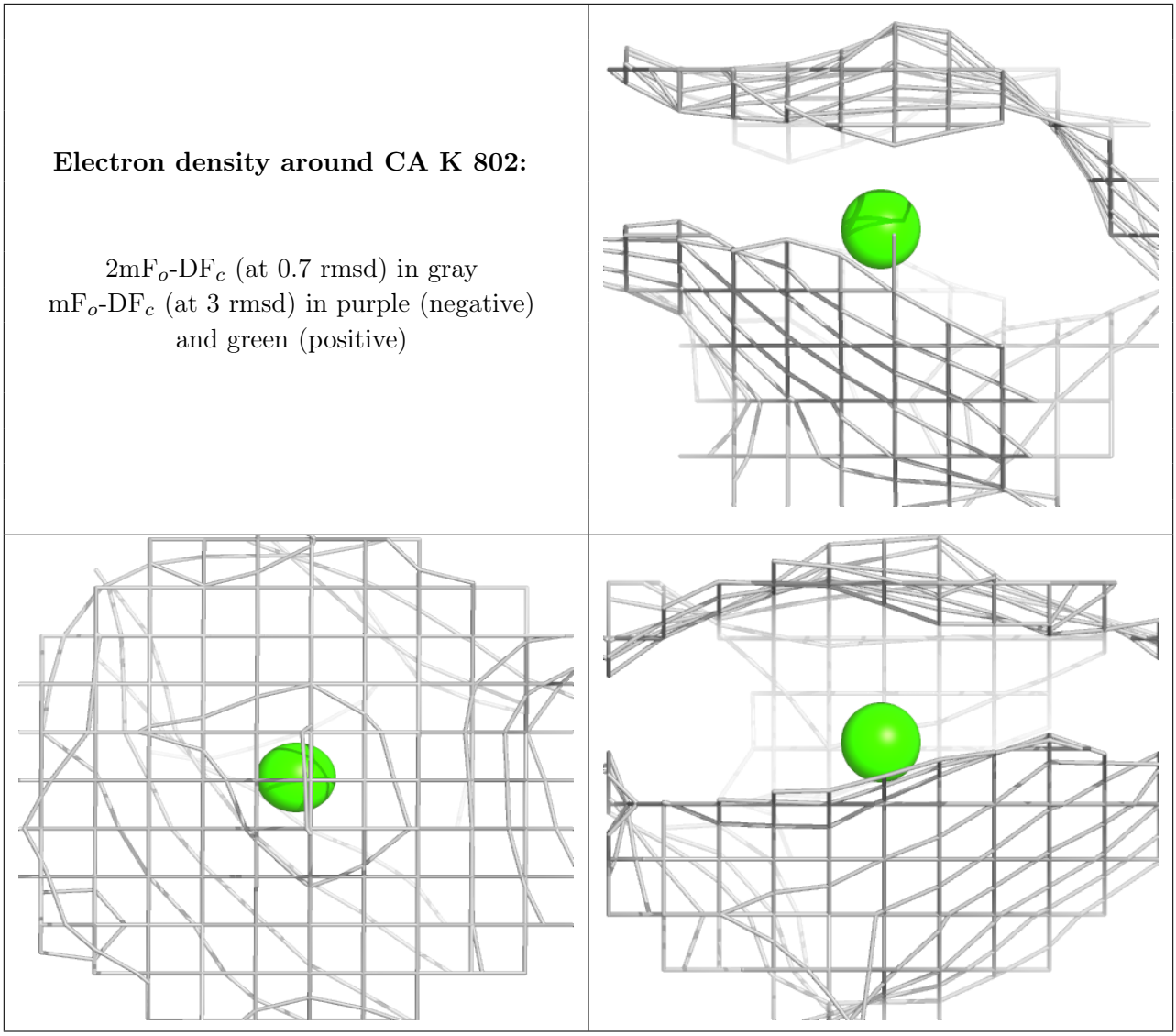
Electron density around CA J 802:

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



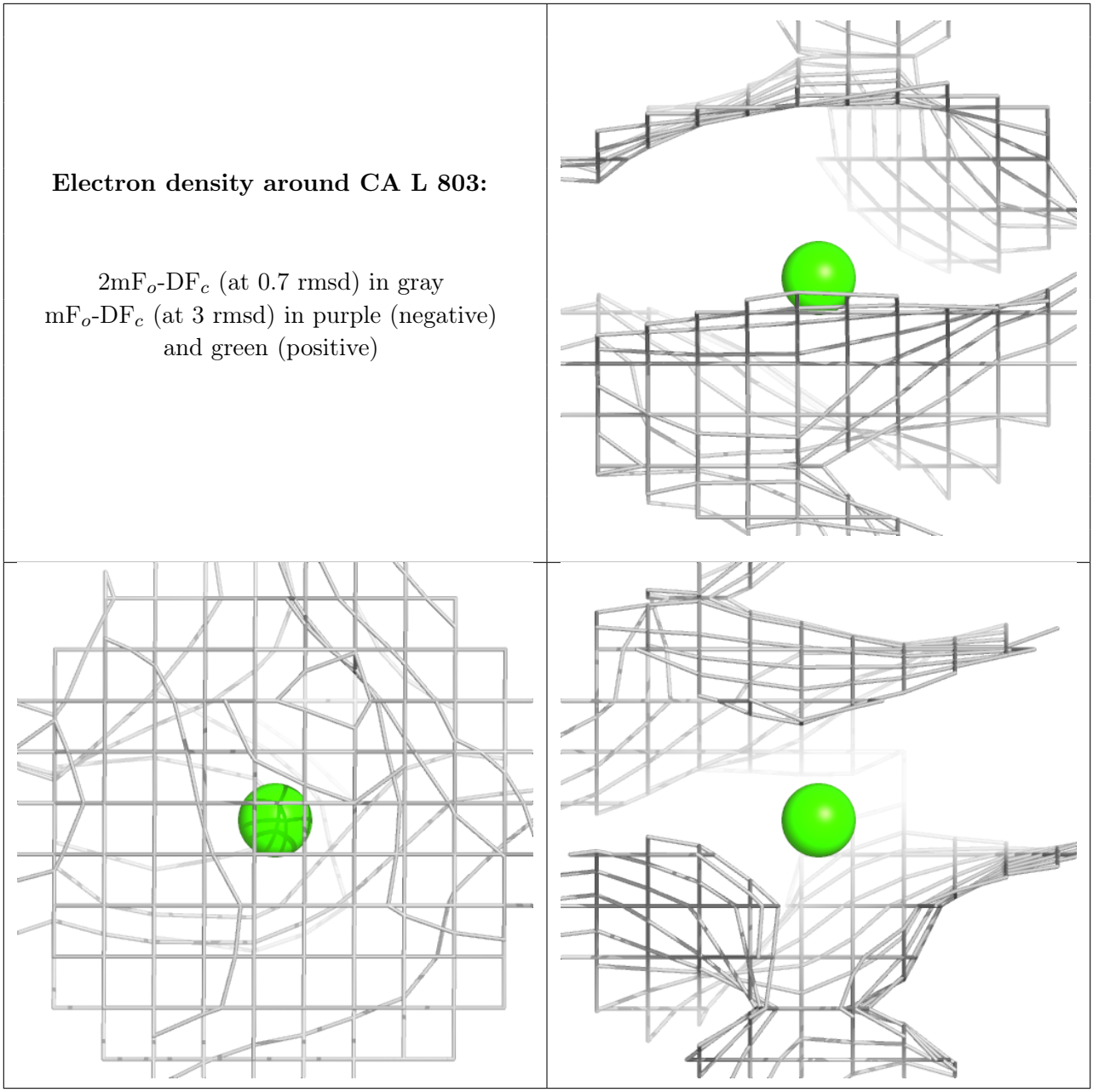
Electron density around CA K 802:

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



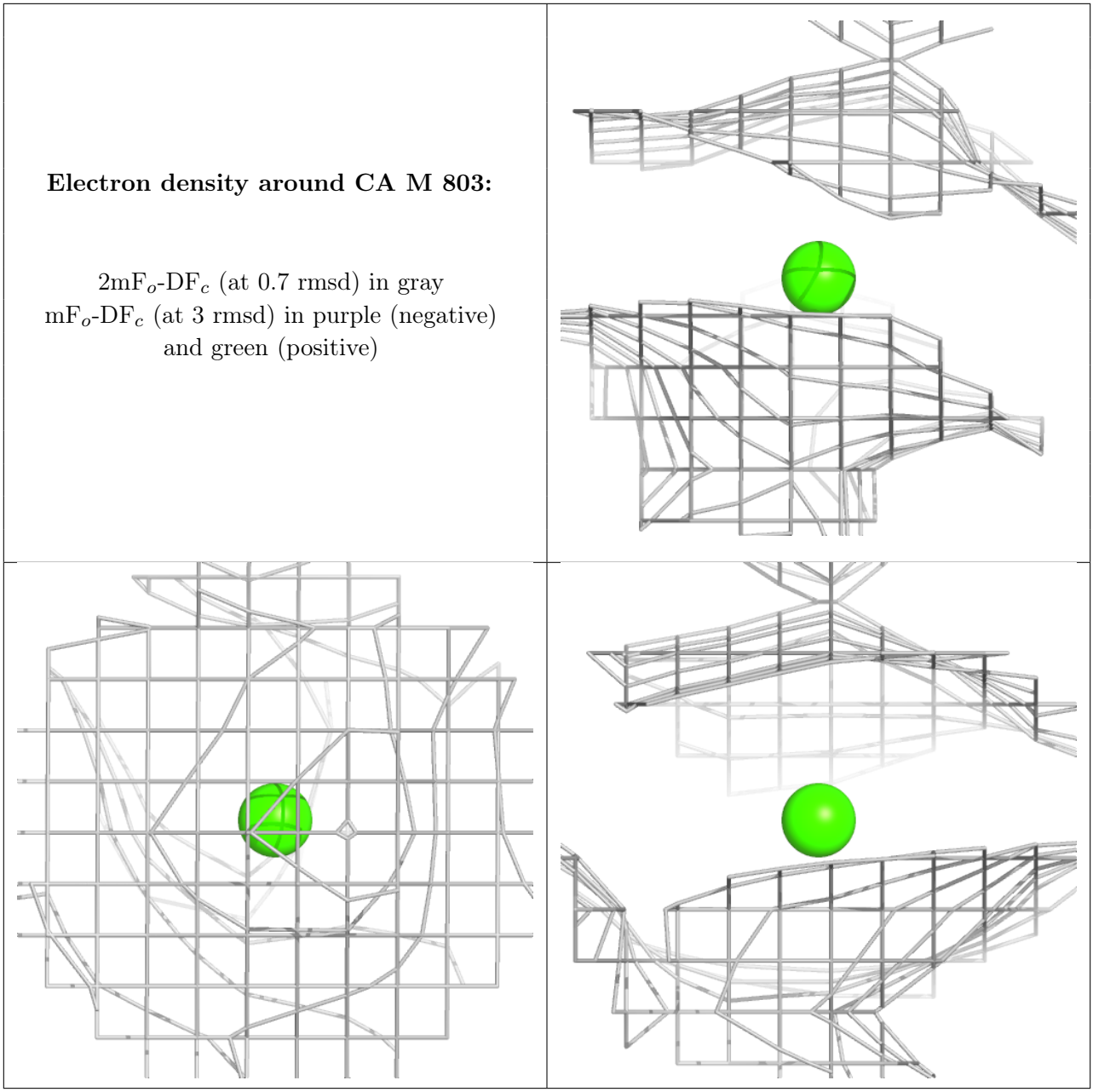
Electron density around CA L 803:

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



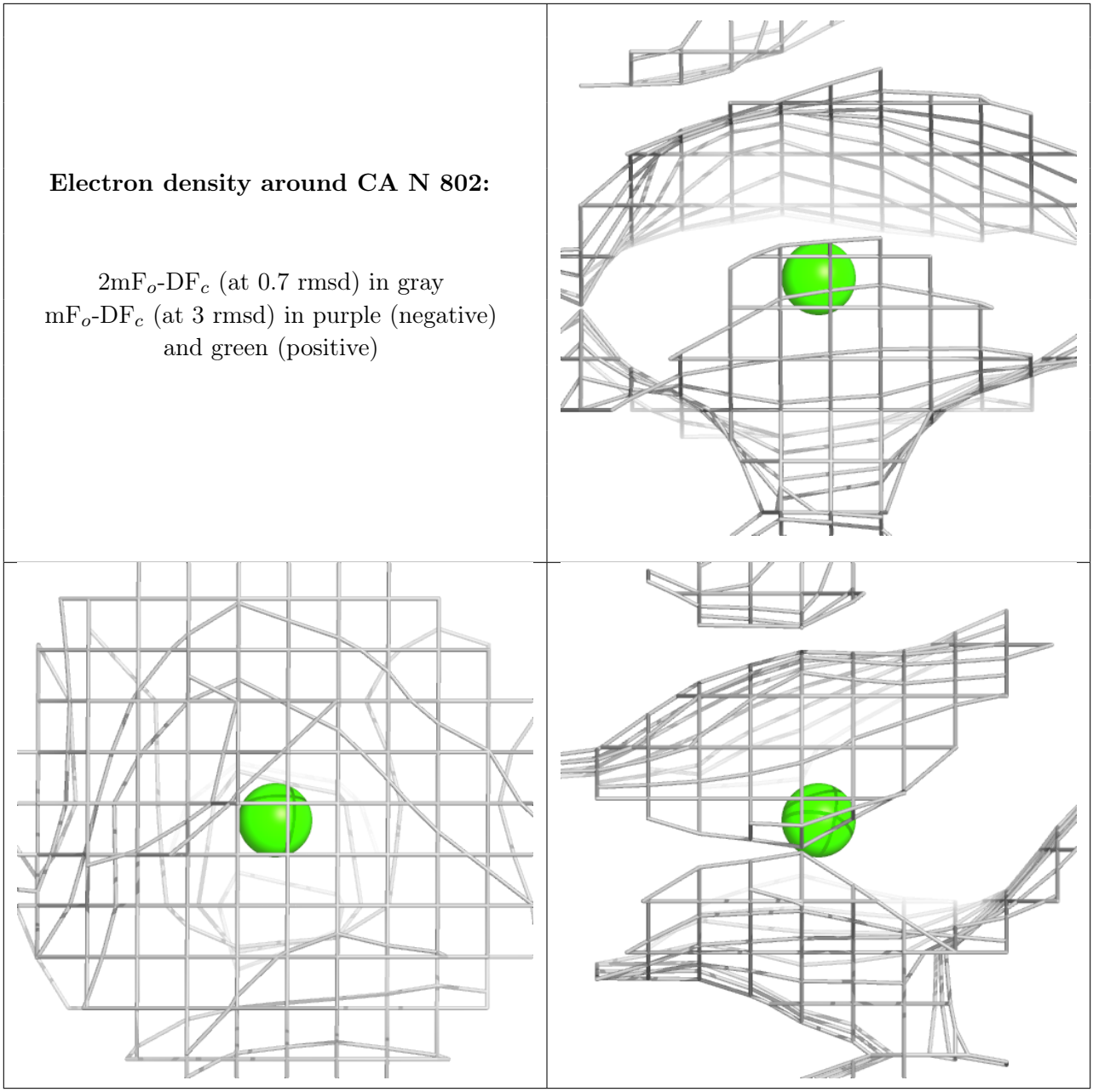
Electron density around CA M 803:

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



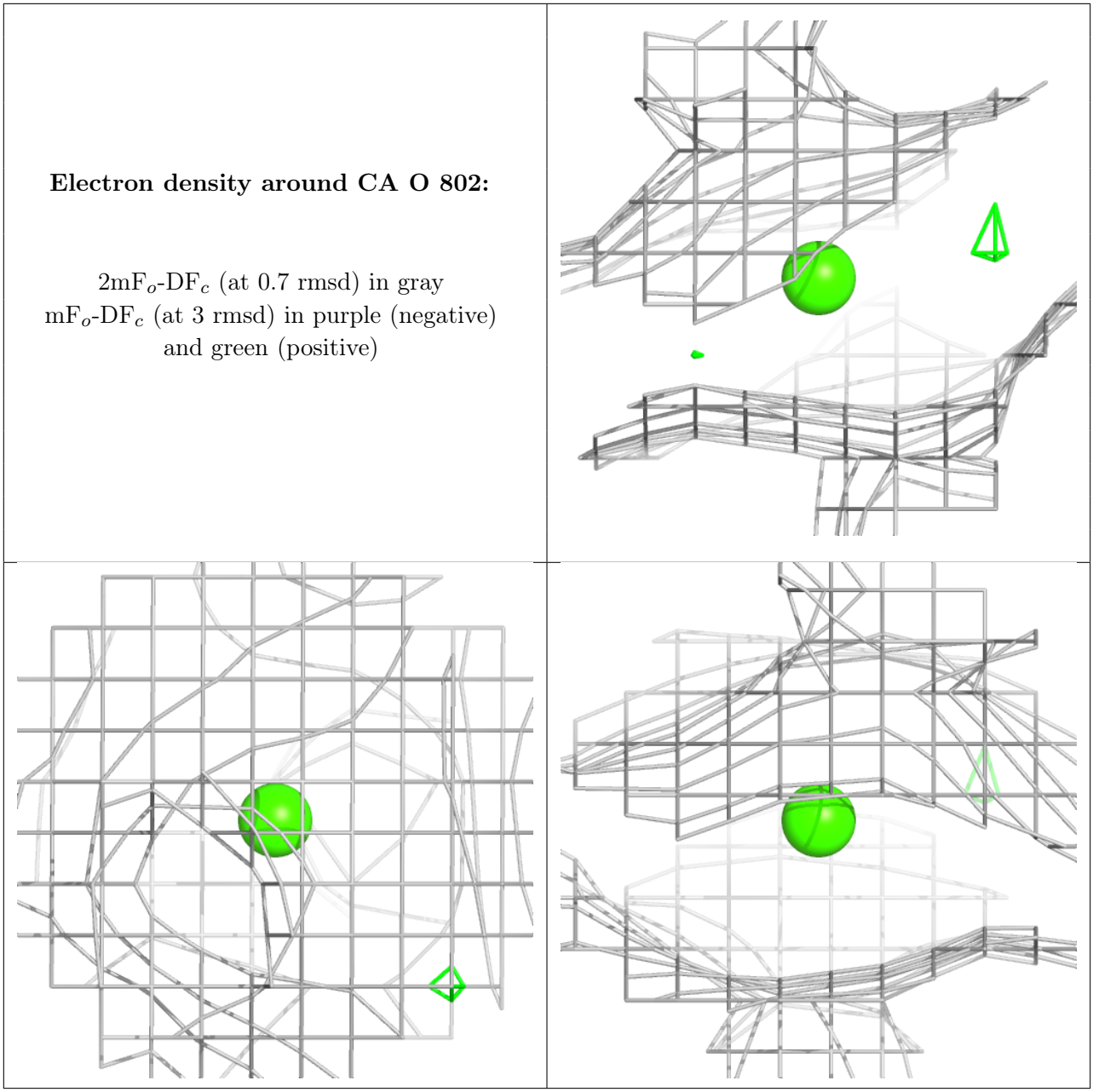
Electron density around CA N 802:

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



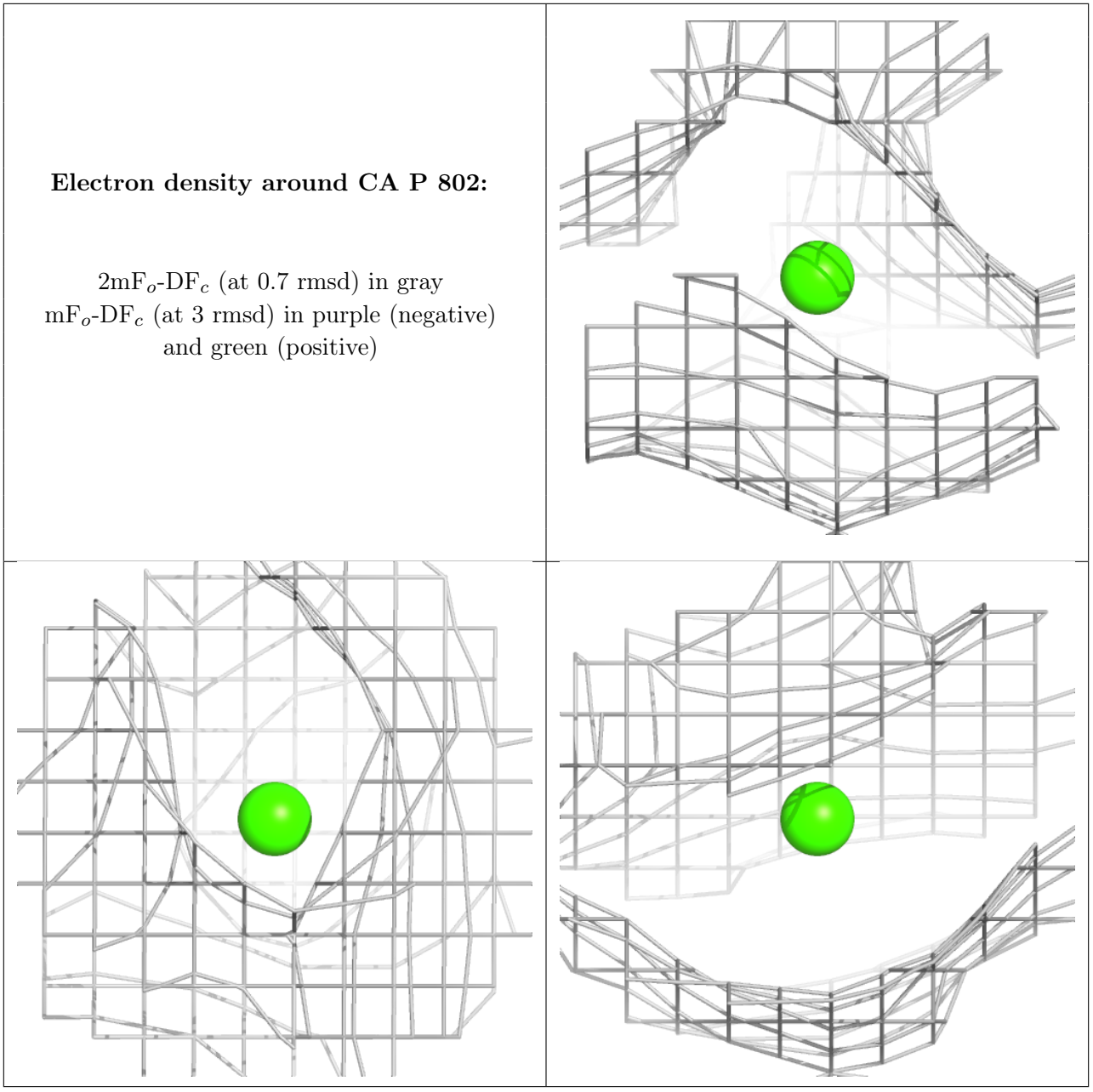
Electron density around CA O 802:

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



Electron density around CA P 802:

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



6.5 Other polymers

There are no such residues in this entry.