Full wwPDB X-ray Structure Validation Report (i)

Dec 25, 2023 – 04:38 PM JST

PDB ID	:	8WWU
Title	:	1-naphthylamine GS in complex with AMP PNP
Authors	:	Zhang, S.T.; Zhou, N.Y.
Deposited on	:	2023-10-26
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

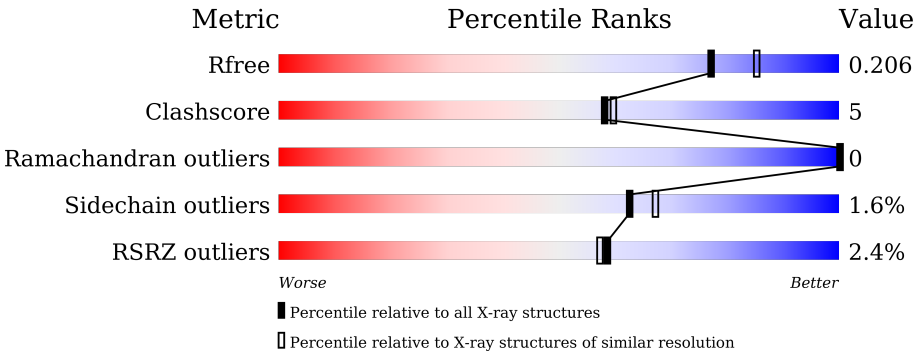
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	510	3% 87% 8% •
1	B	510	4% 83% 13% • •
1	C	510	% 85% 12% •
1	D	510	2% 86% 10% •
1	E	510	3% 84% 11% • •
1	F	510	2% 86% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25382 atoms, of which 78 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3824	2441	642	723	18			
1	B	492	Total	C	N	O	S	0	0	0
			3848	2454	646	730	18			
1	C	491	Total	C	N	O	S	0	0	0
			3839	2448	644	729	18			
1	D	492	Total	C	N	O	S	0	0	0
			3848	2454	646	730	18			
1	E	488	Total	C	N	O	S	0	0	0
			3816	2433	641	724	18			
1	F	488	Total	C	N	O	S	0	0	0
			3816	2433	641	724	18			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
A	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
A	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
A	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
A	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
A	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
A	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
A	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
A	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
A	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
A	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
A	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
A	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
A	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
A	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
A	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
A	69	ALA	THR	conflict	UNP A0A7Y1Q2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
A	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
A	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
A	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
A	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
A	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
A	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
A	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1
A	?	-	ILE	deletion	UNP A0A7Y1Q2L1
A	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
A	101	THR	SER	conflict	UNP A0A7Y1Q2L1
A	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
A	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
A	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
A	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
B	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
B	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
B	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
B	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
B	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
B	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
B	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
B	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
B	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
B	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
B	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
B	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
B	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
B	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
B	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
B	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
B	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
B	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
B	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
B	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
B	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
B	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
B	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
B	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
B	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1
B	?	-	ILE	deletion	UNP A0A7Y1Q2L1
B	99	ASN	SER	conflict	UNP A0A7Y1Q2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	101	THR	SER	conflict	UNP A0A7Y1Q2L1
B	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
B	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
B	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
B	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
C	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
C	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
C	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
C	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
C	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
C	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
C	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
C	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
C	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
C	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
C	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
C	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
C	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
C	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
C	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
C	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
C	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
C	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
C	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
C	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
C	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
C	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
C	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
C	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
C	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1
C	?	-	ILE	deletion	UNP A0A7Y1Q2L1
C	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
C	101	THR	SER	conflict	UNP A0A7Y1Q2L1
C	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
C	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
C	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
C	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
D	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
D	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
D	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
D	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
D	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
D	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
D	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
D	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
D	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
D	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
D	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
D	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
D	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
D	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
D	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
D	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
D	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
D	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
D	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
D	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
D	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
D	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
D	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
D	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1
D	?	-	ILE	deletion	UNP A0A7Y1Q2L1
D	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
D	101	THR	SER	conflict	UNP A0A7Y1Q2L1
D	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
D	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
D	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
D	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
E	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
E	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
E	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
E	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
E	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
E	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
E	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
E	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
E	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
E	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
E	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
E	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
E	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
E	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
E	0	GLY	-	expression tag	UNP A0A7Y1Q2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
E	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
E	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
E	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
E	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
E	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
E	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
E	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
E	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
E	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1
E	?	-	ILE	deletion	UNP A0A7Y1Q2L1
E	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
E	101	THR	SER	conflict	UNP A0A7Y1Q2L1
E	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
E	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
E	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
E	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
F	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
F	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
F	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
F	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
F	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
F	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
F	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
F	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
F	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
F	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
F	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
F	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
F	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
F	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
F	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
F	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
F	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
F	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
F	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
F	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
F	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
F	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
F	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
F	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
F	93	GLU	GLY	conflict	UNP A0A7Y1Q2L1

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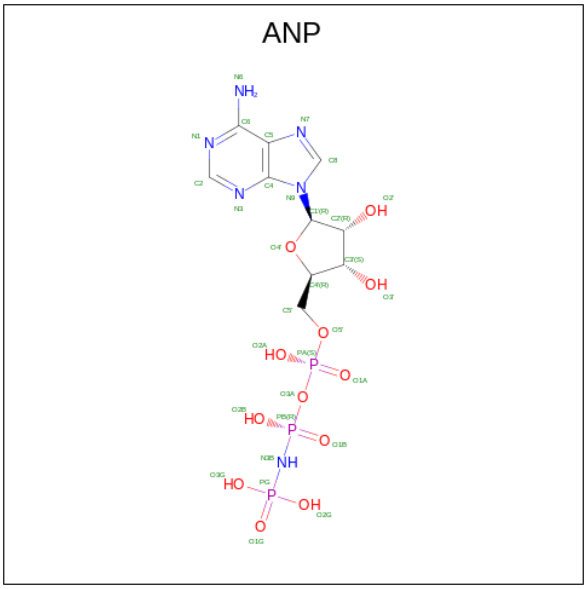
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ILE	deletion	UNP A0A7Y1Q2L1
F	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
F	101	THR	SER	conflict	UNP A0A7Y1Q2L1
F	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
F	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
F	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
F	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	C	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	D	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	E	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	F	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0
3	B	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0
3	D	2	Total Mn 2 2	0	0
3	E	2	Total Mn 2 2	0	0
3	F	2	Total Mn 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	334	Total O 334 334	0	0
5	B	335	Total O 335 335	0	0
5	C	387	Total O 387 387	0	0
5	D	355	Total O 355 355	0	0
5	E	325	Total O 325 325	0	0

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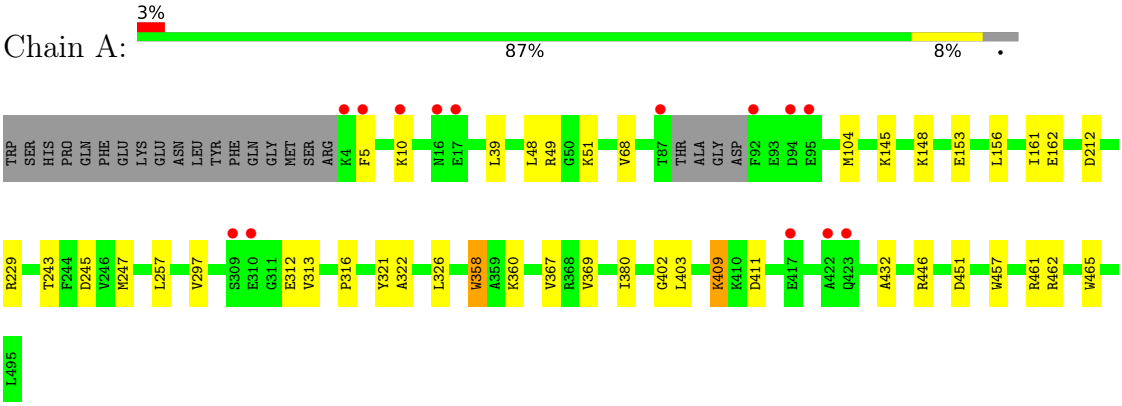
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	373	Total 373	O 373	0	0

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.

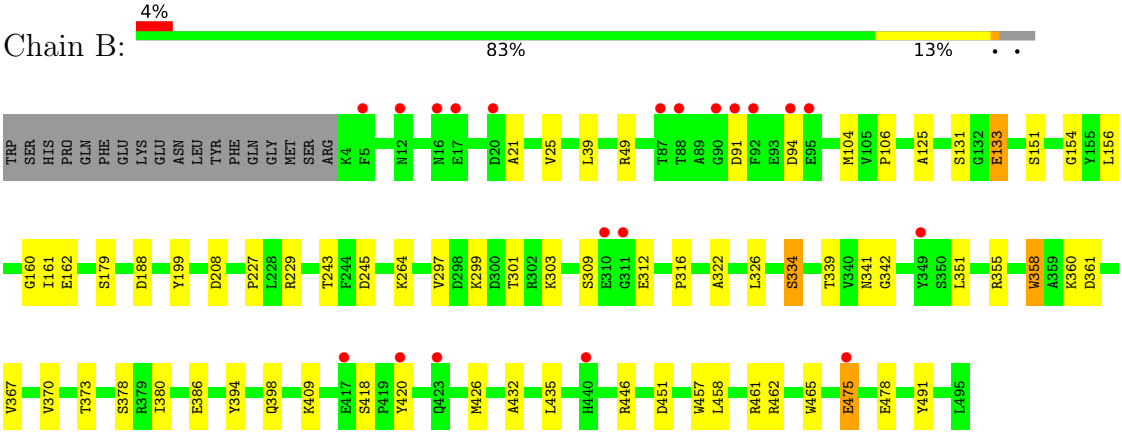
- Molecule 1: Glutamine synthetase

Chain A:



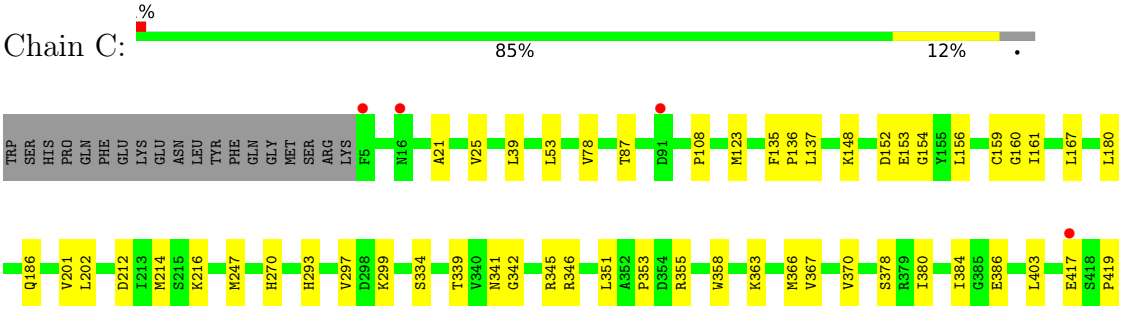
- Molecule 1: Glutamine synthetase

Chain B:



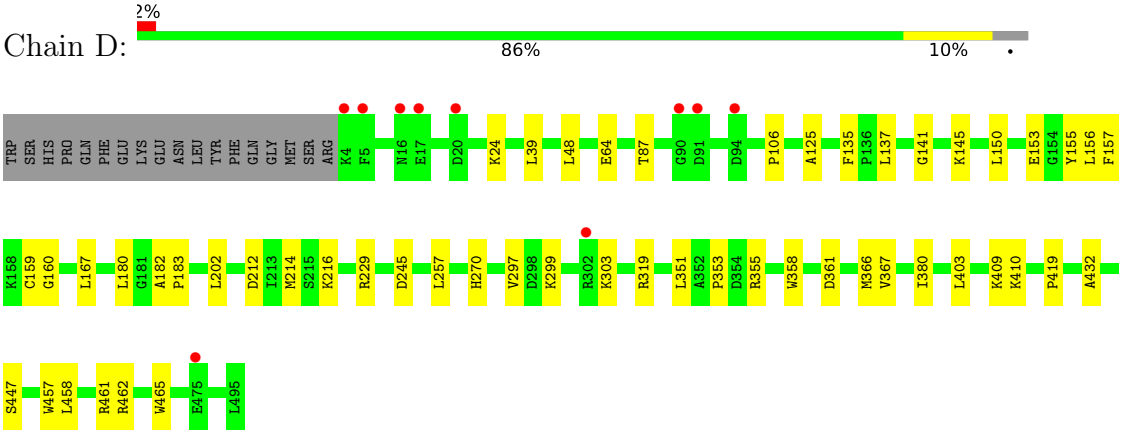
- Molecule 1: Glutamine synthetase

Chain C:



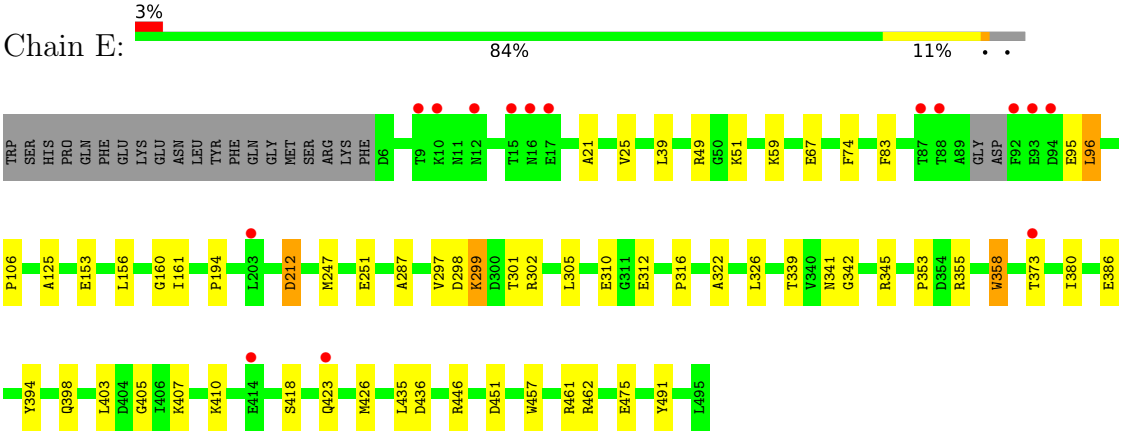
• Molecule 1: Glutamine synthetase

Chain D:



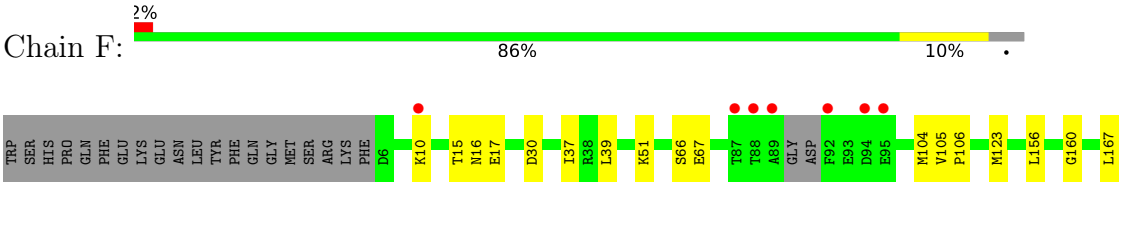
• Molecule 1: Glutamine synthetase

Chain E:



• Molecule 1: Glutamine synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.69Å 140.57Å 217.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.82 – 2.00 49.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.82-2.00) 98.4 (49.69-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.14_3260: 000)	Depositor
R, R_{free}	0.179 , 0.206 0.181 , 0.206	Depositor DCC
R_{free} test set	12596 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	1.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25382	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 38.26 % 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 3.7872e-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: MG, ANP, MN

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	0.38	0/3918	0.57	0/5313
1	B	0.35	0/3943	0.56	0/5349
1	C	0.39	0/3934	0.58	0/5338
1	D	0.36	0/3943	0.56	0/5349
1	E	0.36	0/3909	0.57	0/5303
1	F	0.37	0/3909	0.57	0/5303
All	All	0.37	0/23556	0.57	0/31955

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3824	0	3757	28	0
1	B	3848	0	3777	53	0
1	C	3839	0	3764	46	0
1	D	3848	0	3777	29	0
1	E	3816	0	3747	42	0
1	F	3816	0	3747	29	0
2	A	31	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	13	13	1	0
2	C	31	13	13	1	0
2	D	31	13	13	1	0
2	E	31	13	13	1	0
2	F	31	13	13	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	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
5	A	334	0	0	3	0
5	B	335	0	0	5	0
5	C	387	0	0	2	0
5	D	355	0	0	1	0
5	E	325	0	0	6	0
5	F	373	0	0	1	0
All	All	25304	78	22647	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (220) 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:B:301:THR:OG1	1:B:303:LYS:HG3	1.57	1.01
1:B:154:GLY:HA2	1:B:299:LYS:HE2	1.64	0.79
1:F:15:THR:HG22	1:F:17:GLU:H	1.52	0.73
1:A:39:LEU:HG	1:A:104:MET:HE2	1.71	0.72
1:C:339:THR:HG22	1:C:341:ASN:N	2.05	0.71
1:E:310:GLU:OE2	1:E:373:THR:HG21	1.90	0.70
1:D:39:LEU:HD21	1:D:106:PRO:HB3	1.72	0.69
1:B:154:GLY:HA2	1:B:299:LYS:CE	2.24	0.68
1:E:339:THR:HG22	1:E:341:ASN:N	2.09	0.68
1:B:339:THR:HG22	1:B:341:ASN:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LEU:HD11	1:B:358:TRP:HB3	1.76	0.67
1:C:108:PRO:HA	1:C:123:MET:CE	2.24	0.67
1:E:339:THR:HG21	5:E:757:HOH:O	1.96	0.65
1:D:141:GLY:O	1:D:145:LYS:HG3	1.98	0.64
1:D:156:LEU:HD21	1:D:299:LYS:HG3	1.80	0.64
1:D:87:THR:HG23	1:E:418:SER:OG	1.99	0.62
1:B:339:THR:HG22	1:B:341:ASN:H	1.64	0.62
1:D:48:LEU:HD21	1:D:257:LEU:HD21	1.82	0.61
1:C:153:GLU:HG3	1:C:403:LEU:HD11	1.81	0.61
1:E:39:LEU:HD11	1:E:106:PRO:HG3	1.83	0.61
1:A:313:VAL:CG2	1:A:360:LYS:HD3	2.31	0.61
1:C:148:LYS:HE2	1:C:152:ASP:OD1	2.01	0.61
1:E:339:THR:HG22	1:E:341:ASN:H	1.66	0.60
1:C:339:THR:HG22	1:C:341:ASN:H	1.66	0.60
1:B:339:THR:HG23	1:B:491:TYR:CE2	2.36	0.60
1:C:87:THR:HG23	1:F:418:SER:OG	2.01	0.59
1:B:39:LEU:HD21	1:B:106:PRO:HB3	1.84	0.59
1:C:417:GLU:O	1:C:417:GLU:HG3	2.00	0.59
1:B:367:VAL:HG13	1:B:380:ILE:HG23	1.85	0.59
1:B:355:ARG:NH2	1:B:420:TYR:O	2.35	0.58
1:D:167:LEU:HD22	1:D:214:MET:CE	2.33	0.58
1:E:339:THR:HG23	1:E:491:TYR:CE2	2.39	0.58
1:B:39:LEU:HB3	1:B:104:MET:CE	2.33	0.58
1:C:353:PRO:HB3	1:C:366:MET:HA	1.85	0.58
1:B:301:THR:OG1	1:B:303:LYS:CG	2.43	0.58
1:C:353:PRO:HG2	1:C:384:ILE:HD13	1.86	0.58
1:F:312:GLU:OE2	1:F:316:PRO:HD3	2.04	0.57
1:E:312:GLU:OE2	1:E:316:PRO:HD3	2.04	0.57
1:B:39:LEU:HD13	1:B:104:MET:HE2	1.85	0.57
1:E:39:LEU:HD22	1:E:125:ALA:HB2	1.86	0.57
1:B:39:LEU:HB3	1:B:104:MET:HE1	1.86	0.56
1:A:312:GLU:OE2	1:A:316:PRO:HD3	2.05	0.56
1:B:334:SER:HB2	5:B:638:HOH:O	2.03	0.56
1:B:301:THR:HG1	1:B:303:LYS:HG3	1.70	0.56
1:B:339:THR:HG21	5:B:692:HOH:O	2.06	0.56
1:B:91:ASP:HB3	1:B:94:ASP:HB3	1.87	0.56
1:A:313:VAL:HG22	1:A:369:VAL:HG11	1.88	0.55
1:A:229:ARG:HD2	1:A:245:ASP:OD1	2.07	0.55
1:D:353:PRO:HB3	1:D:366:MET:HA	1.89	0.55
1:E:298:ASP:HB3	1:E:301:THR:OG1	2.05	0.55
1:A:51:LYS:NZ	5:A:602:HOH:O	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:HG13	1:A:380:ILE:HG23	1.90	0.54
1:A:446:ARG:HD3	1:A:451:ASP:OD1	2.07	0.54
1:D:156:LEU:CD2	1:D:299:LYS:HG3	2.38	0.54
1:F:229:ARG:HD2	1:F:245:ASP:OD1	2.08	0.54
1:A:68:VAL:HG11	1:A:104:MET:SD	2.48	0.54
1:C:339:THR:HG22	1:C:342:GLY:H	1.72	0.54
1:B:339:THR:HB	1:B:386:GLU:OE2	2.09	0.53
1:F:105:VAL:HG23	1:F:105:VAL:O	2.09	0.53
1:B:39:LEU:HD22	1:B:125:ALA:HB2	1.90	0.53
1:B:229:ARG:HD2	1:B:245:ASP:OD1	2.10	0.52
1:E:156:LEU:HD21	1:E:299:LYS:HG3	1.91	0.52
1:B:432:ALA:HB2	1:B:465:TRP:CE2	2.44	0.52
1:E:355:ARG:HG2	1:E:426:MET:SD	2.50	0.52
1:E:475:GLU:HB2	5:E:656:HOH:O	2.10	0.52
1:A:161:ILE:HD12	1:A:247:MET:CE	2.40	0.51
1:D:355:ARG:HD2	1:D:419:PRO:O	2.11	0.51
1:D:156:LEU:HB2	1:D:297:VAL:HG22	1.93	0.51
1:D:319:ARG:HD3	5:D:688:HOH:O	2.11	0.50
1:C:39:LEU:HD22	1:C:53:LEU:HD11	1.94	0.50
1:C:423:GLN:CD	5:C:611:HOH:O	2.50	0.50
1:F:435:LEU:HD13	1:F:462:ARG:HG2	1.93	0.50
1:A:313:VAL:HG23	1:A:360:LYS:HE3	1.94	0.50
1:C:339:THR:HB	1:C:386:GLU:OE1	2.10	0.50
1:C:353:PRO:HG2	1:C:384:ILE:CD1	2.42	0.50
1:E:59:LYS:HE3	5:E:850:HOH:O	2.12	0.49
1:A:212:ASP:OD1	1:A:212:ASP:N	2.44	0.49
1:E:339:THR:CG2	1:E:341:ASN:H	2.25	0.49
1:C:334:SER:HB3	1:C:457:TRP:HE1	1.78	0.49
1:C:339:THR:CG2	1:C:341:ASN:H	2.24	0.49
1:B:355:ARG:HG2	1:B:426:MET:SD	2.52	0.48
1:B:21:ALA:O	1:B:25:VAL:HG23	2.13	0.48
1:B:446:ARG:HD2	5:B:887:HOH:O	2.13	0.48
1:E:339:THR:HB	1:E:386:GLU:OE2	2.14	0.48
1:A:313:VAL:HG23	1:A:360:LYS:CE	2.43	0.48
1:C:167:LEU:HD22	1:C:214:MET:CE	2.43	0.48
1:C:345:ARG:HD3	5:C:622:HOH:O	2.12	0.48
1:C:346:ARG:NE	1:C:384:ILE:HD11	2.28	0.48
1:A:153:GLU:HG3	1:A:403:LEU:HD11	1.96	0.48
1:C:108:PRO:HA	1:C:123:MET:HE2	1.94	0.48
1:E:339:THR:HG22	1:E:342:GLY:H	1.79	0.48
1:B:339:THR:CG2	1:B:341:ASN:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HD3	1:C:270:HIS:CE1	2.48	0.47
1:C:339:THR:HG23	1:C:491:TYR:CE2	2.49	0.47
1:E:457:TRP:O	1:E:461:ARG:HG2	2.14	0.47
1:B:309:SER:HA	1:B:373:THR:HG23	1.96	0.47
1:C:212:ASP:OD1	1:C:212:ASP:N	2.46	0.47
1:A:39:LEU:CG	1:A:104:MET:HE2	2.43	0.47
1:B:339:THR:HG23	1:B:491:TYR:CZ	2.49	0.47
1:E:212:ASP:N	1:E:212:ASP:OD1	2.46	0.47
1:F:234:GLU:HG2	1:F:241:GLU:HB2	1.96	0.47
1:D:212:ASP:OD1	1:D:212:ASP:N	2.45	0.47
1:E:51:LYS:NZ	1:E:67:GLU:O	2.36	0.47
1:E:405:GLY:HA2	1:E:410:LYS:HG3	1.95	0.47
1:B:199:TYR:CE2	1:F:182:ALA:HA	2.50	0.47
1:E:161:ILE:HA	5:E:604:HOH:O	2.14	0.47
1:D:458:LEU:O	1:D:462:ARG:HG3	2.15	0.47
1:E:326:LEU:HD11	1:E:358:TRP:HB3	1.97	0.47
1:E:423:GLN:NE2	5:E:611:HOH:O	2.47	0.47
1:B:161:ILE:HA	5:B:605:HOH:O	2.15	0.46
1:C:351:LEU:HG	1:C:363:LYS:HB3	1.96	0.46
1:B:151:SER:O	1:B:299:LYS:HE2	2.16	0.46
1:F:212:ASP:OD1	1:F:212:ASP:N	2.46	0.46
1:D:39:LEU:HD22	1:D:125:ALA:HB2	1.98	0.46
1:F:353:PRO:HB3	1:F:366:MET:HA	1.96	0.46
1:E:160:GLY:HA3	2:E:501:ANP:H1'	1.97	0.46
1:C:160:GLY:HA3	2:C:501:ANP:H1'	1.96	0.46
1:A:409:LYS:HB2	1:A:409:LYS:HE2	1.77	0.46
1:C:355:ARG:HD2	1:C:419:PRO:O	2.16	0.46
1:F:51:LYS:NZ	1:F:67:GLU:O	2.36	0.46
1:B:156:LEU:HB2	1:B:297:VAL:HG22	1.98	0.46
1:E:322:ALA:HB2	1:E:380:ILE:HD11	1.97	0.46
1:E:435:LEU:HD13	1:E:462:ARG:HG2	1.98	0.46
1:C:457:TRP:O	1:C:461:ARG:HG2	2.16	0.45
1:A:162:GLU:HG3	1:A:243:THR:HG22	1.98	0.45
1:E:403:LEU:HG	1:E:407:LYS:HE3	1.97	0.45
1:D:432:ALA:HB2	1:D:465:TRP:CE2	2.51	0.45
1:C:156:LEU:HB2	1:C:297:VAL:HG22	1.99	0.45
1:D:150:LEU:HG	1:D:155:TYR:HB2	1.99	0.45
1:D:457:TRP:O	1:D:461:ARG:HG2	2.17	0.45
1:F:355:ARG:HD2	1:F:419:PRO:O	2.17	0.44
1:D:229:ARG:HD2	1:D:245:ASP:OD1	2.16	0.44
1:A:457:TRP:O	1:A:461:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LEU:HD11	1:F:194:PRO:HG2	2.00	0.44
1:B:475:GLU:H	1:B:475:GLU:HG3	1.56	0.44
1:B:154:GLY:CA	1:B:299:LYS:HE2	2.40	0.44
1:C:154:GLY:HA2	1:C:299:LYS:HD3	1.99	0.44
1:D:153:GLU:HG3	1:D:403:LEU:HD11	1.99	0.44
1:E:21:ALA:O	1:E:25:VAL:HG23	2.18	0.44
1:B:162:GLU:HG3	1:B:243:THR:HG22	1.98	0.44
1:C:161:ILE:HD12	1:C:247:MET:CE	2.48	0.44
1:A:321:TYR:CE2	1:A:402:GLY:HA3	2.53	0.44
1:E:297:VAL:CG1	1:E:302:ARG:HA	2.47	0.44
1:E:298:ASP:HB2	1:E:305:LEU:HD21	1.99	0.44
1:B:264:LYS:HE3	5:B:845:HOH:O	2.18	0.44
1:C:21:ALA:O	1:C:25:VAL:HG23	2.18	0.44
1:C:339:THR:CG2	1:C:341:ASN:HB3	2.48	0.44
1:C:370:VAL:O	1:C:378:SER:HA	2.17	0.44
1:F:287:ALA:HB1	1:F:345:ARG:HG3	2.00	0.43
1:F:39:LEU:HD21	1:F:106:PRO:HG3	2.00	0.43
1:A:161:ILE:HA	5:A:611:HOH:O	2.19	0.43
1:B:370:VAL:O	1:B:378:SER:HA	2.17	0.43
1:B:457:TRP:O	1:B:461:ARG:HG2	2.18	0.43
1:E:353:PRO:HD2	5:E:682:HOH:O	2.19	0.43
1:F:367:VAL:HG13	1:F:380:ILE:HG23	2.00	0.43
1:E:96:LEU:HD12	1:E:96:LEU:HA	1.78	0.43
1:C:334:SER:OG	1:C:435:LEU:HD23	2.18	0.43
1:F:357:ALA:HB2	1:F:424:VAL:HG21	2.00	0.43
1:B:322:ALA:HB2	1:B:380:ILE:HD11	2.01	0.43
1:C:367:VAL:HG13	1:C:380:ILE:HG23	2.00	0.43
1:A:39:LEU:HG	1:A:104:MET:CE	2.46	0.43
1:B:312:GLU:OE2	1:B:316:PRO:HD3	2.18	0.43
1:D:160:GLY:HA3	2:D:501:ANP:H1'	2.01	0.43
1:F:66:SER:HB3	1:F:104:MET:HE3	2.00	0.43
1:F:264:LYS:HE3	5:F:893:HOH:O	2.18	0.43
1:F:265:GLN:O	1:F:269:ARG:HG2	2.18	0.43
1:B:339:THR:CG2	1:B:341:ASN:HB3	2.49	0.42
1:B:394:TYR:O	1:B:398:GLN:HG2	2.18	0.42
1:E:394:TYR:O	1:E:398:GLN:HG2	2.19	0.42
1:D:216:LYS:HD3	1:D:270:HIS:CE1	2.54	0.42
1:E:339:THR:HG23	1:E:491:TYR:CZ	2.53	0.42
1:E:153:GLU:HG3	1:E:403:LEU:HD11	2.02	0.42
1:B:446:ARG:HD3	1:B:451:ASP:OD1	2.19	0.42
1:D:182:ALA:HB1	1:D:183:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:H	1:B:133:GLU:HG2	1.55	0.42
1:B:360:LYS:HG3	1:B:361:ASP:OD2	2.19	0.42
1:D:180:LEU:HD11	1:E:194:PRO:HG2	2.00	0.42
1:A:432:ALA:HB2	1:A:465:TRP:CE2	2.55	0.42
1:B:339:THR:HG22	1:B:342:GLY:H	1.85	0.42
1:C:159:CYS:HA	1:C:293:HIS:O	2.19	0.42
1:E:74:PHE:CG	1:E:83:PHE:HB2	2.55	0.42
1:A:326:LEU:HD11	1:A:358:TRP:HB3	2.02	0.42
1:C:78:VAL:HG11	1:C:186:GLN:HG2	2.02	0.42
1:E:247:MET:CE	1:E:251:GLU:HG2	2.50	0.42
1:E:287:ALA:HB1	1:E:345:ARG:HG3	2.01	0.42
1:D:367:VAL:HG13	1:D:380:ILE:HG23	2.02	0.42
1:F:160:GLY:HA3	2:F:501:ANP:H1'	2.02	0.42
1:B:160:GLY:HA3	2:B:501:ANP:H1'	2.01	0.41
1:E:436:ASP:OD2	1:E:462:ARG:NH2	2.51	0.41
1:C:216:LYS:HD3	1:C:270:HIS:NE2	2.35	0.41
1:F:37:ILE:HG21	1:F:123:MET:CE	2.50	0.41
1:B:49:ARG:HA	1:D:202:LEU:O	2.20	0.41
1:F:15:THR:HG22	1:F:16:ASN:N	2.35	0.41
1:C:346:ARG:CZ	1:C:384:ILE:HD11	2.50	0.41
1:D:135:PHE:CE2	1:D:137:LEU:HB2	2.56	0.41
1:A:48:LEU:HD21	1:A:257:LEU:HD21	2.03	0.41
1:A:156:LEU:HB2	1:A:297:VAL:HG22	2.03	0.41
1:C:432:ALA:HB2	1:C:465:TRP:CE2	2.55	0.41
1:F:403:LEU:HG	1:F:407:LYS:HE2	2.03	0.41
1:B:208:ASP:OD2	1:F:269:ARG:HD3	2.19	0.41
1:C:39:LEU:HD22	1:C:53:LEU:CD1	2.50	0.41
1:F:457:TRP:O	1:F:461:ARG:HG2	2.21	0.41
1:B:179:SER:HB3	1:B:188:ASP:HB2	2.02	0.41
1:B:227:PRO:HB2	1:B:245:ASP:HB2	2.03	0.41
1:B:458:LEU:O	1:B:462:ARG:HG3	2.21	0.41
1:C:135:PHE:CE2	1:C:137:LEU:HB2	2.55	0.41
1:F:105:VAL:O	1:F:105:VAL:CG2	2.68	0.41
1:D:150:LEU:CD2	1:D:157:PHE:HB2	2.51	0.41
1:D:157:PHE:CE2	1:D:159:CYS:HB2	2.56	0.41
1:A:322:ALA:HB2	1:A:380:ILE:HD11	2.04	0.40
1:C:135:PHE:CD1	1:C:136:PRO:HD2	2.56	0.40
1:F:156:LEU:HB2	1:F:297:VAL:CG2	2.51	0.40
1:A:321:TYR:CD2	1:A:402:GLY:HA3	2.56	0.40
1:C:201:VAL:HG22	1:C:202:LEU:HG	2.03	0.40
1:C:353:PRO:HB3	1:C:366:MET:CA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LEU:HD23	1:D:351:LEU:HA	1.89	0.40
1:E:446:ARG:NH1	1:E:451:ASP:OD1	2.49	0.40
1:A:462:ARG:HD3	5:A:618:HOH:O	2.22	0.40
1:B:435:LEU:HD13	1:B:462:ARG:HG2	2.03	0.40
1:F:156:LEU:HB2	1:F:297:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/510 (95%)	479 (99%)	5 (1%)	0	100	100
1	B	490/510 (96%)	485 (99%)	5 (1%)	0	100	100
1	C	489/510 (96%)	483 (99%)	6 (1%)	0	100	100
1	D	490/510 (96%)	484 (99%)	6 (1%)	0	100	100
1	E	484/510 (95%)	479 (99%)	5 (1%)	0	100	100
1	F	484/510 (95%)	480 (99%)	4 (1%)	0	100	100
All	All	2921/3060 (96%)	2890 (99%)	31 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	408/427 (96%)	400 (98%)	8 (2%)	55	58
1	B	410/427 (96%)	401 (98%)	9 (2%)	52	55
1	C	409/427 (96%)	407 (100%)	2 (0%)	88	92
1	D	410/427 (96%)	402 (98%)	8 (2%)	55	58
1	E	407/427 (95%)	401 (98%)	6 (2%)	65	69
1	F	407/427 (95%)	401 (98%)	6 (2%)	65	69
All	All	2451/2562 (96%)	2412 (98%)	39 (2%)	62	67

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	10	LYS
1	A	49	ARG
1	A	145	LYS
1	A	148	LYS
1	A	358	TRP
1	A	409	LYS
1	A	411	ASP
1	B	131	SER
1	B	133	GLU
1	B	334	SER
1	B	351	LEU
1	B	358	TRP
1	B	409	LYS
1	B	418	SER
1	B	475	GLU
1	B	478	GLU
1	C	358	TRP
1	C	423	GLN
1	D	24	LYS
1	D	64	GLU
1	D	303	LYS
1	D	358	TRP
1	D	361	ASP
1	D	409	LYS
1	D	410	LYS
1	D	447	SER
1	E	49	ARG
1	E	95	GLU
1	E	96	LEU

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Mol	Chain	Res	Type
1	E	212	ASP
1	E	299	LYS
1	E	358	TRP
1	F	10	LYS
1	F	30	ASP
1	F	167	LEU
1	F	358	TRP
1	F	394	TYR
1	F	443	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ANP	F	501	3,4	29,33,33	1.17	4 (13%)	31,52,52	1.19	4 (12%)
2	ANP	A	501	3,4	29,33,33	1.15	3 (10%)	31,52,52	2.10	6 (19%)
2	ANP	D	501	3,4	29,33,33	1.25	4 (13%)	31,52,52	1.12	3 (9%)
2	ANP	C	501	3,4	29,33,33	1.17	4 (13%)	31,52,52	1.15	4 (12%)
2	ANP	E	501	3,4	29,33,33	1.18	5 (17%)	31,52,52	1.26	3 (9%)
2	ANP	B	501	3,4	29,33,33	1.21	4 (13%)	31,52,52	1.39	4 (12%)

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	ANP	F	501	3,4	-	5/14/38/38	0/3/3/3
2	ANP	A	501	3,4	-	6/14/38/38	0/3/3/3
2	ANP	D	501	3,4	-	4/14/38/38	0/3/3/3
2	ANP	C	501	3,4	-	2/14/38/38	0/3/3/3
2	ANP	E	501	3,4	-	5/14/38/38	0/3/3/3
2	ANP	B	501	3,4	-	4/14/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ANP	PG-O2G	-3.30	1.47	1.56
2	A	501	ANP	PG-O2G	-3.27	1.48	1.56
2	D	501	ANP	PG-N3B	3.25	1.71	1.63
2	C	501	ANP	PG-N3B	3.13	1.71	1.63
2	B	501	ANP	PG-O3G	-3.07	1.48	1.56
2	F	501	ANP	PG-N3B	3.04	1.71	1.63
2	A	501	ANP	PG-O3G	-3.03	1.48	1.56
2	D	501	ANP	PG-O1G	2.93	1.50	1.46
2	E	501	ANP	PG-O2G	-2.69	1.49	1.56
2	E	501	ANP	PG-O3G	-2.58	1.49	1.56
2	B	501	ANP	PB-O2B	-2.55	1.49	1.56
2	E	501	ANP	PG-O1G	2.55	1.50	1.46
2	D	501	ANP	PB-O1B	2.54	1.50	1.46
2	C	501	ANP	PB-O1B	2.51	1.50	1.46
2	F	501	ANP	PG-O1G	2.51	1.50	1.46
2	E	501	ANP	PB-O2B	-2.42	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ANP	PB-O2B	-2.40	1.50	1.56
2	C	501	ANP	PG-O1G	2.36	1.49	1.46
2	D	501	ANP	PB-N3B	2.31	1.69	1.63
2	F	501	ANP	PB-O1B	2.30	1.49	1.46
2	F	501	ANP	PB-N3B	2.27	1.69	1.63
2	C	501	ANP	PB-N3B	2.24	1.69	1.63
2	E	501	ANP	PB-O1B	2.07	1.49	1.46
2	B	501	ANP	PG-O1G	2.00	1.49	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	ANP	O3G-PG-O1G	-9.10	90.57	113.45
2	B	501	ANP	O2G-PG-O1G	-4.64	101.78	113.45
2	E	501	ANP	O2B-PB-O1B	4.14	118.60	109.92
2	A	501	ANP	O2B-PB-O1B	3.99	118.28	109.92
2	A	501	ANP	O1G-PG-N3B	-3.22	107.03	111.77
2	B	501	ANP	O3G-PG-O1G	-3.15	105.52	113.45
2	B	501	ANP	O2B-PB-O1B	3.13	116.48	109.92
2	D	501	ANP	O3A-PB-N3B	3.11	115.22	106.59
2	F	501	ANP	PB-O3A-PA	-2.92	122.33	132.62
2	C	501	ANP	O3G-PG-O1G	-2.88	106.22	113.45
2	D	501	ANP	PB-O3A-PA	-2.71	123.08	132.62
2	C	501	ANP	C5-C6-N6	2.58	124.27	120.35
2	F	501	ANP	C5-C6-N6	2.49	124.13	120.35
2	C	501	ANP	PB-O3A-PA	-2.45	124.00	132.62
2	E	501	ANP	O2G-PG-O1G	-2.40	107.42	113.45
2	F	501	ANP	O3A-PB-N3B	2.36	113.14	106.59
2	A	501	ANP	C5-C6-N6	2.33	123.89	120.35
2	F	501	ANP	O1G-PG-N3B	-2.32	108.35	111.77
2	B	501	ANP	C5-C6-N6	2.32	123.88	120.35
2	E	501	ANP	C5-C6-N6	2.29	123.84	120.35
2	D	501	ANP	O2G-PG-O1G	-2.24	107.83	113.45
2	C	501	ANP	O1G-PG-N3B	-2.21	108.51	111.77
2	A	501	ANP	O3A-PB-N3B	2.19	112.66	106.59
2	A	501	ANP	O2G-PG-O1G	-2.15	108.05	113.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	501	ANP	PA-O3A-PB-O2B
2	B	501	ANP	PA-O3A-PB-O1B
2	B	501	ANP	PA-O3A-PB-O2B
2	B	501	ANP	O4'-C4'-C5'-O5'
2	C	501	ANP	O4'-C4'-C5'-O5'
2	D	501	ANP	O4'-C4'-C5'-O5'
2	E	501	ANP	PG-N3B-PB-O1B
2	E	501	ANP	PA-O3A-PB-O1B
2	F	501	ANP	PB-N3B-PG-O1G
2	F	501	ANP	PG-N3B-PB-O1B
2	F	501	ANP	O4'-C4'-C5'-O5'
2	A	501	ANP	O4'-C4'-C5'-O5'
2	A	501	ANP	C3'-C4'-C5'-O5'
2	E	501	ANP	O4'-C4'-C5'-O5'
2	B	501	ANP	C3'-C4'-C5'-O5'
2	C	501	ANP	C3'-C4'-C5'-O5'
2	D	501	ANP	C3'-C4'-C5'-O5'
2	F	501	ANP	C3'-C4'-C5'-O5'
2	D	501	ANP	PB-O3A-PA-O1A
2	E	501	ANP	C3'-C4'-C5'-O5'
2	A	501	ANP	PB-O3A-PA-O5'
2	E	501	ANP	PB-O3A-PA-O2A
2	F	501	ANP	PB-O3A-PA-O2A
2	A	501	ANP	PG-N3B-PB-O3A
2	D	501	ANP	PB-N3B-PG-O1G

There are no ring outliers.

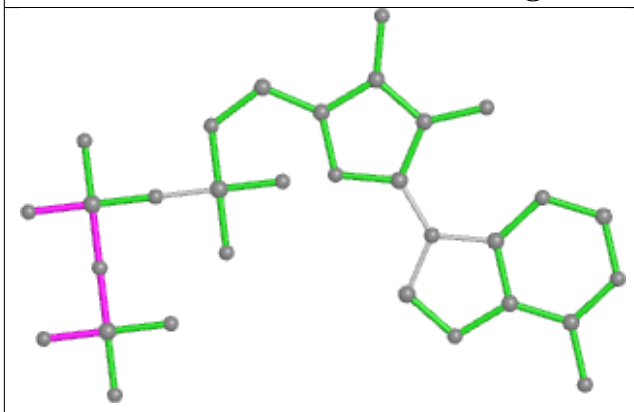
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	ANP	1	0
2	D	501	ANP	1	0
2	C	501	ANP	1	0
2	E	501	ANP	1	0
2	B	501	ANP	1	0

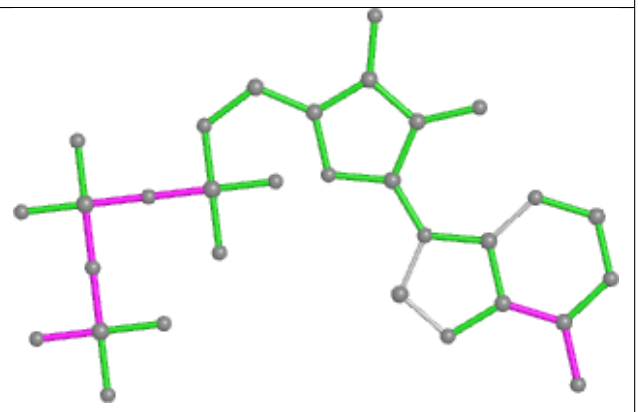
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

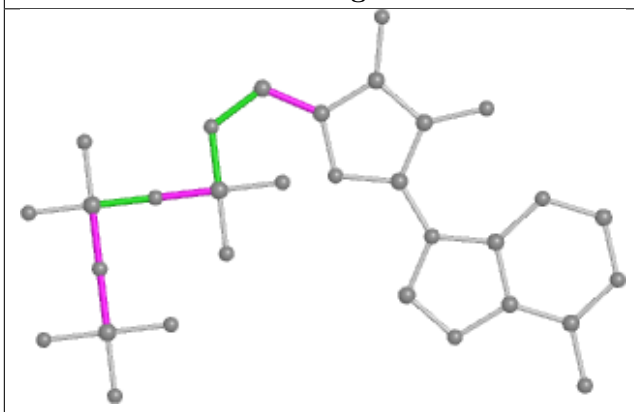
Ligand ANP F 501



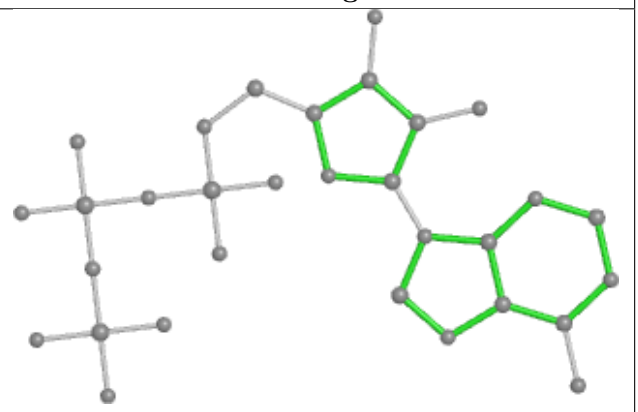
Bond lengths



Bond angles

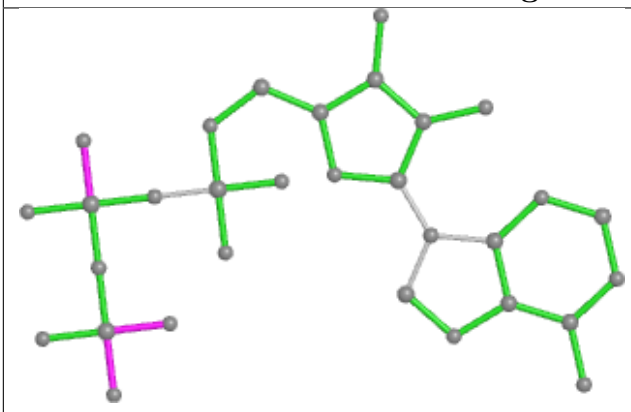


Torsions



Rings

Ligand ANP A 501



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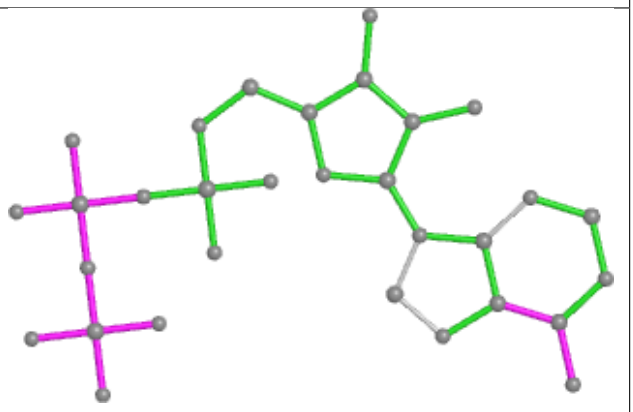

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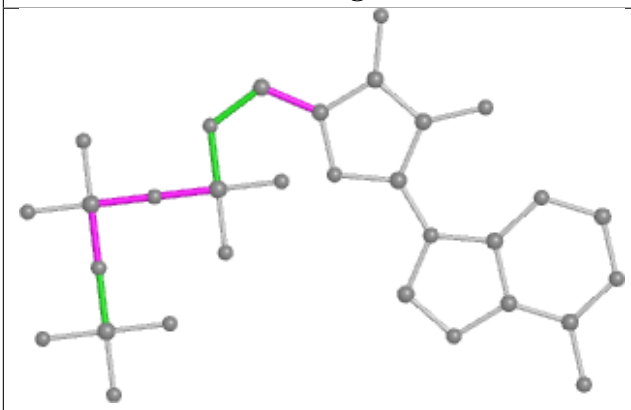

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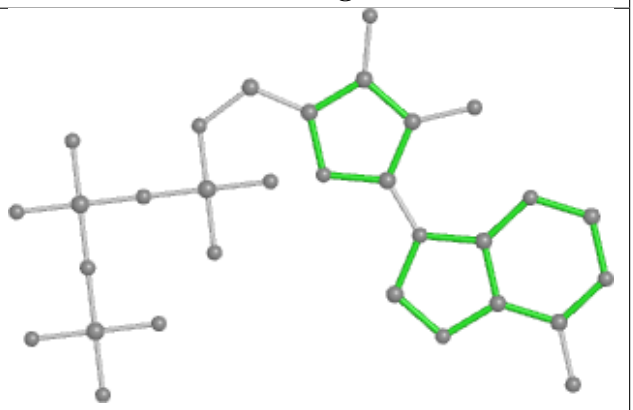
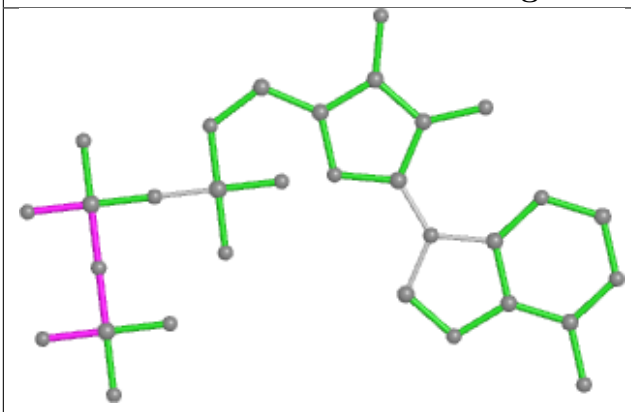
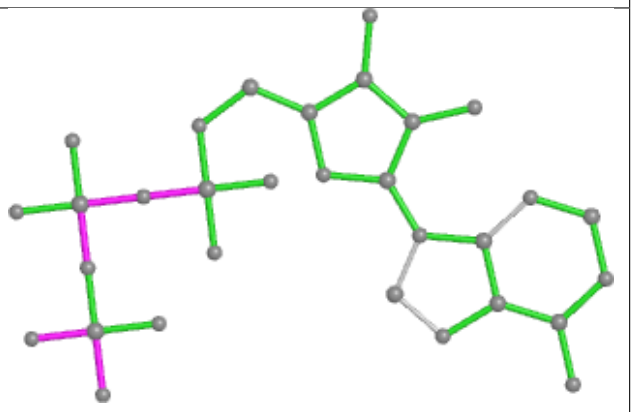


Rings

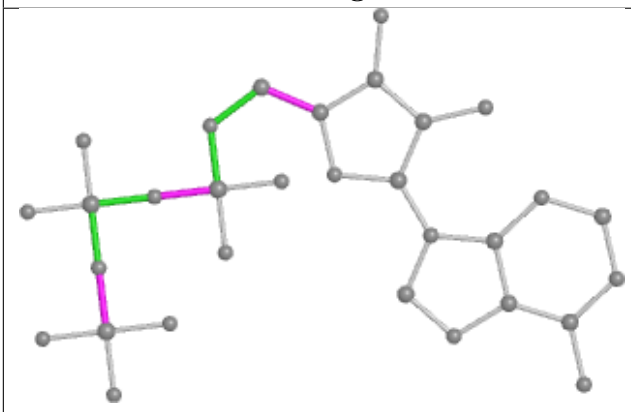
Ligand ANP D 501



Bond lengths



Bond angles



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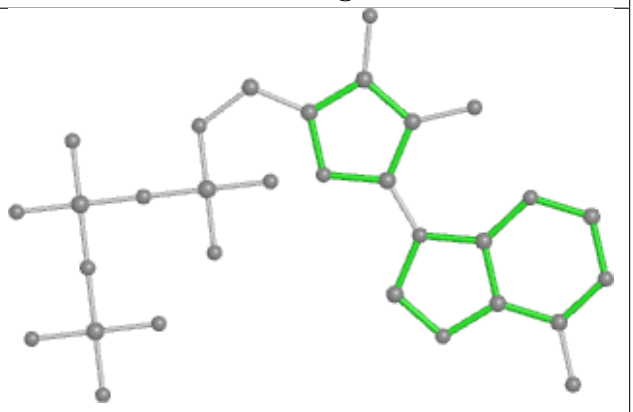
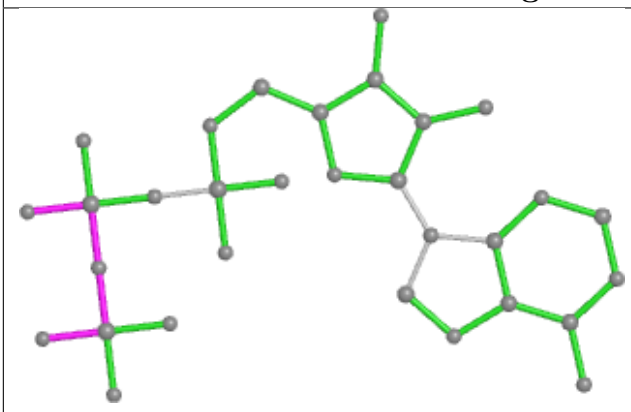
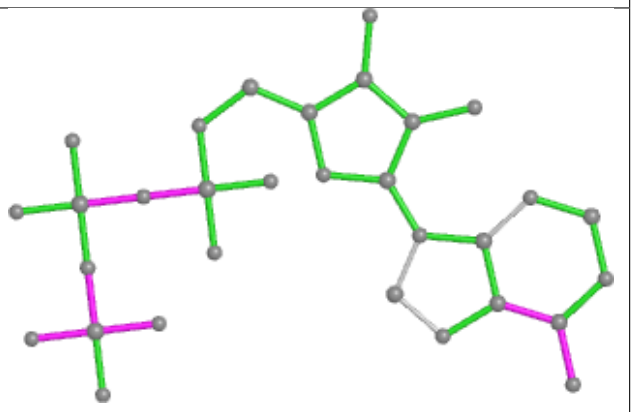


Rings

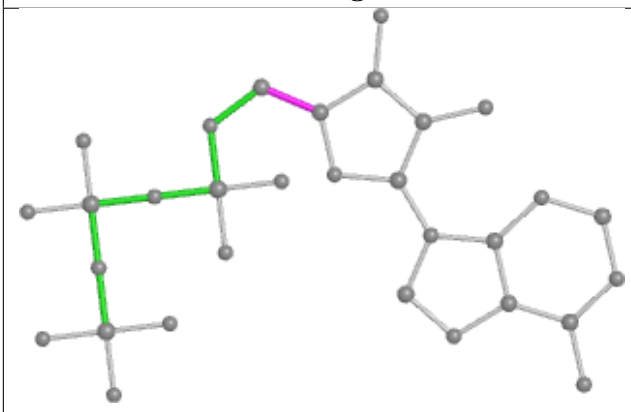
Ligand ANP C 501



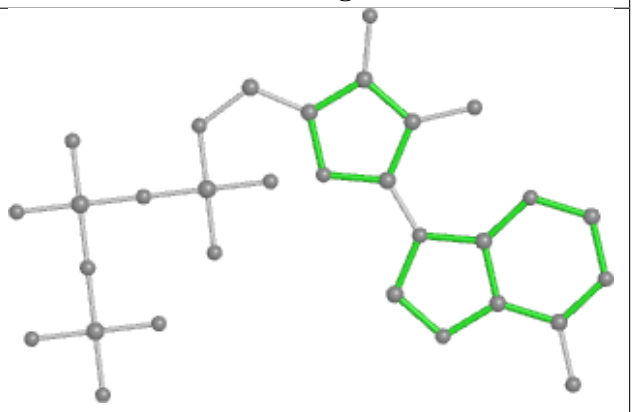
Bond lengths



Bond angles

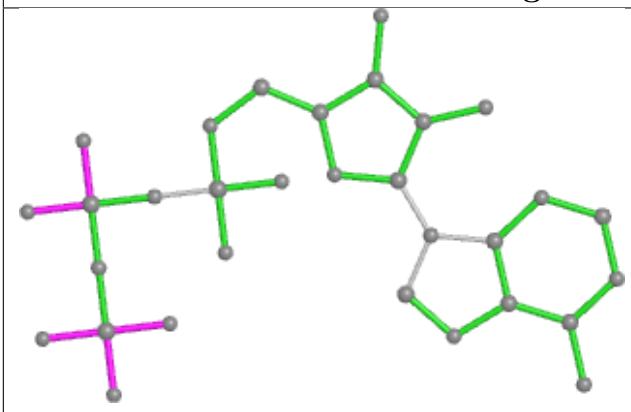


Torsions

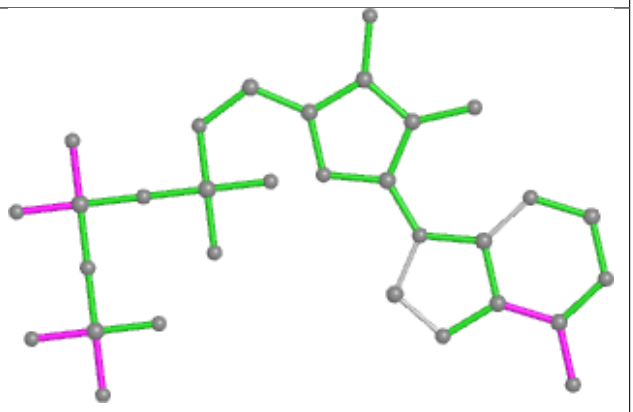


Rings

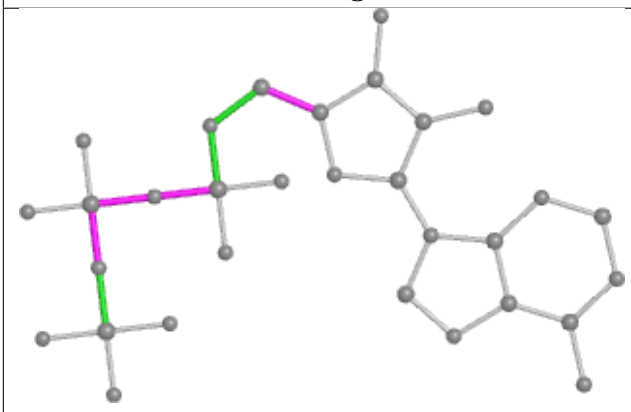
Ligand ANP E 501



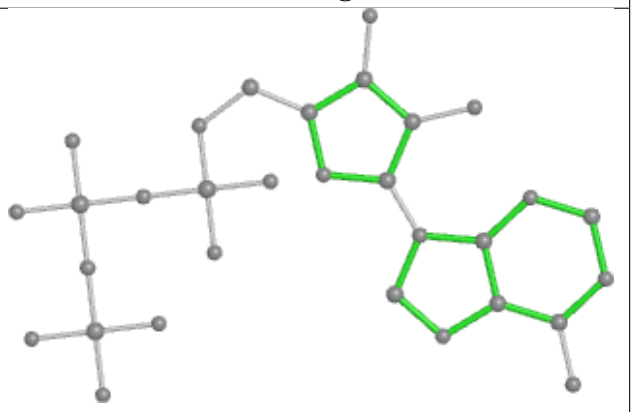
Bond lengths



Bond angles

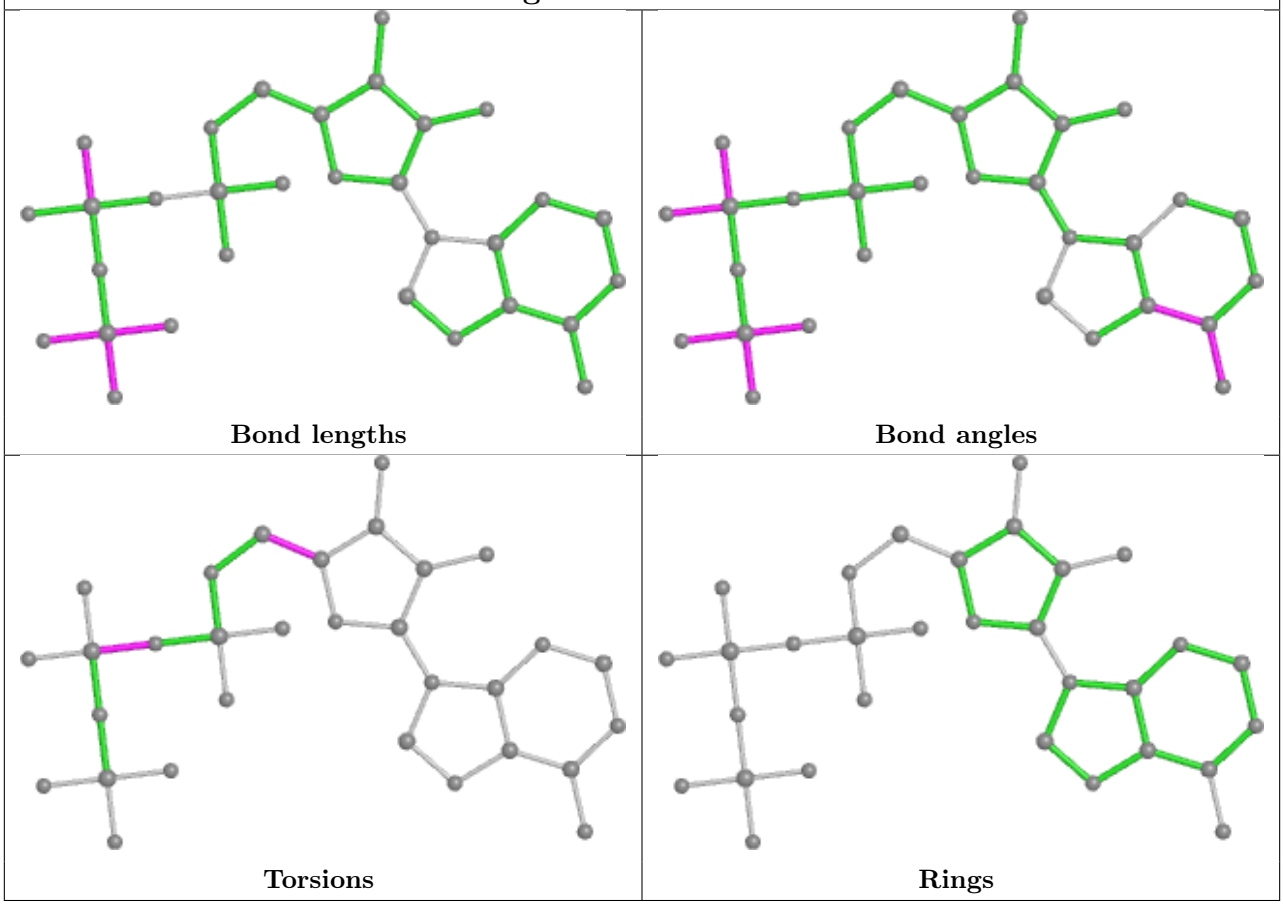


Torsions



Rings

Ligand ANP B 501



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	488/510 (95%)	-0.10	14 (2%)	51	50	17, 27, 49, 72	0
1	B	492/510 (96%)	-0.02	20 (4%)	37	36	18, 29, 50, 72	0
1	C	491/510 (96%)	-0.30	5 (1%)	82	81	17, 26, 43, 58	0
1	D	492/510 (96%)	-0.20	10 (2%)	65	63	18, 28, 47, 66	0
1	E	488/510 (95%)	-0.20	15 (3%)	49	48	17, 28, 48, 74	0
1	F	488/510 (95%)	-0.26	8 (1%)	72	70	16, 26, 44, 65	0
All	All	2939/3060 (96%)	-0.18	72 (2%)	59	57	16, 27, 48, 74	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	94	ASP	6.8
1	A	423	GLN	4.5
1	F	88	THR	4.1
1	D	17	GLU	4.0
1	B	417	GLU	3.8
1	F	89	ALA	3.7
1	A	5	PHE	3.6
1	F	92	PHE	3.6
1	E	87	THR	3.5
1	C	417	GLU	3.4
1	B	311	GLY	3.4
1	B	87	THR	3.4
1	B	94	ASP	3.3
1	A	4	LYS	3.3
1	B	90	GLY	3.2
1	B	91	ASP	3.2
1	E	423	GLN	3.2
1	A	92	PHE	3.1
1	E	88	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	3.0
1	B	88	THR	3.0
1	B	5	PHE	3.0
1	B	420	TYR	3.0
1	E	16	ASN	3.0
1	B	440	HIS	2.9
1	A	310	GLU	2.9
1	F	95	GLU	2.9
1	C	475	GLU	2.8
1	A	417	GLU	2.8
1	B	17	GLU	2.8
1	E	10	LYS	2.8
1	D	5	PHE	2.7
1	D	475	GLU	2.7
1	E	12	ASN	2.7
1	E	94	ASP	2.7
1	D	16	ASN	2.7
1	E	17	GLU	2.6
1	B	92	PHE	2.6
1	A	95	GLU	2.6
1	C	5	PHE	2.6
1	A	309	SER	2.5
1	D	90	GLY	2.5
1	E	93	GLU	2.5
1	E	9	THR	2.4
1	B	310	GLU	2.4
1	B	95	GLU	2.4
1	D	94	ASP	2.4
1	F	10	LYS	2.4
1	F	87	THR	2.3
1	F	310	GLU	2.3
1	A	16	ASN	2.3
1	B	12	ASN	2.3
1	B	16	ASN	2.3
1	A	10	LYS	2.3
1	B	423	GLN	2.3
1	A	17	GLU	2.2
1	C	91	ASP	2.2
1	D	20	ASP	2.2
1	D	91	ASP	2.2
1	B	475	GLU	2.1
1	C	16	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	ASP	2.1
1	A	87	THR	2.1
1	D	302	ARG	2.1
1	E	92	PHE	2.1
1	B	349	TYR	2.1
1	E	414	GLU	2.1
1	E	203	LEU	2.1
1	A	422	ALA	2.0
1	E	15	THR	2.0
1	E	373	THR	2.0
1	D	4	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	F	504	1/1	0.43	0.23	30,30,30,30	0
4	MG	D	504	1/1	0.56	0.17	30,30,30,30	0
4	MG	C	504	1/1	0.79	0.15	30,30,30,30	0
4	MG	B	504	1/1	0.86	0.10	39,39,39,39	0
3	MN	D	502	1/1	0.87	0.06	54,54,54,54	0
2	ANP	E	501	31/31	0.90	0.12	25,34,46,49	0
4	MG	A	504	1/1	0.90	0.06	34,34,34,34	0
3	MN	F	502	1/1	0.91	0.05	53,53,53,53	0
3	MN	C	502	1/1	0.91	0.10	47,47,47,47	0
2	ANP	F	501	31/31	0.91	0.11	20,28,45,54	0
2	ANP	D	501	31/31	0.92	0.11	23,32,40,50	0
4	MG	E	504	1/1	0.93	0.06	30,30,30,30	0

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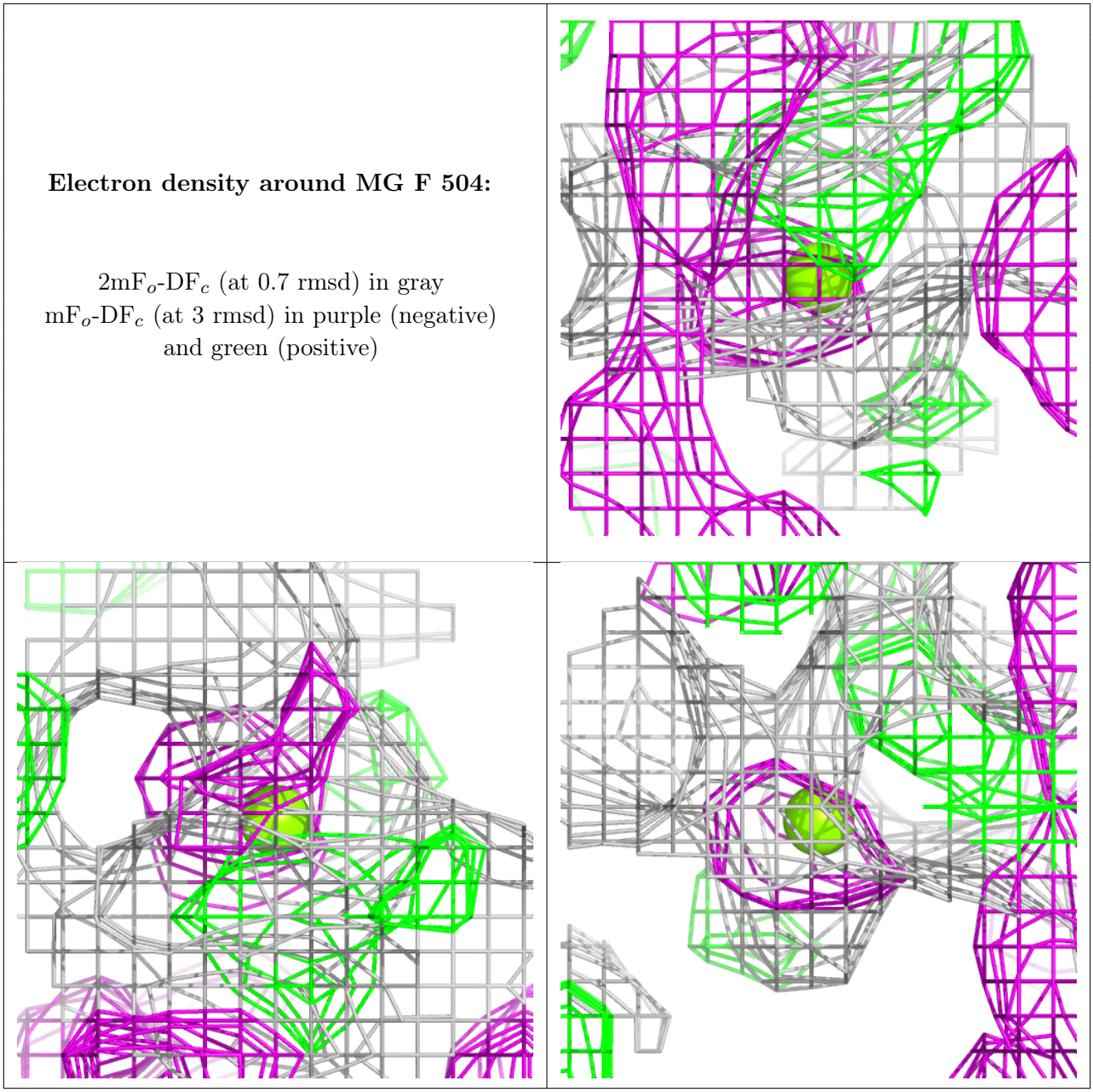
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ANP	B	501	31/31	0.93	0.10	22,29,40,54	0
3	MN	E	502	1/1	0.94	0.06	55,55,55,55	0
2	ANP	A	501	31/31	0.94	0.09	23,31,37,48	0
2	ANP	C	501	31/31	0.95	0.09	20,26,37,47	0
3	MN	B	502	1/1	0.96	0.07	53,53,53,53	0
3	MN	A	502	1/1	0.97	0.06	50,50,50,50	0
3	MN	D	503	1/1	0.98	0.05	36,36,36,36	0
3	MN	A	503	1/1	0.98	0.03	34,34,34,34	0
3	MN	E	503	1/1	0.98	0.05	33,33,33,33	0
3	MN	C	503	1/1	0.98	0.03	32,32,32,32	0
3	MN	B	503	1/1	0.98	0.03	37,37,37,37	0
3	MN	F	503	1/1	0.99	0.03	32,32,32,32	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.

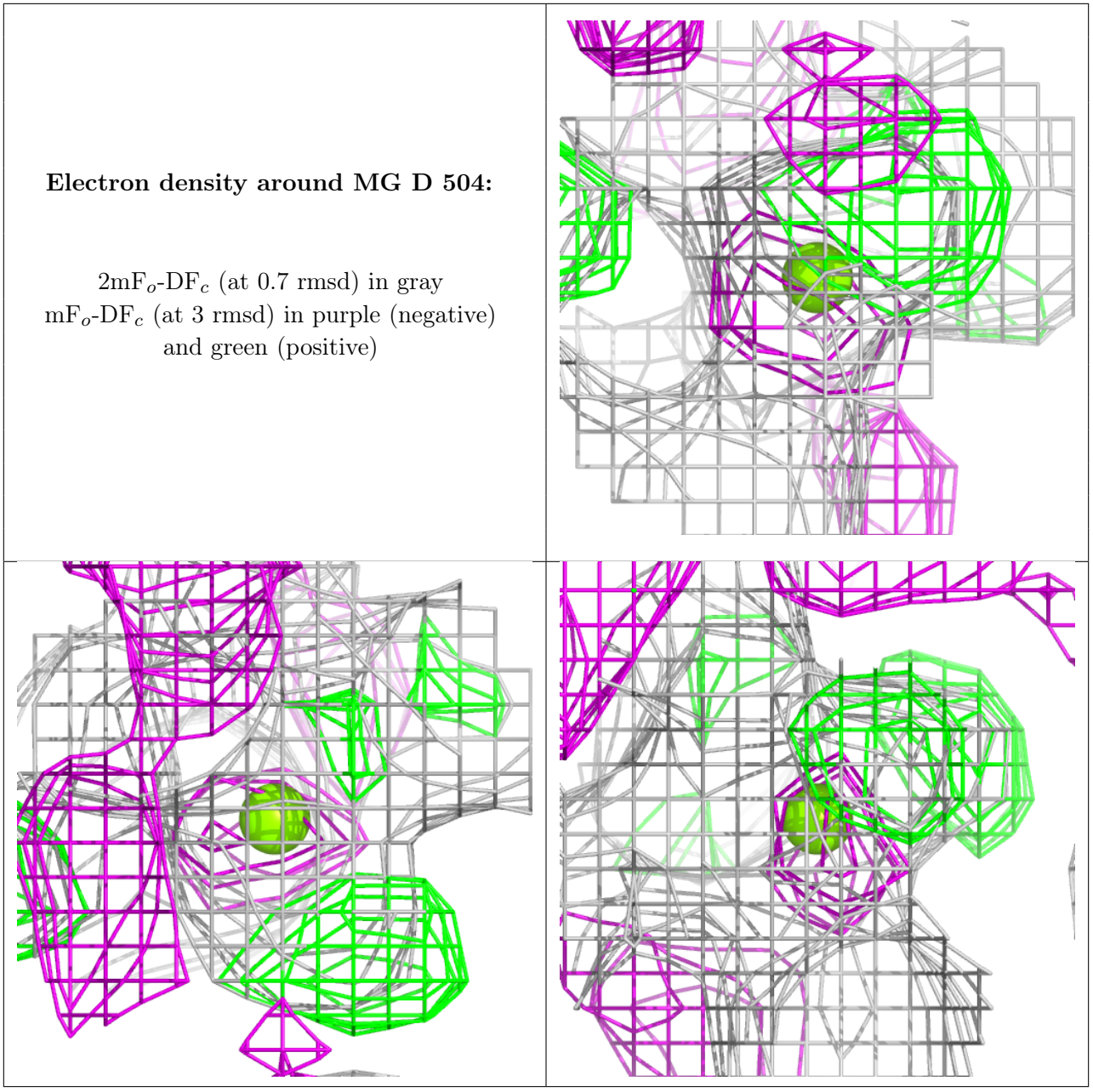
Electron density around MG F 504:

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



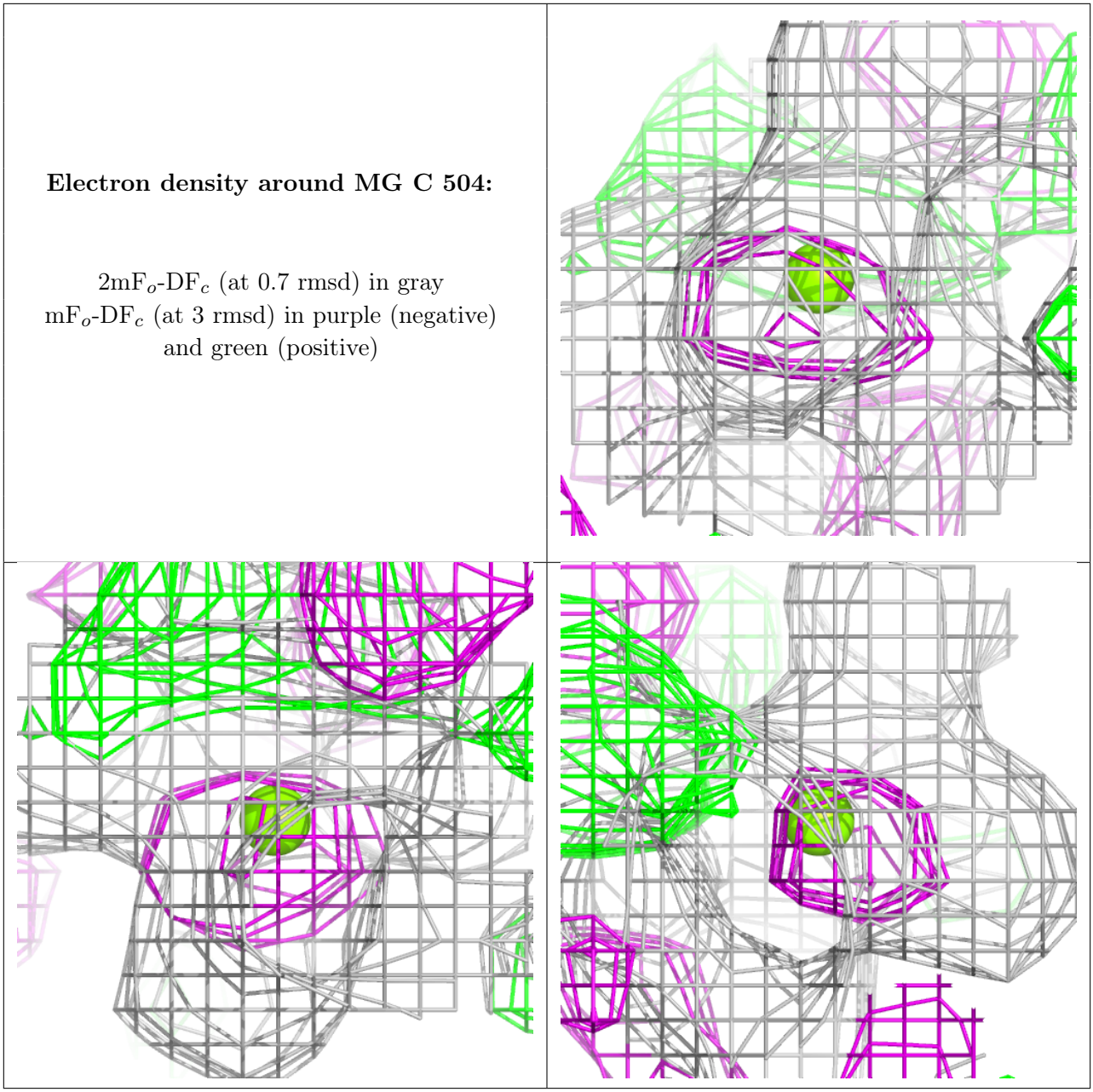
Electron density around MG D 504:

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



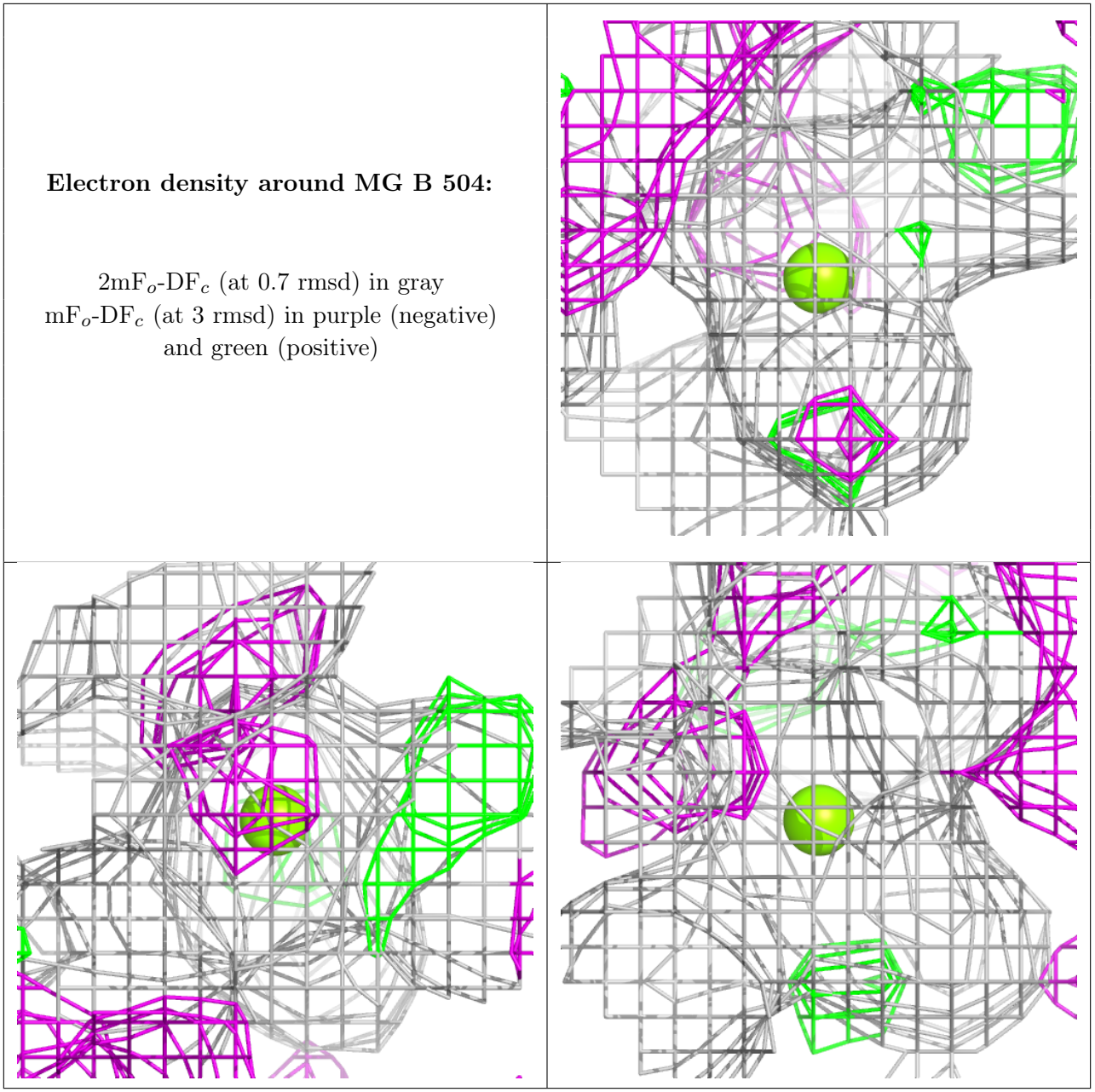
Electron density around MG C 504:

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



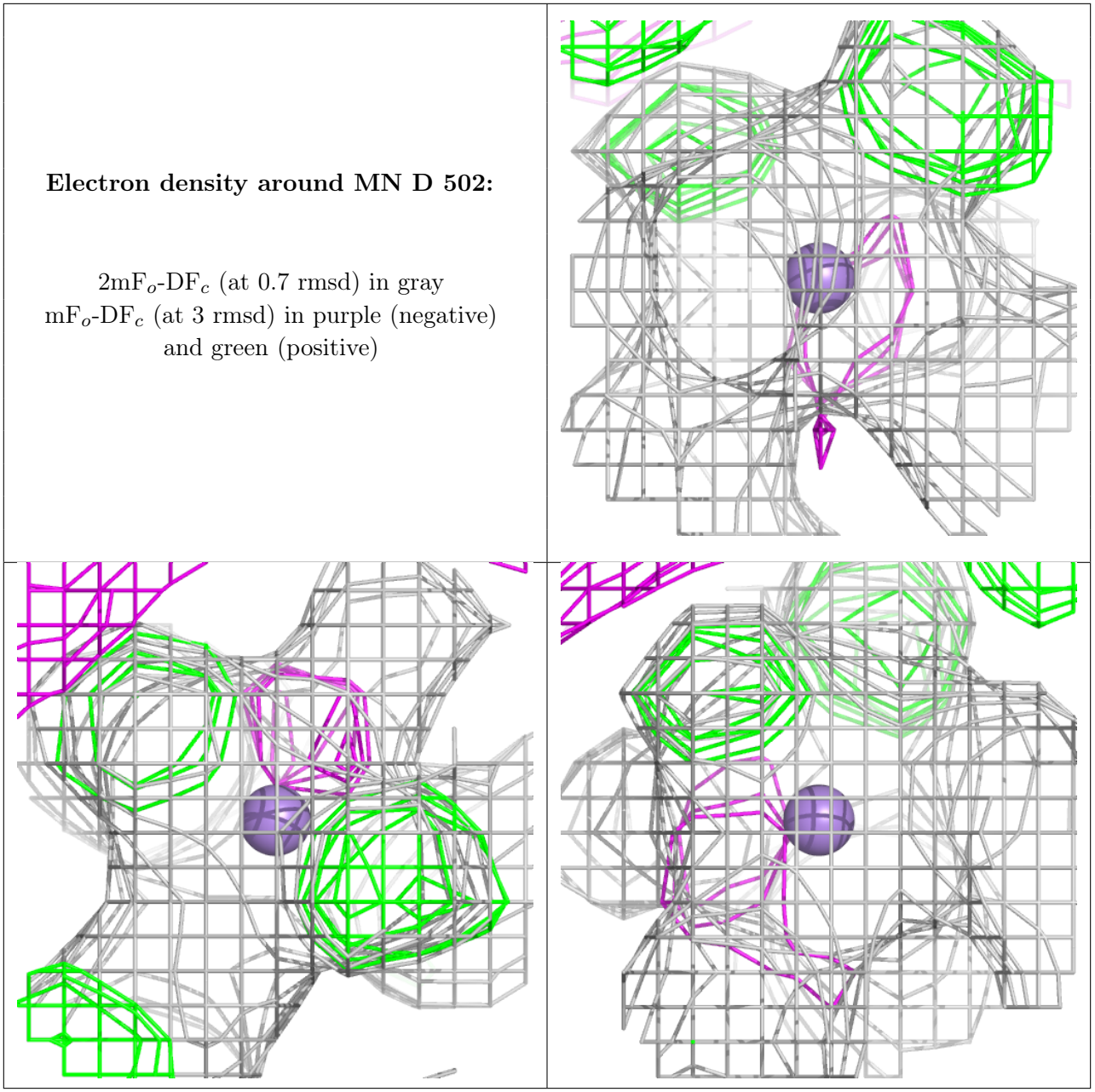
Electron density around MG B 504:

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



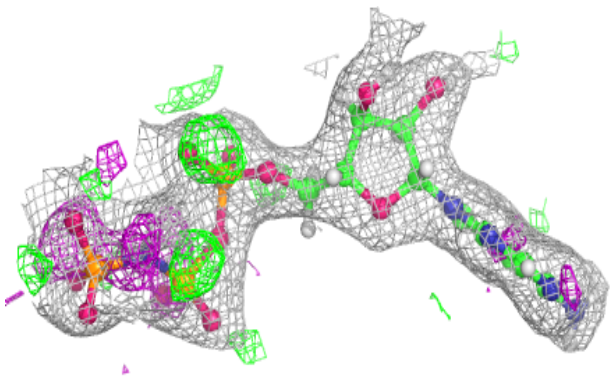
Electron density around MN D 502:

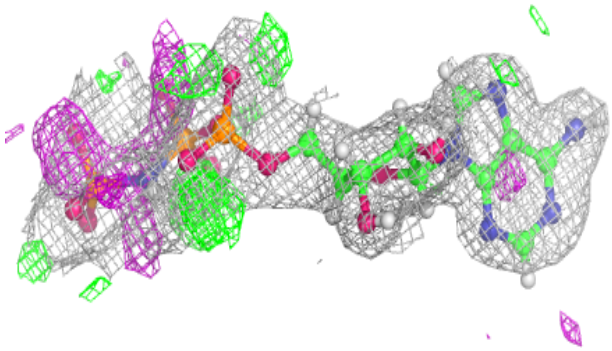
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

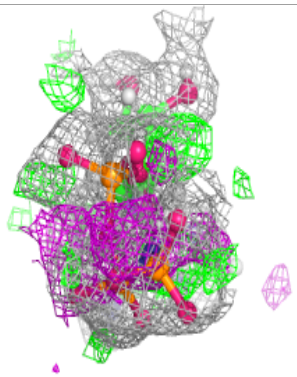


Electron density around ANP E 501:

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

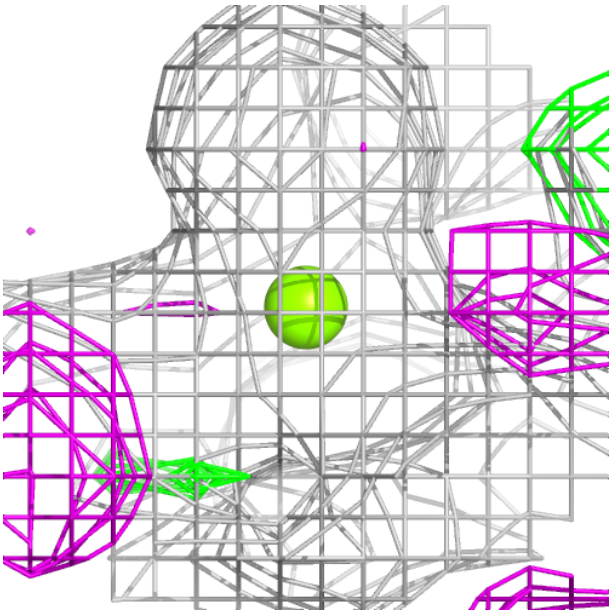


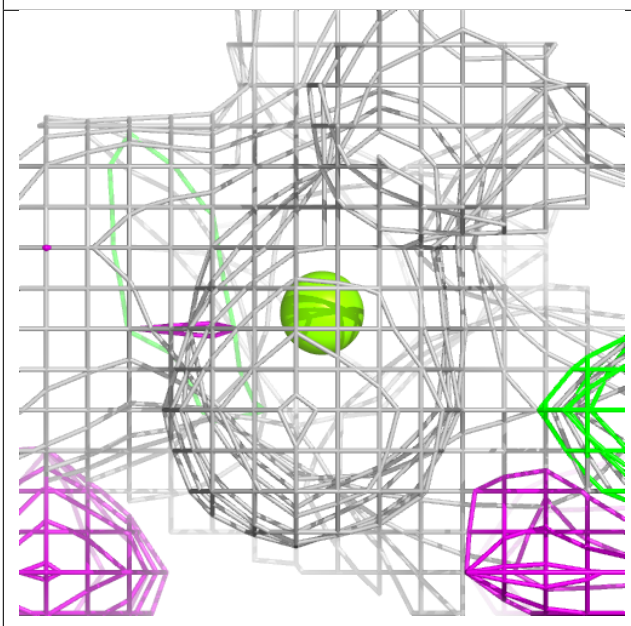


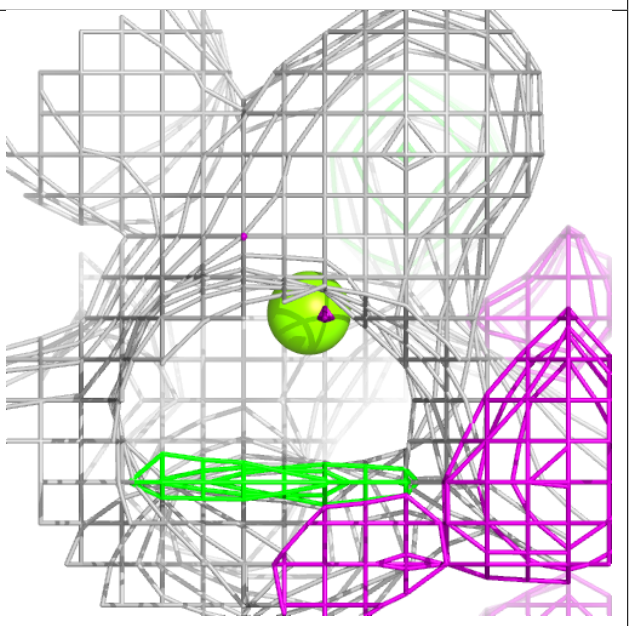


Electron density around MG A 504:

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

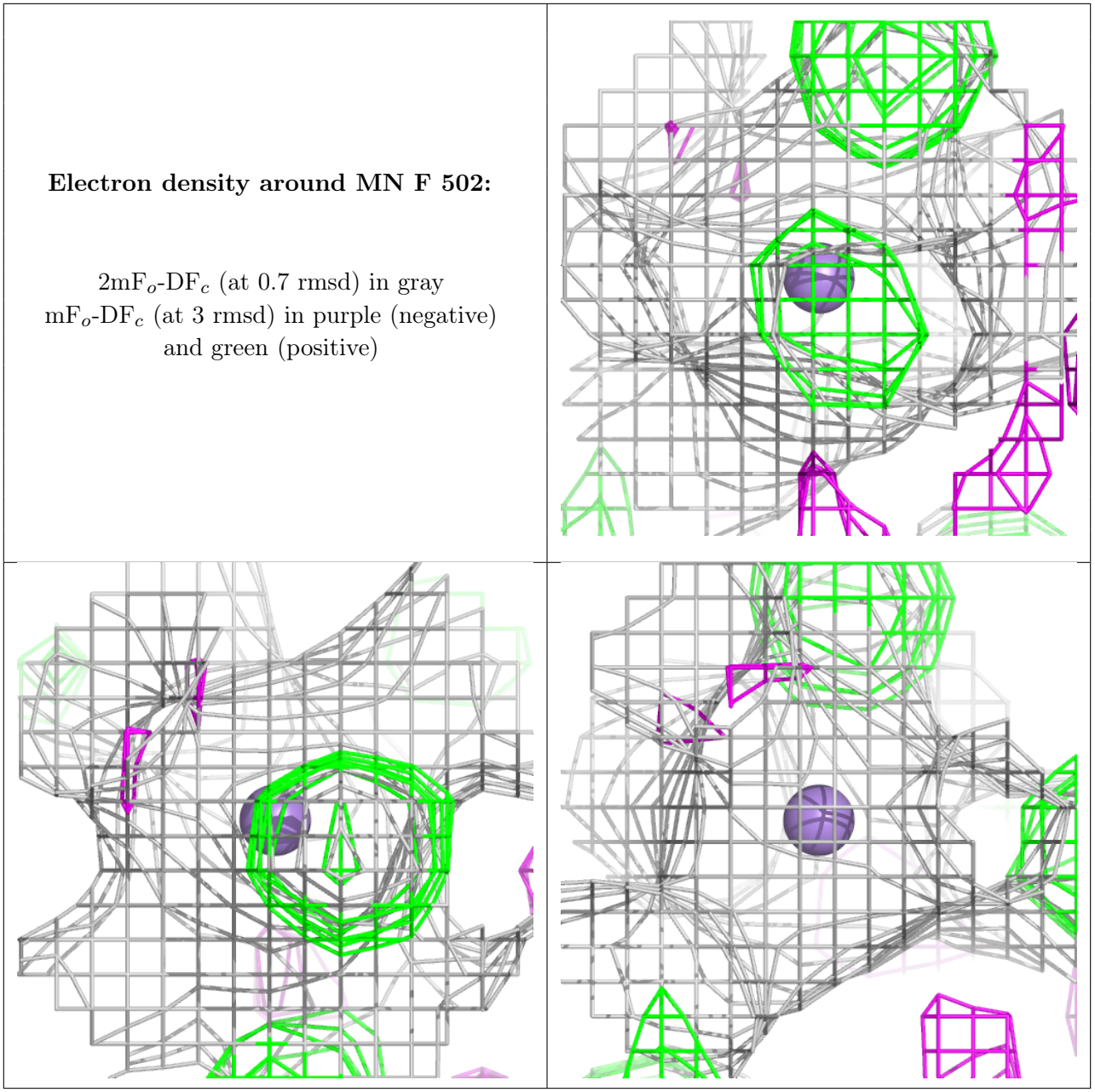






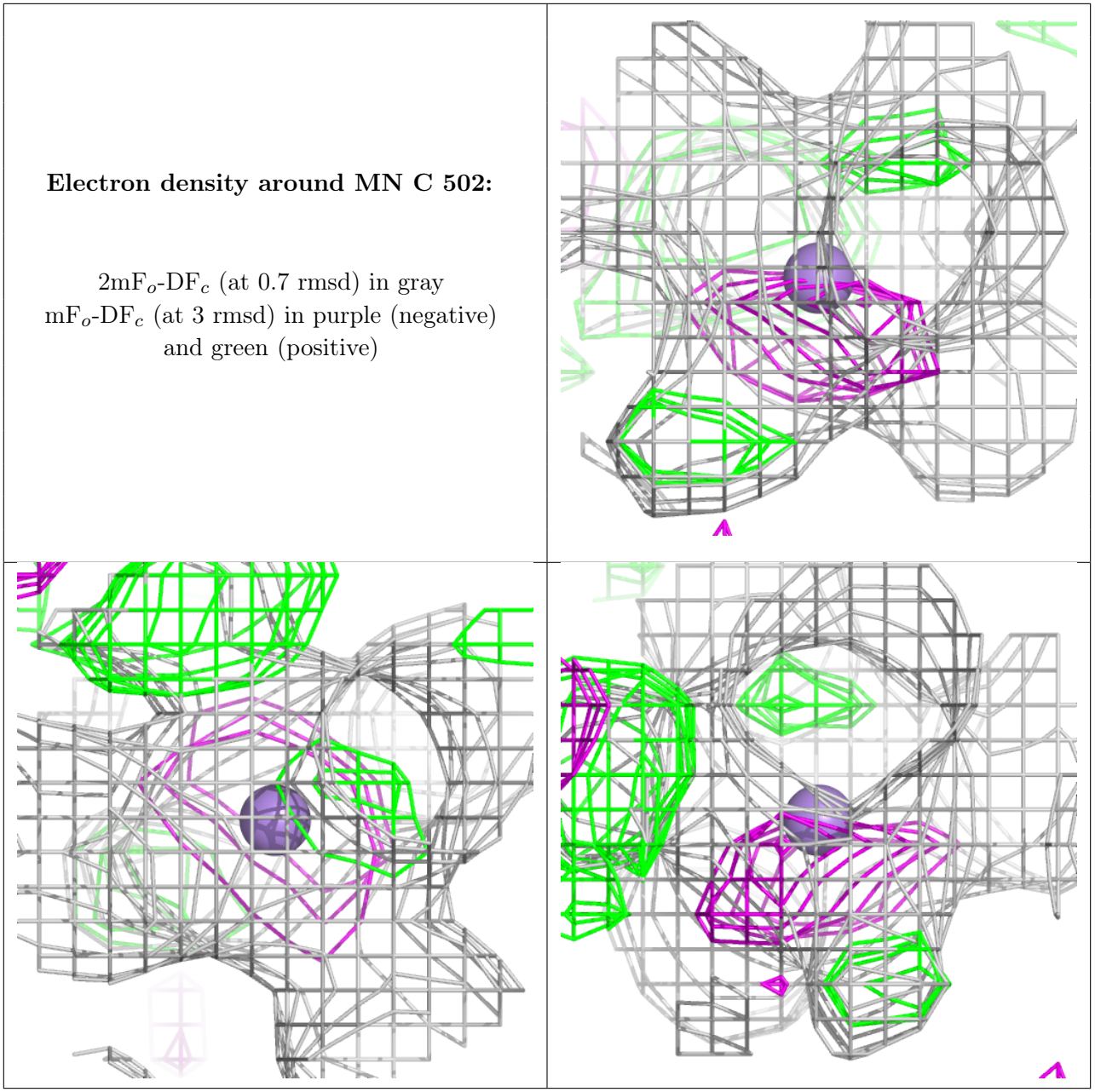
Electron density around MN F 502:

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



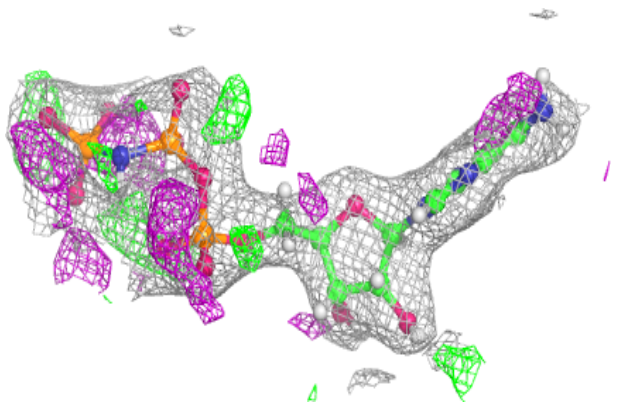
Electron density around MN C 502:

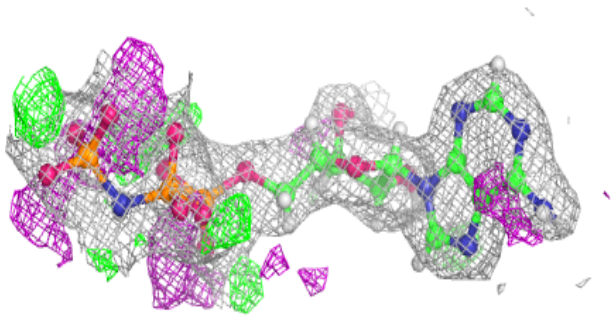
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

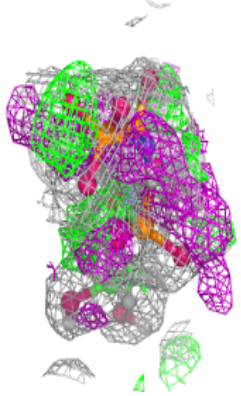


Electron density around ANP F 501:

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

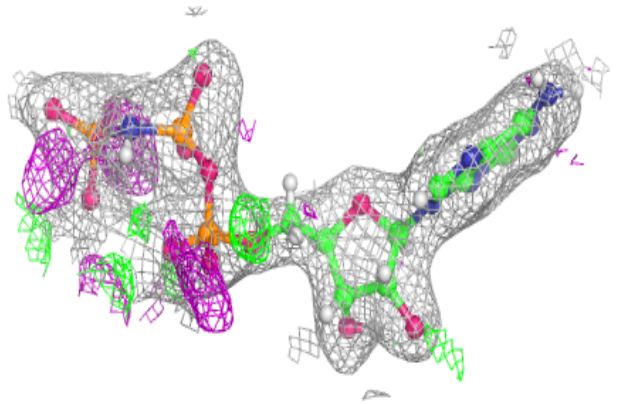


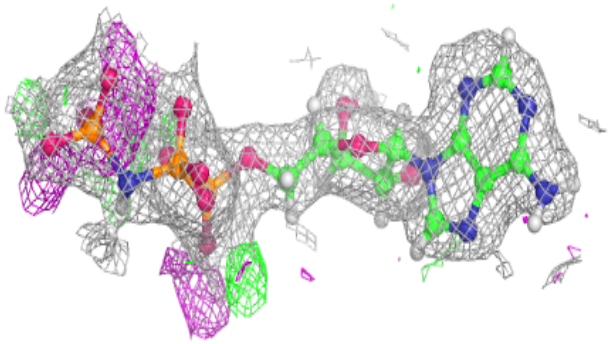


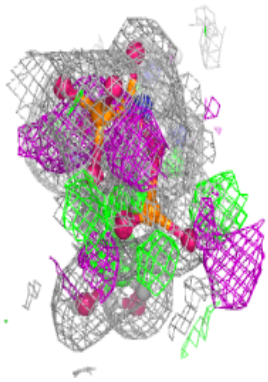


Electron density around ANP D 501:

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

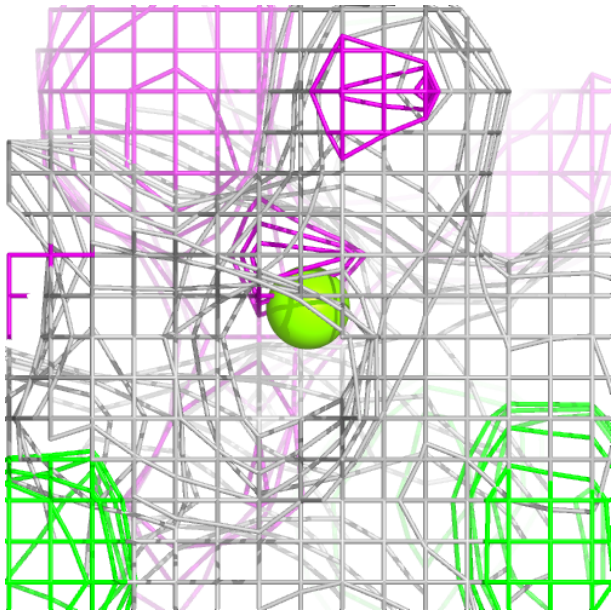


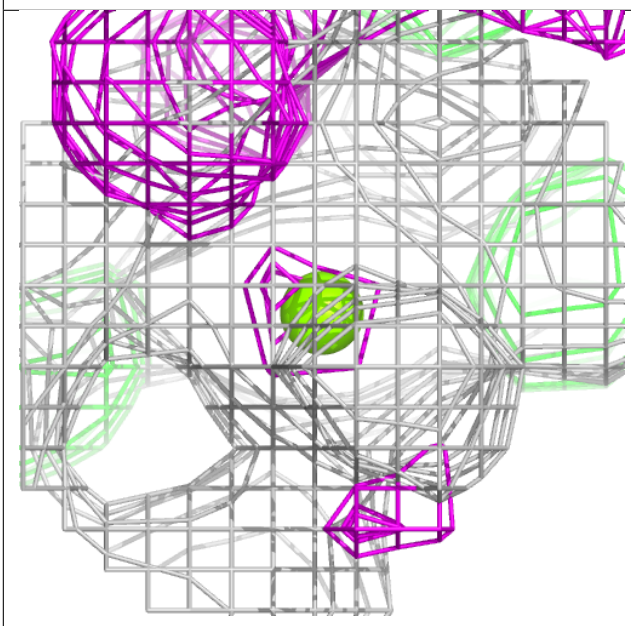


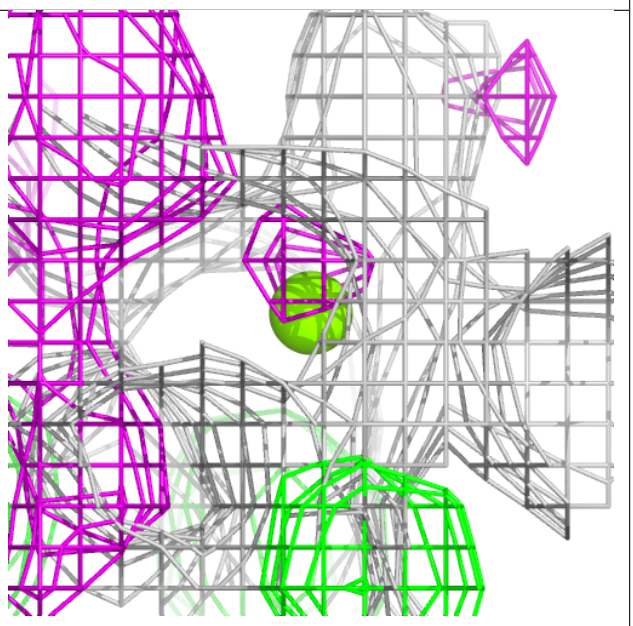


Electron density around MG E 504:

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

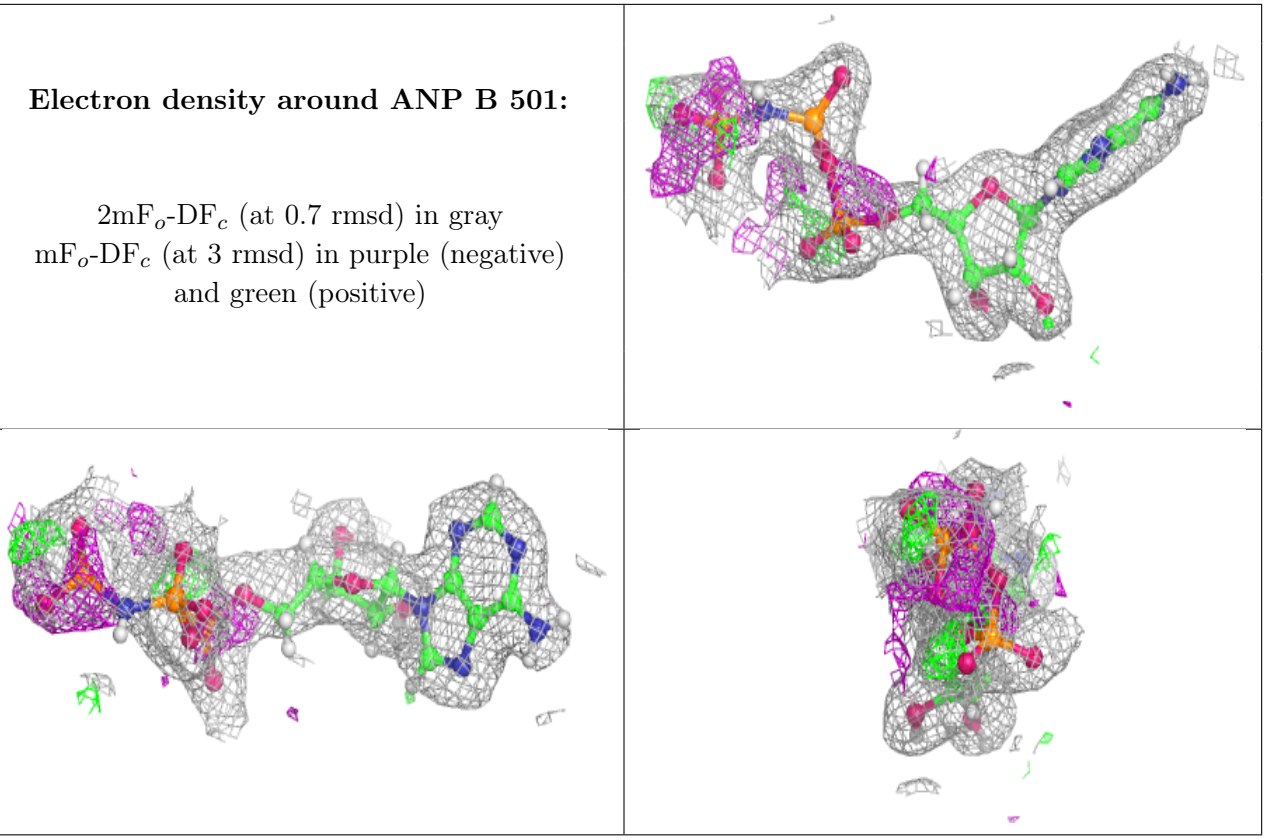






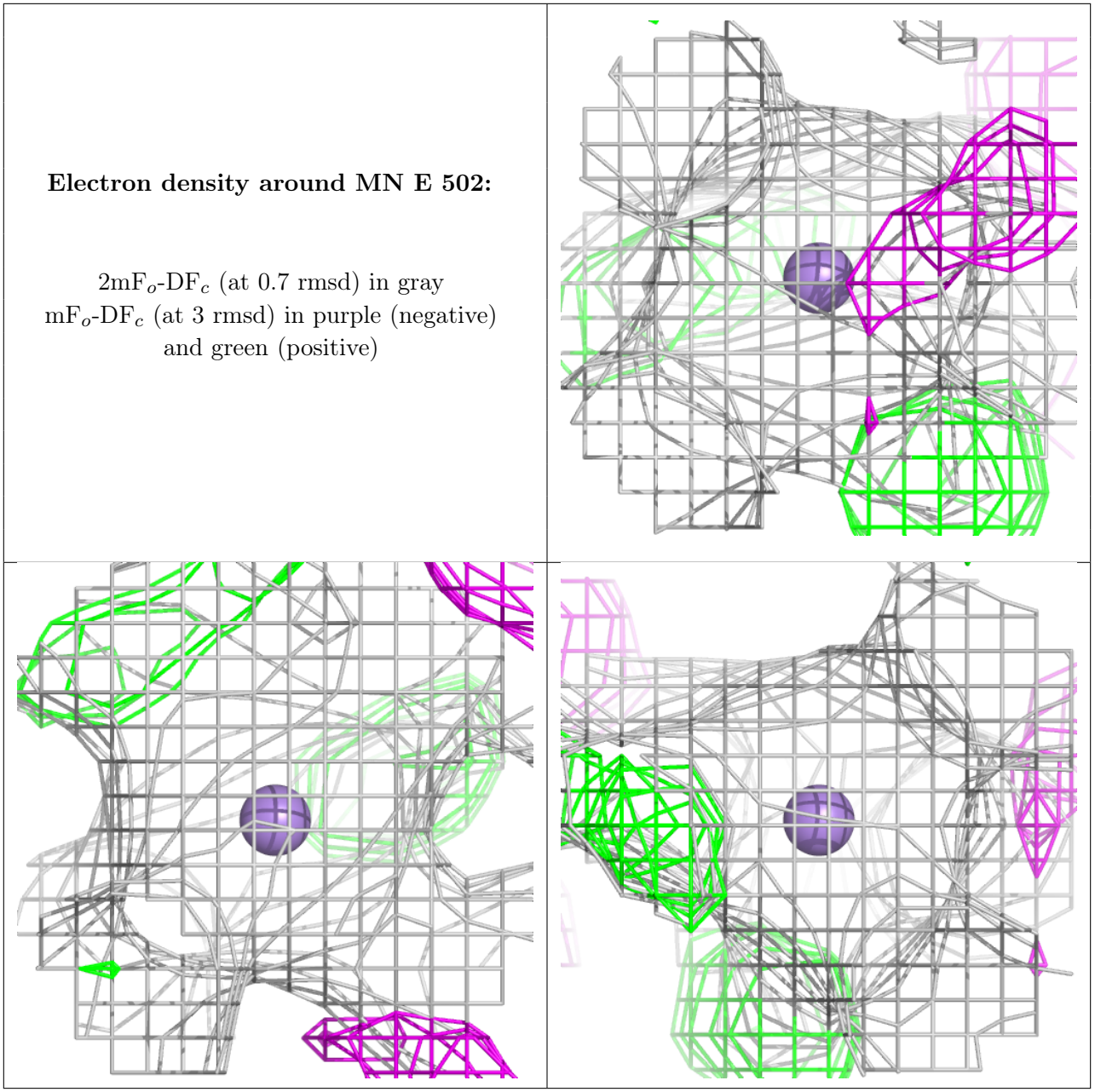
Electron density around ANP B 501:

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



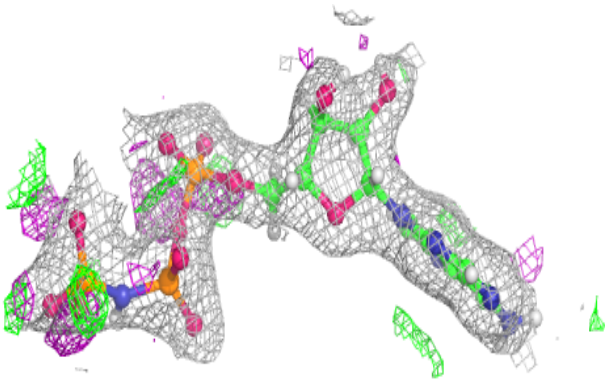
Electron density around MN E 502:

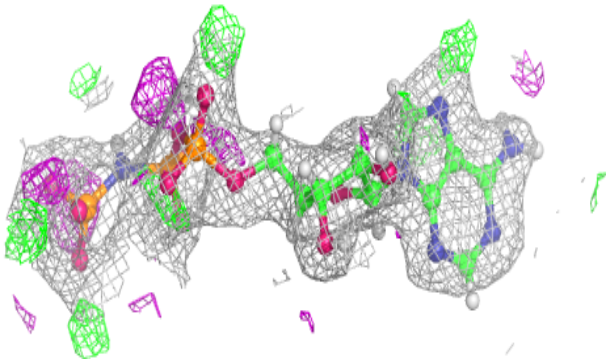
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

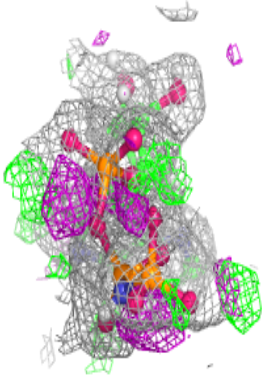


Electron density around ANP A 501:

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

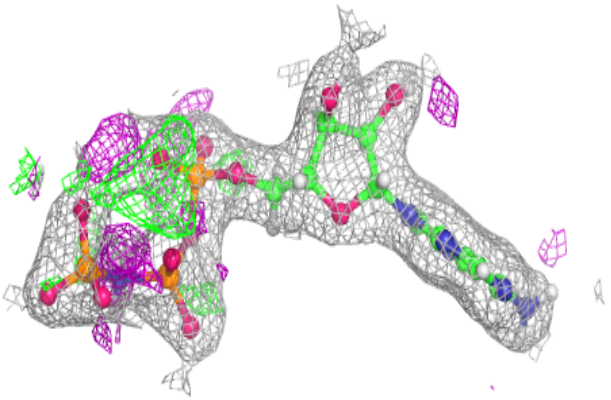


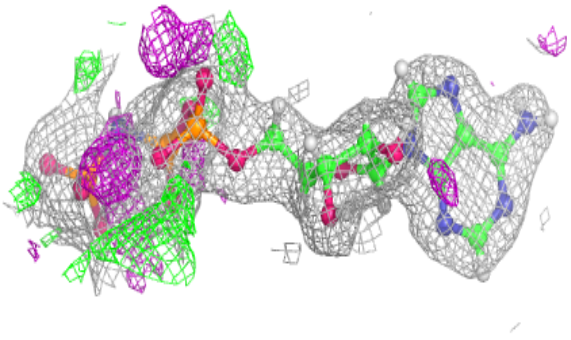


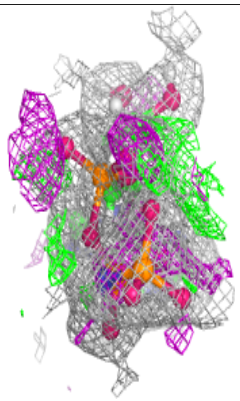


Electron density around ANP C 501:

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

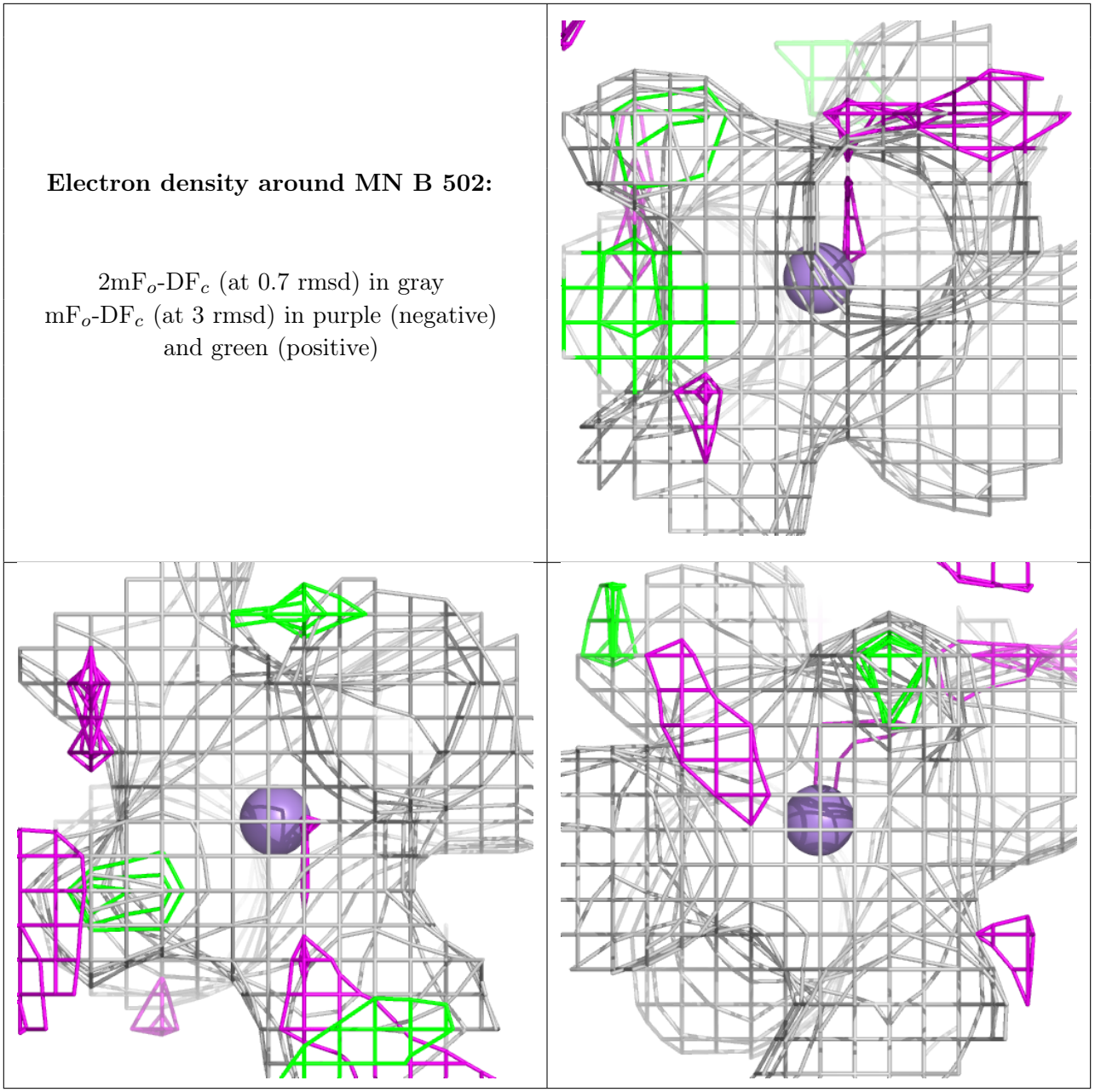






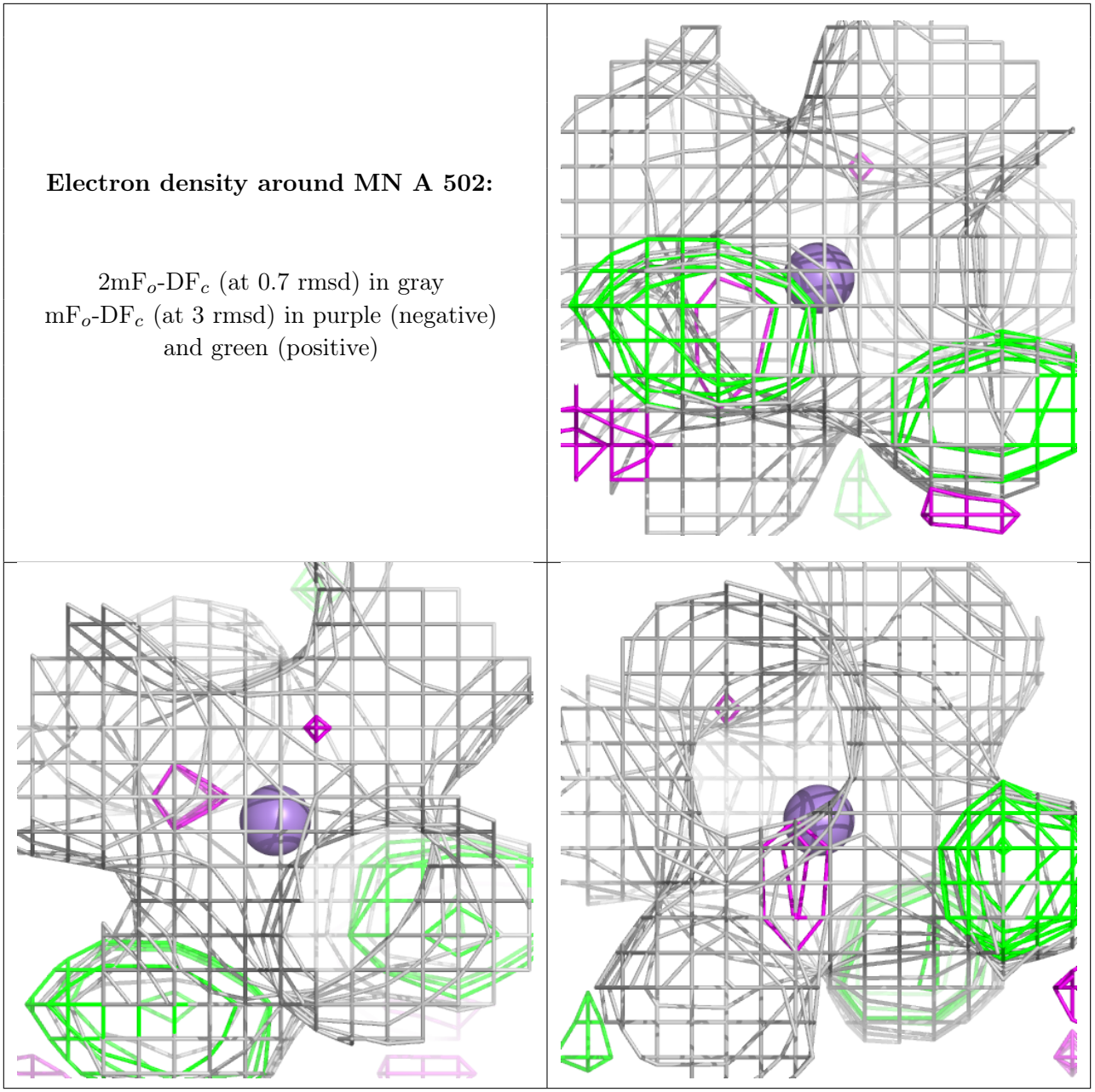
Electron density around MN B 502:

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



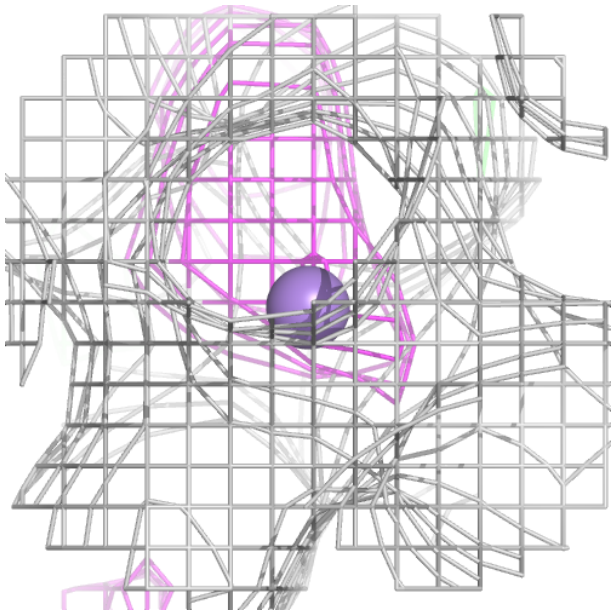
Electron density around MN A 502:

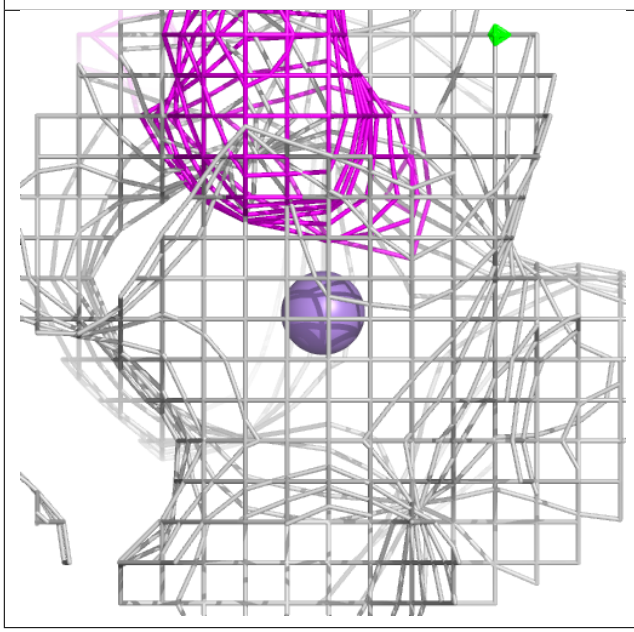
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

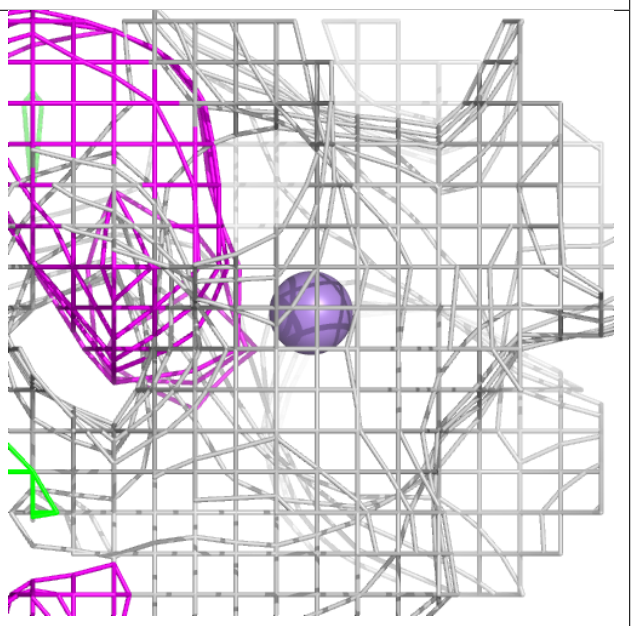


Electron density around MN D 503:

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

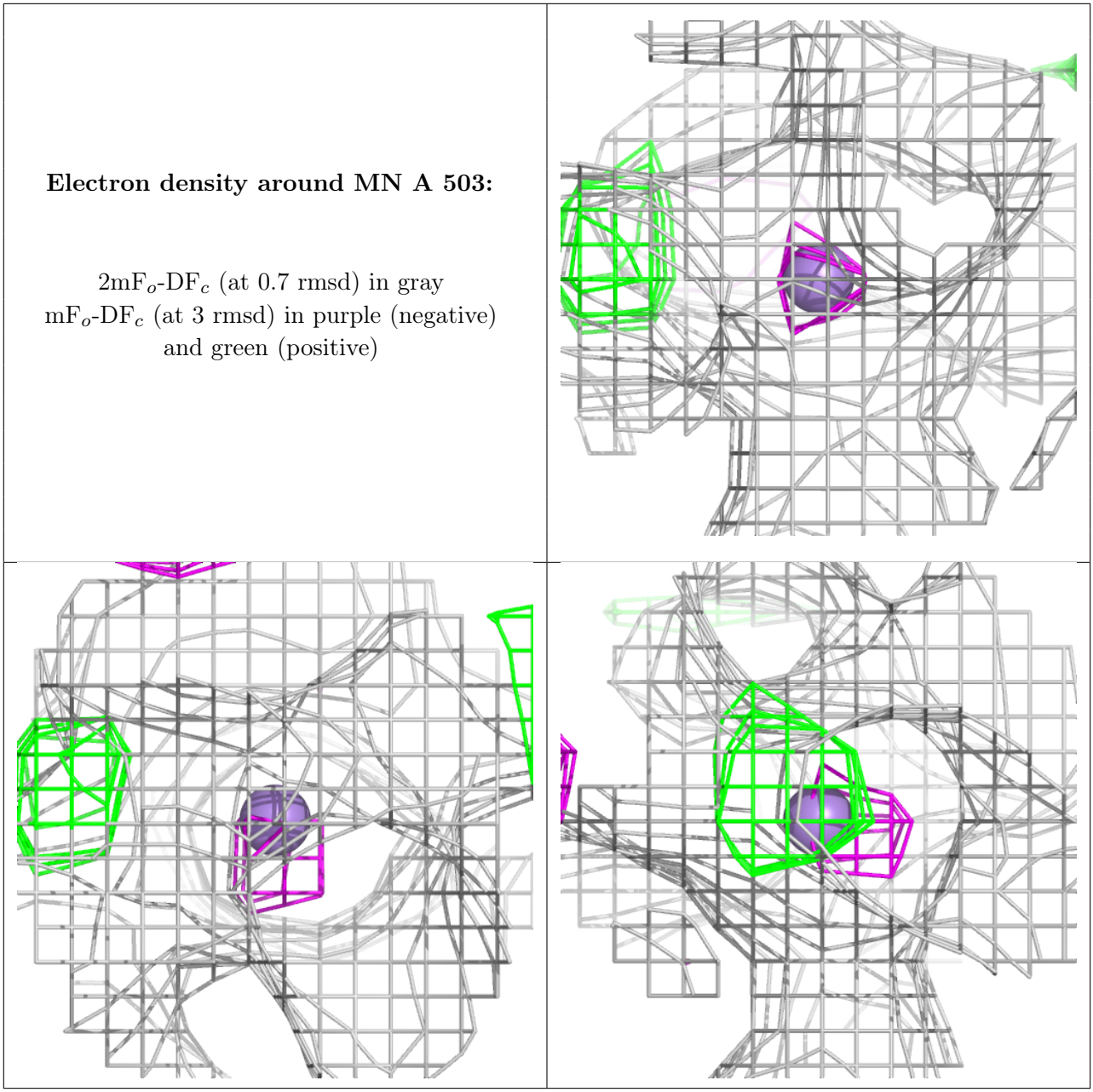






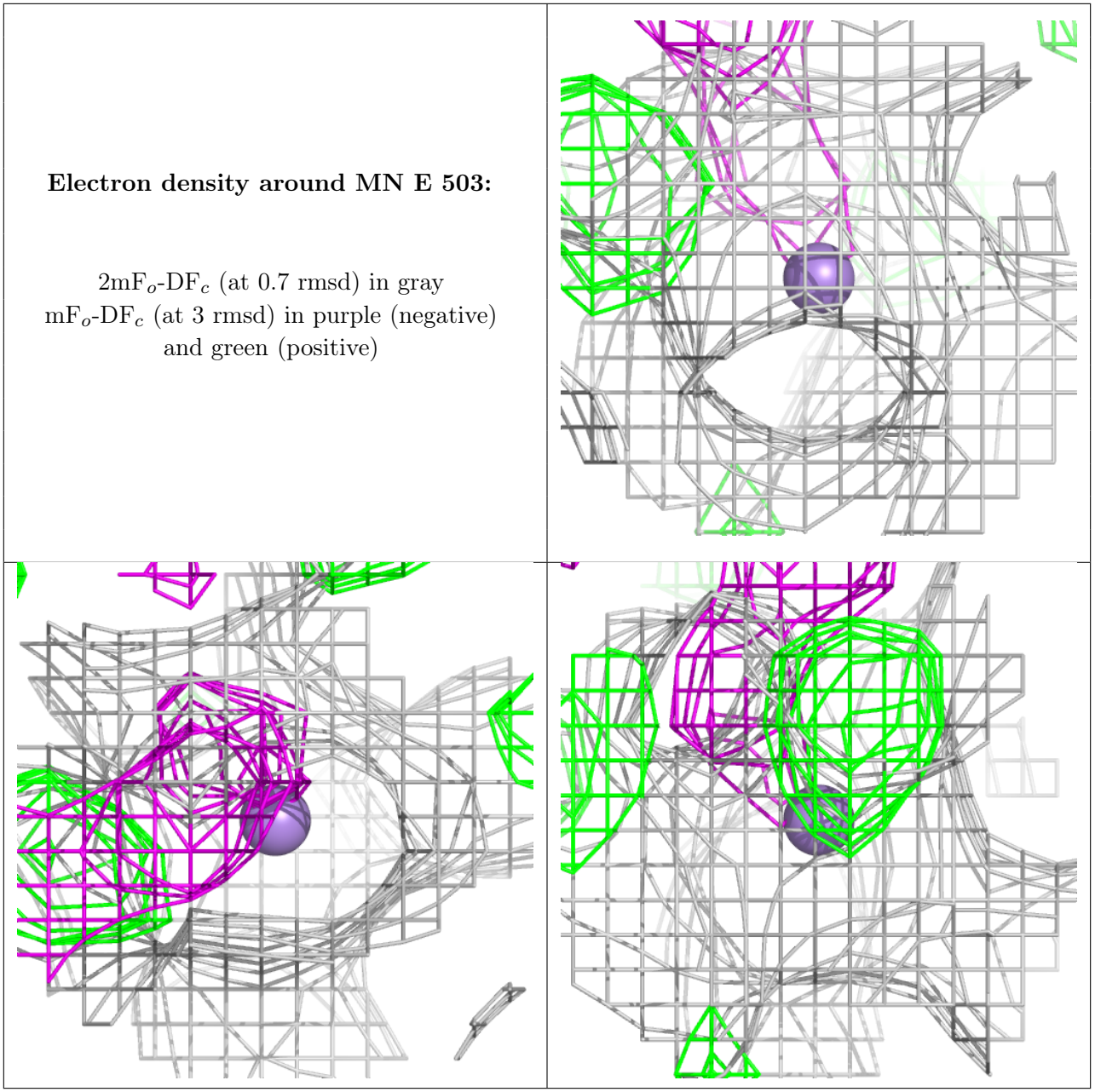
Electron density around MN A 503:

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



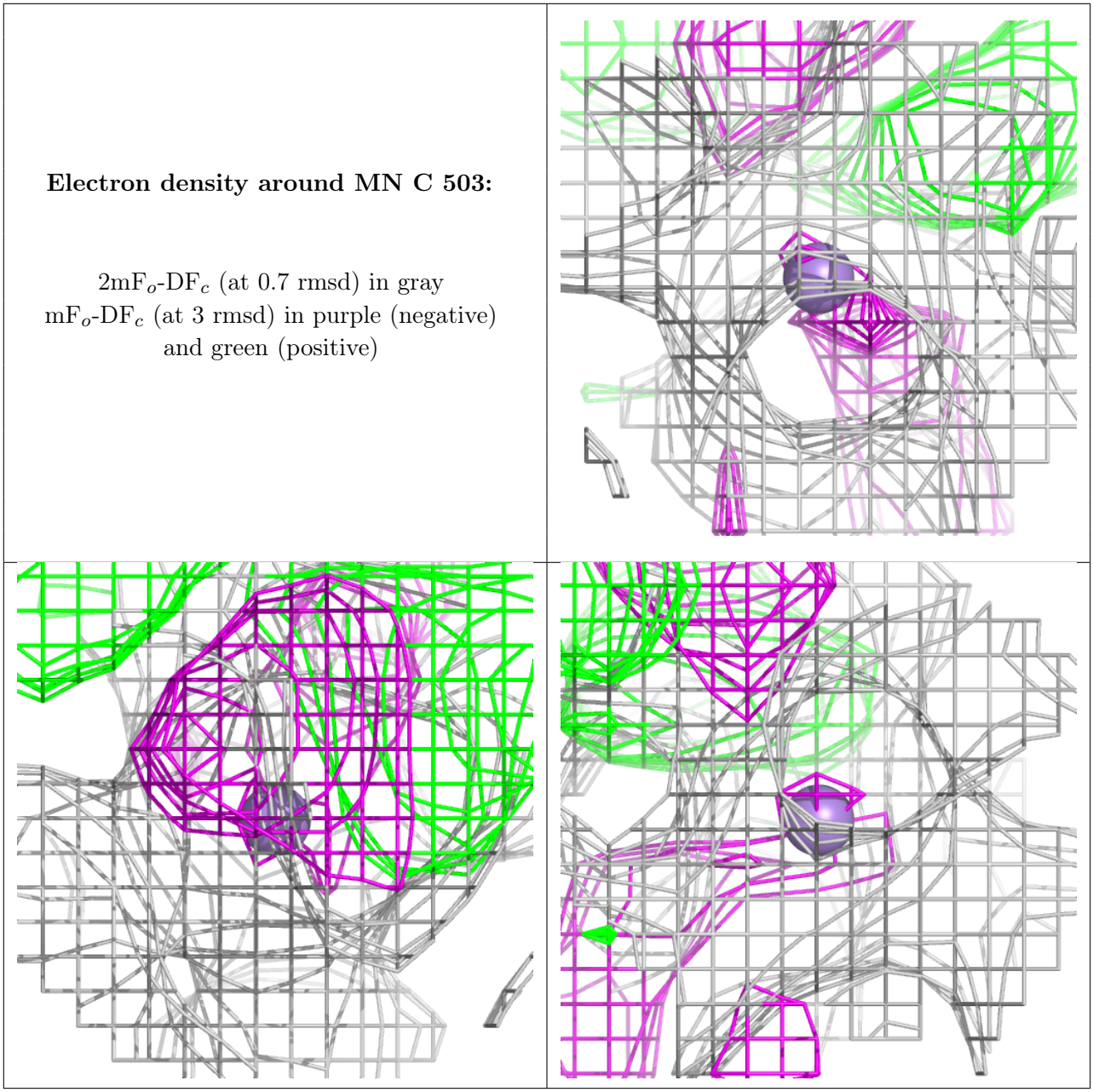
Electron density around MN E 503:

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



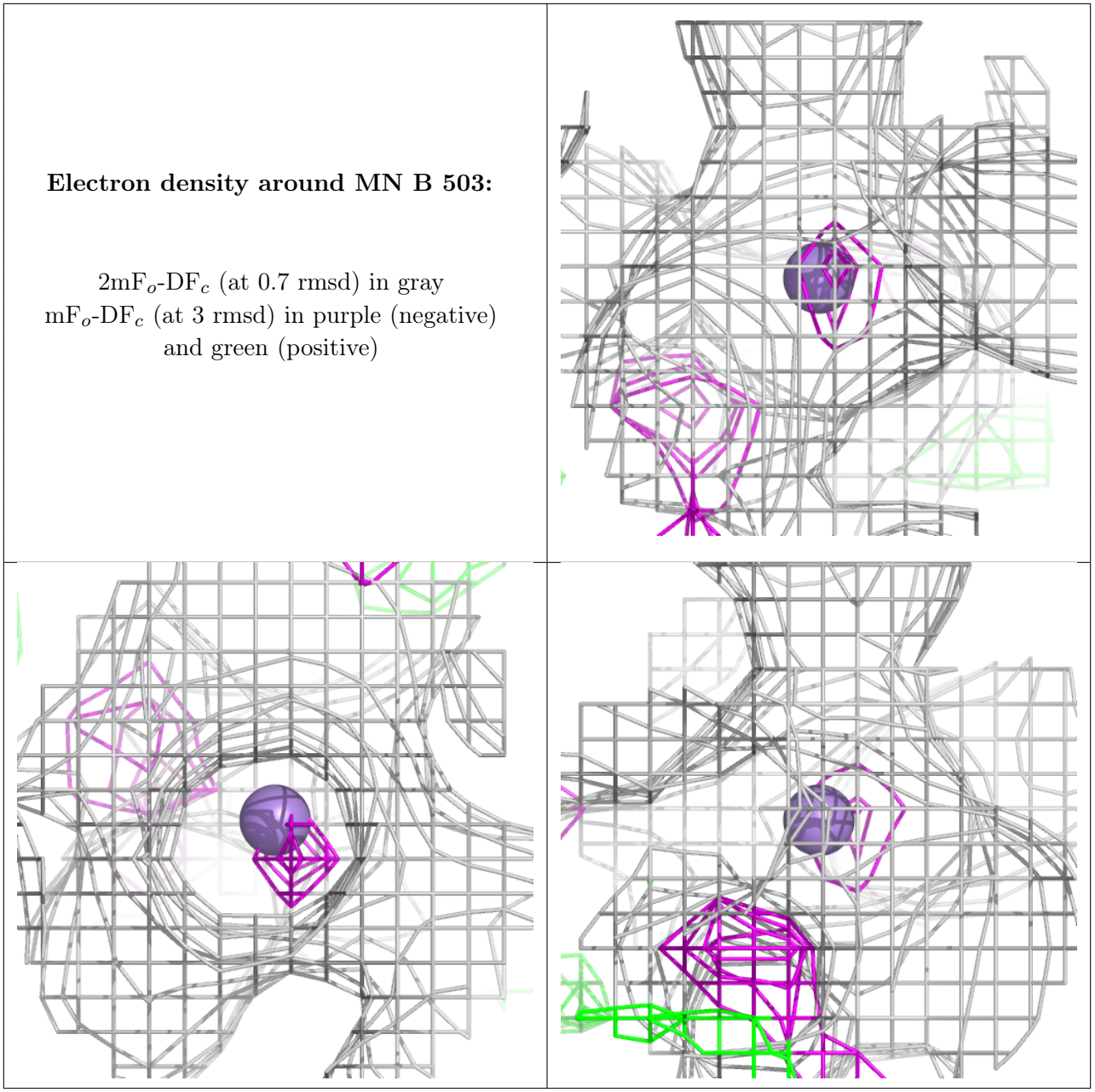
Electron density around MN C 503:

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



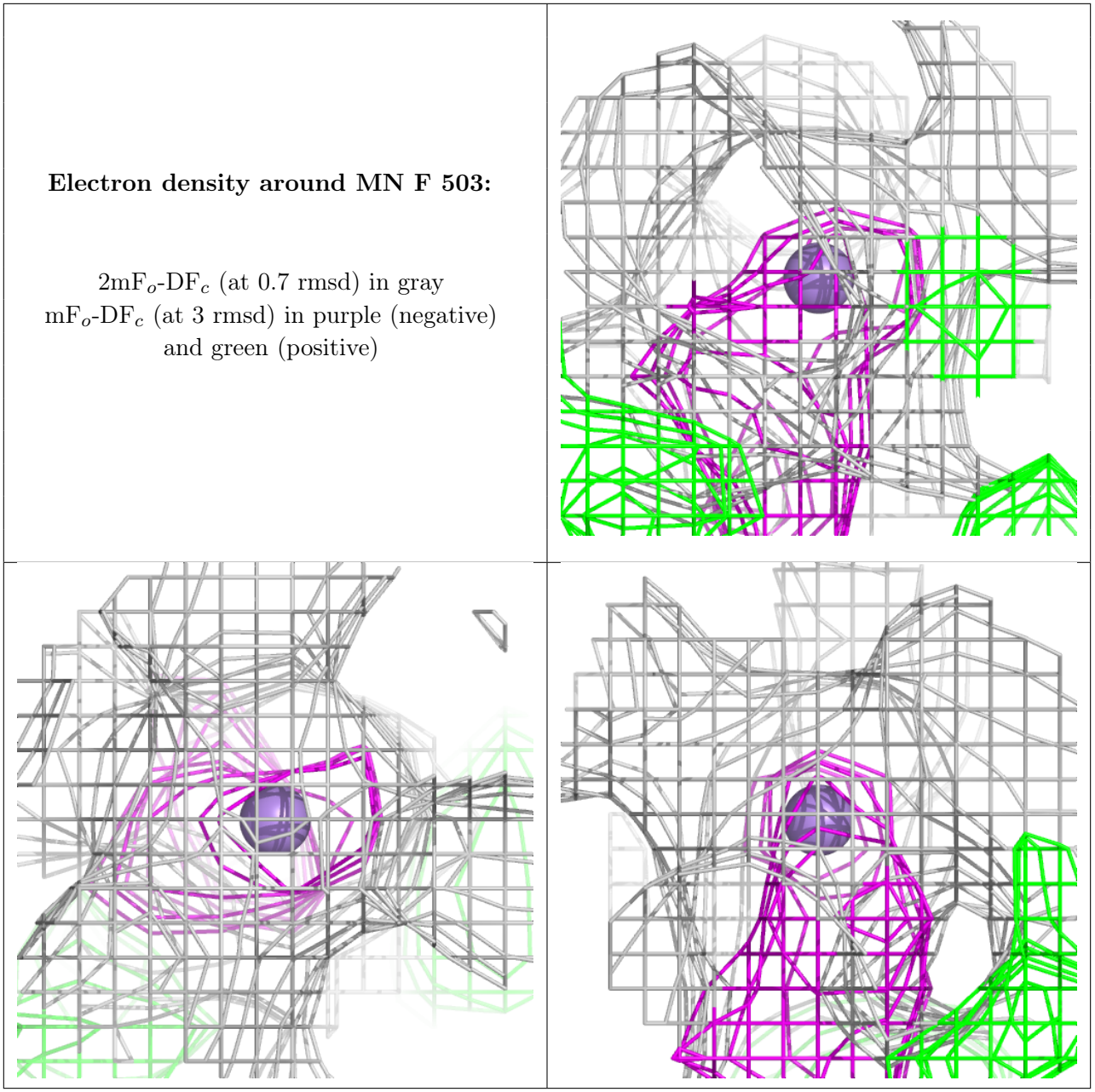
Electron density around MN B 503:

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



Electron density around MN F 503:

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



6.5 Other polymers (i)

There are no such residues in this entry.