wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 12:37 AM EDT

PDB ID	:	8DBA
Title	:	Crystal structure of dodecameric KaiC
Authors	:	Padua, R.A.P.; Grant, T.; Pitsawong, W.; Hoemberger, M.S.; Otten, R.; Bradshaw, N.; Grigorieff, N.; Kern, D.
Deposited on	:	2022-06-14
Resolution	:	3.50 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 (i)) were used in the production of this report:

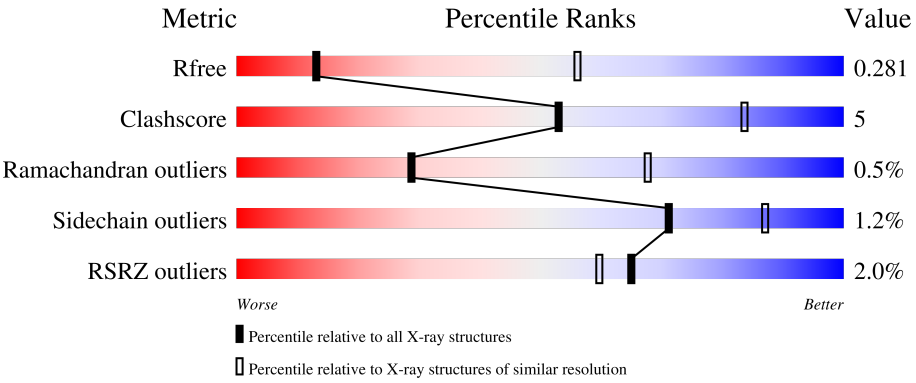
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	568	2% 79% 10% 11%
1	B	568	2% 77% 11% 11%
1	C	568	% 77% 12% • 11%
1	D	568	2% 76% 13% • 10%
1	E	568	% 81% 9% • 10%

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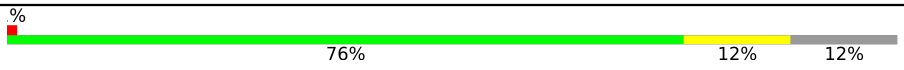
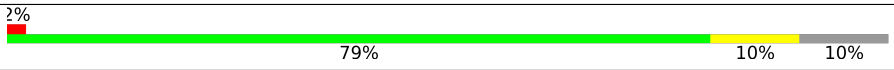
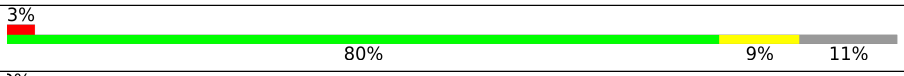
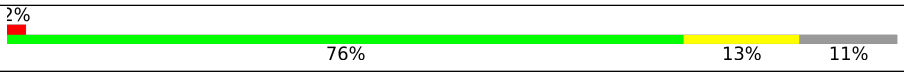
Mol	Chain	Length	Quality of chain
1	F	568	
1	G	568	
1	H	568	
1	I	568	
1	J	568	
1	K	568	
1	L	568	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 93625 atoms, of which 46166 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 Circadian clock protein KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	507	Total	C	H	N	O	S	0	0	0
			7689	2443	3810	701	719	16			
1	B	505	Total	C	H	N	O	S	0	0	0
			7687	2435	3812	700	724	16			
1	C	508	Total	C	H	N	O	S	0	0	0
			7706	2442	3821	705	722	16			
1	D	510	Total	C	H	N	O	S	0	0	0
			7775	2466	3859	711	723	16			
1	E	511	Total	C	H	N	O	S	0	0	0
			7778	2460	3862	706	734	16			
1	F	500	Total	C	H	N	O	S	0	0	0
			7662	2421	3810	698	717	16			
1	G	518	Total	C	H	N	O	S	0	0	0
			7908	2513	3913	718	748	16			
1	H	509	Total	C	H	N	O	S	0	0	0
			7797	2459	3887	704	731	16			
1	I	494	Total	C	H	N	O	S	0	0	0
			7514	2402	3695	690	711	16			
1	J	510	Total	C	H	N	O	S	0	0	0
			7714	2459	3812	699	728	16			
1	K	508	Total	C	H	N	O	S	0	0	0
			7706	2444	3822	702	722	16			
1	L	503	Total	C	H	N	O	S	0	0	0
			7674	2444	3786	706	722	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B9KWX8
A	0	ALA	-	expression tag	UNP B9KWX8
B	-1	GLY	-	expression tag	UNP B9KWX8
B	0	ALA	-	expression tag	UNP B9KWX8
C	-1	GLY	-	expression tag	UNP B9KWX8

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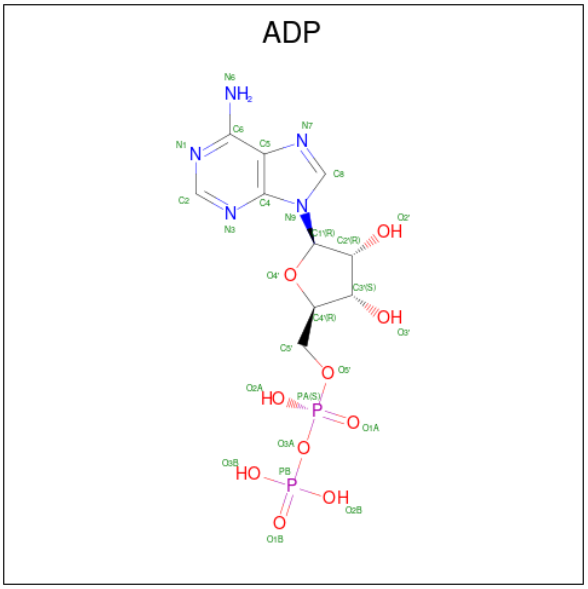
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP B9KWX8
D	-1	GLY	-	expression tag	UNP B9KWX8
D	0	ALA	-	expression tag	UNP B9KWX8
E	-1	GLY	-	expression tag	UNP B9KWX8
E	0	ALA	-	expression tag	UNP B9KWX8
F	-1	GLY	-	expression tag	UNP B9KWX8
F	0	ALA	-	expression tag	UNP B9KWX8
G	-1	GLY	-	expression tag	UNP B9KWX8
G	0	ALA	-	expression tag	UNP B9KWX8
H	-1	GLY	-	expression tag	UNP B9KWX8
H	0	ALA	-	expression tag	UNP B9KWX8
I	-1	GLY	-	expression tag	UNP B9KWX8
I	0	ALA	-	expression tag	UNP B9KWX8
J	-1	GLY	-	expression tag	UNP B9KWX8
J	0	ALA	-	expression tag	UNP B9KWX8
K	-1	GLY	-	expression tag	UNP B9KWX8
K	0	ALA	-	expression tag	UNP B9KWX8
L	-1	GLY	-	expression tag	UNP B9KWX8
L	0	ALA	-	expression tag	UNP B9KWX8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	F	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	G	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	G	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	H	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	H	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	I	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	I	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	J	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	J	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	K	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	K	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	L	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	L	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	G	3	Total	Mg	0	0
			3	3		
3	H	2	Total	Mg	0	0
			2	2		
3	I	2	Total	Mg	0	0
			2	2		
3	J	2	Total	Mg	0	0
			2	2		
3	K	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	4	Total	O	0	0
			4	4		
4	C	7	Total	O	0	0
			7	7		
4	D	6	Total	O	0	0
			6	6		

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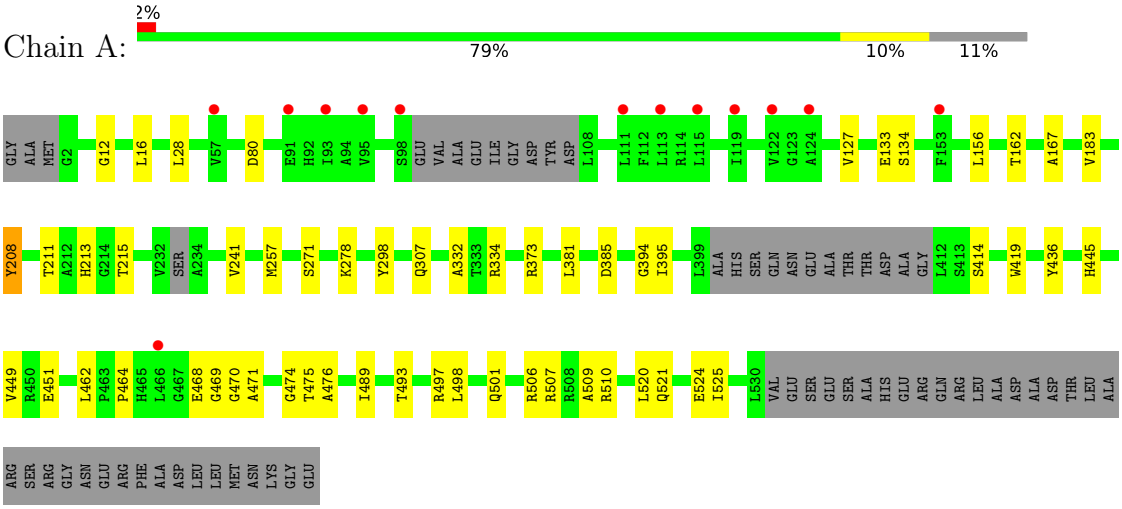
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	6	Total O 6 6	0	0
4	F	6	Total O 6 6	0	0
4	G	5	Total O 5 5	0	0
4	H	5	Total O 5 5	0	0
4	I	7	Total O 7 7	0	0
4	J	5	Total O 5 5	0	0
4	K	6	Total O 6 6	0	0
4	L	5	Total O 5 5	0	0

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.

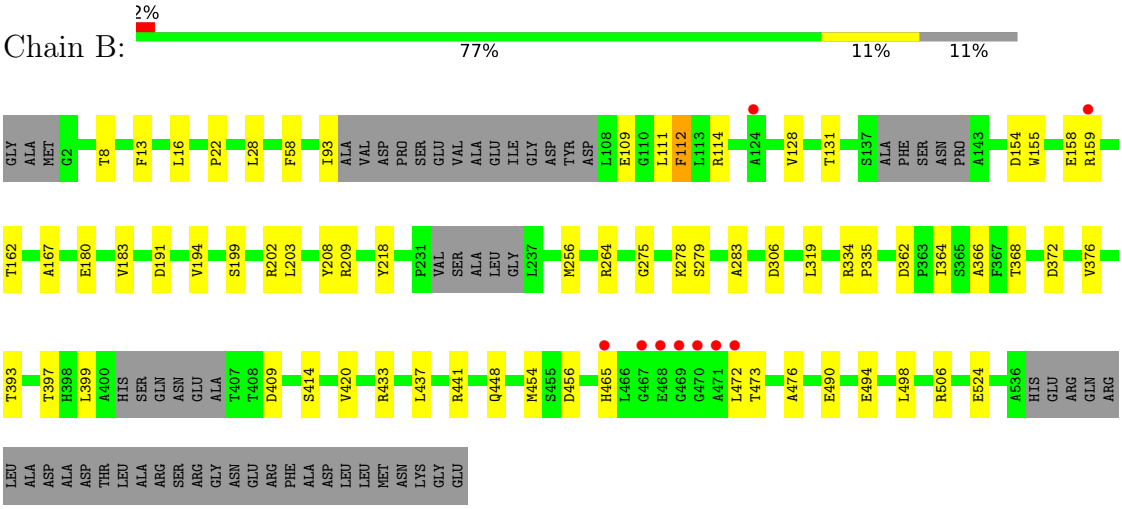
• Molecule 1: Circadian clock protein KaiC

Chain A:



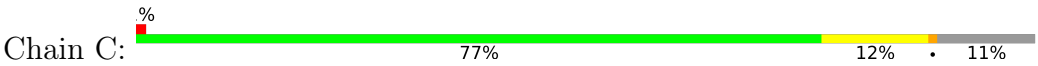
• Molecule 1: Circadian clock protein KaiC

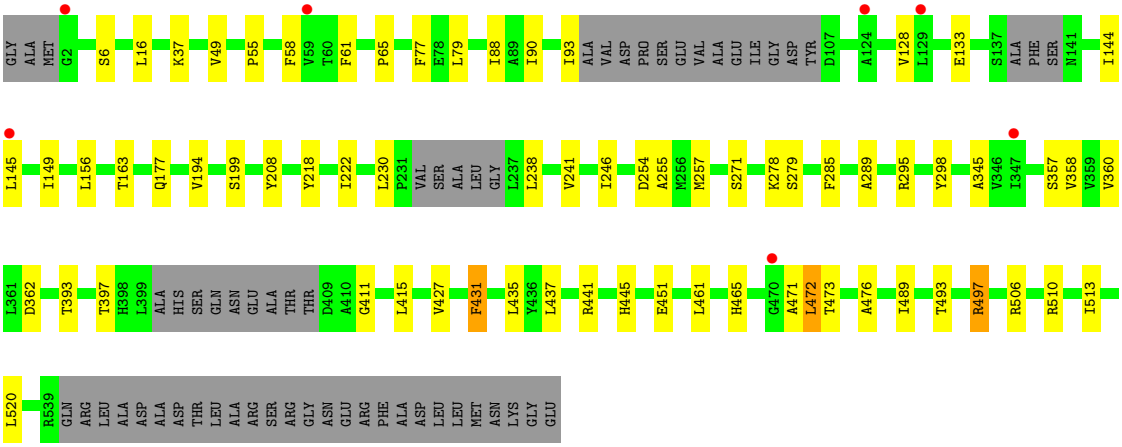
Chain B:



• Molecule 1: Circadian clock protein KaiC

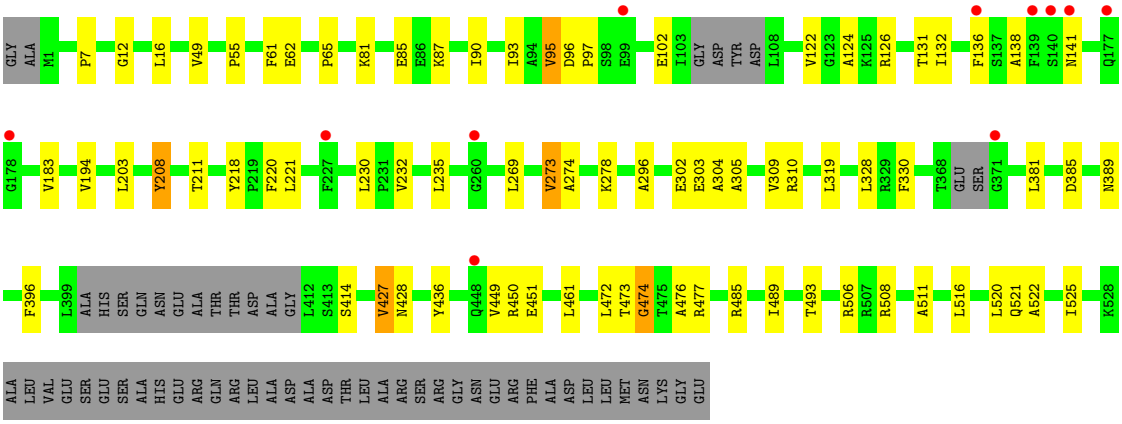
Chain C:





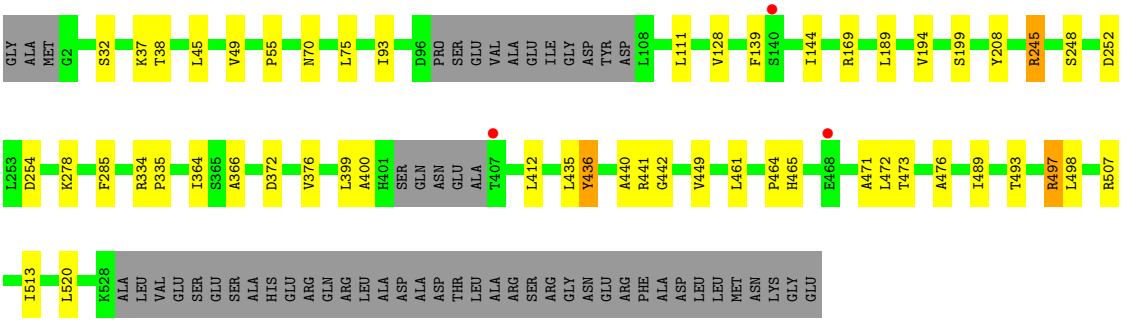
• Molecule 1: Circadian clock protein KaiC

Chain D:



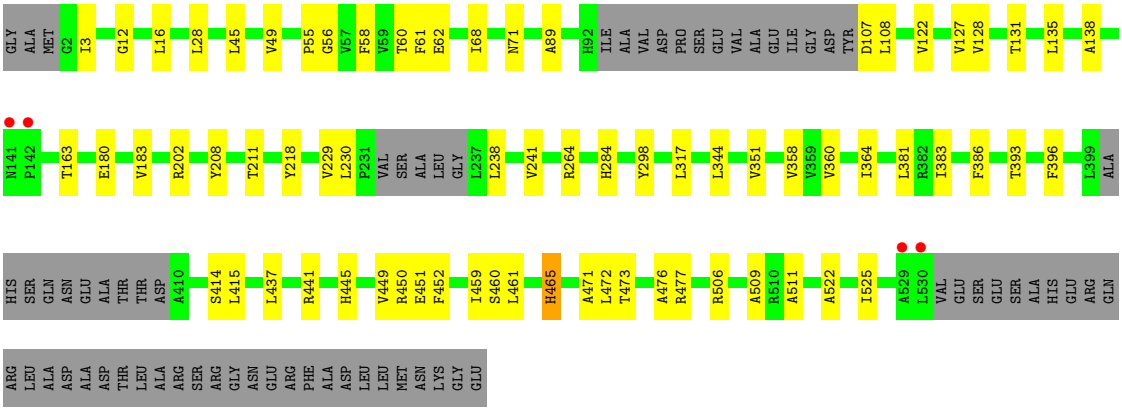
• Molecule 1: Circadian clock protein KaiC

Chain E:



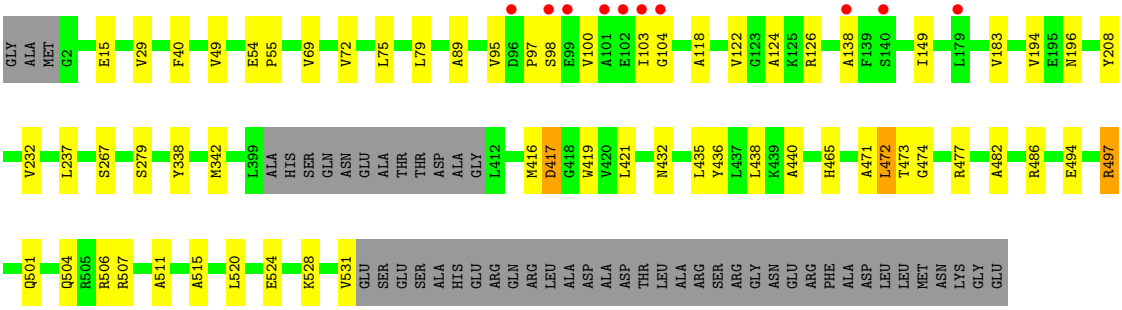
• Molecule 1: Circadian clock protein KaiC

Chain F:



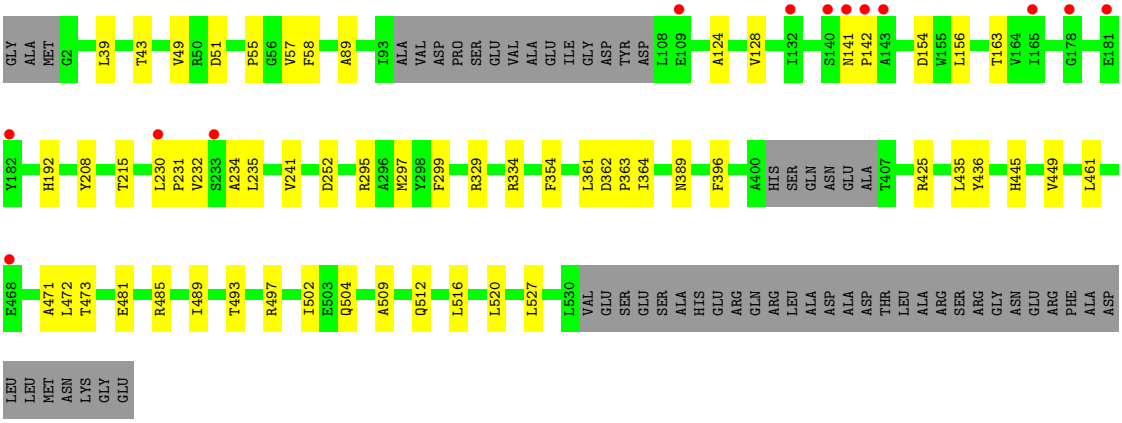
• Molecule 1: Circadian clock protein KaiC

Chain G:



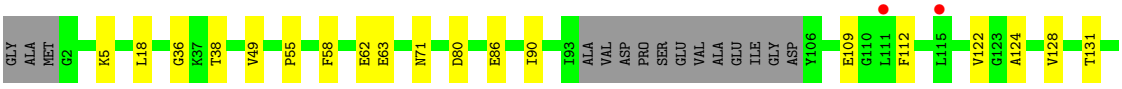
• Molecule 1: Circadian clock protein KaiC

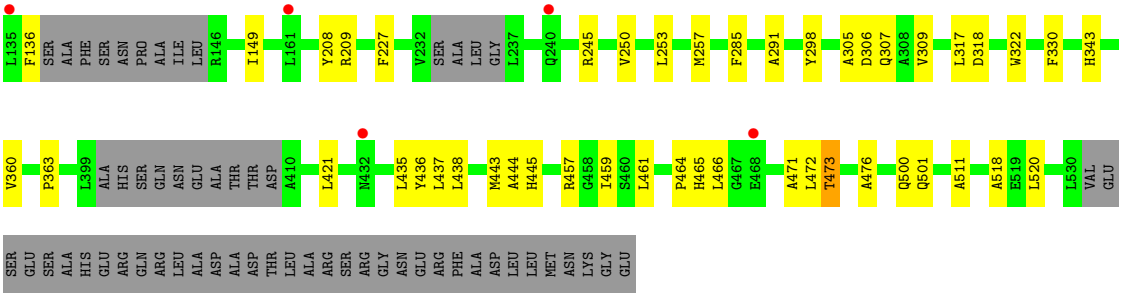
Chain H:



• Molecule 1: Circadian clock protein KaiC

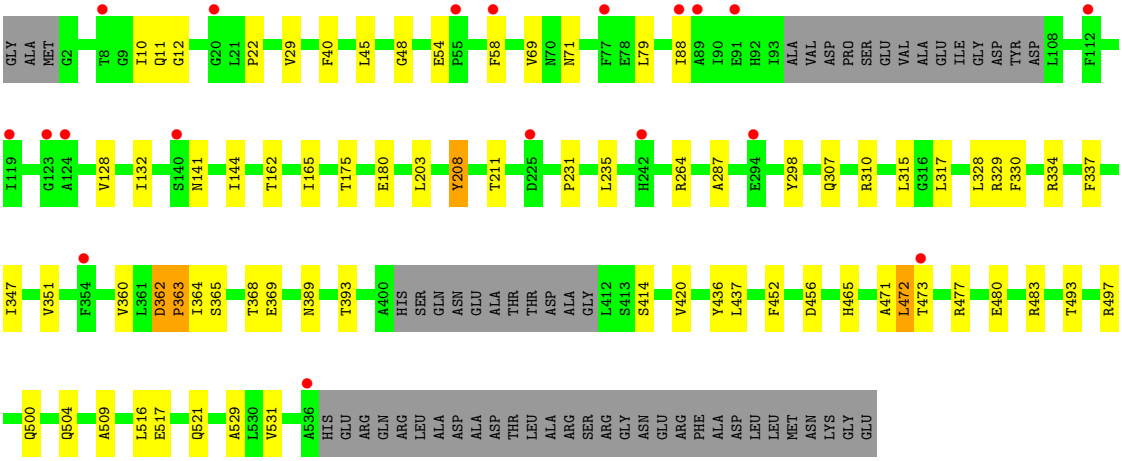
Chain I:





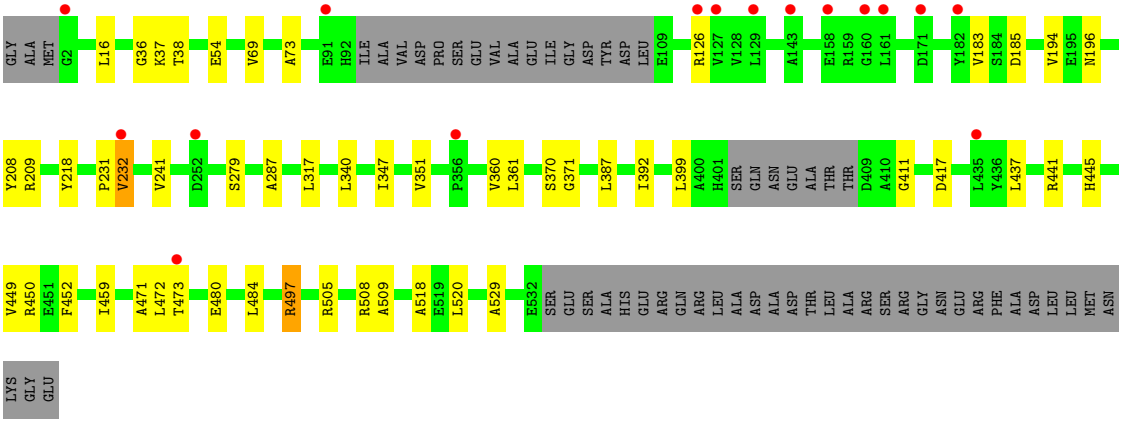
• Molecule 1: Circadian clock protein KaiC

Chain J:



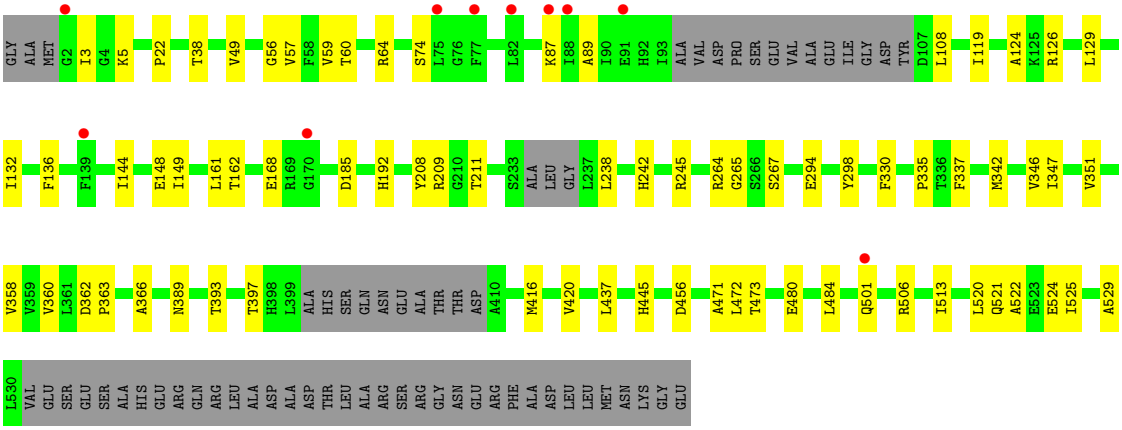
• Molecule 1: Circadian clock protein KaiC

Chain K:



• Molecule 1: Circadian clock protein KaiC

Chain L:


GLY ALA MET G2 I3 G4 K5 P22 T38 V49 G56 V57 F58 V59 T60 R64 S74 L75 G76 F77 L82 K87 I88 A89 I90 E91 H92 I93 ALA VAL ASP PRO SER GLU VAL ALA GLU ILE GLY ASP TYR D107 L108 I119 A124 K125 R126 L129
I132 F136 F139 I144 E148 I149 L161 T162 E168 R169 G170 D185 H192 Y208 R209 G210 T211 S233 ALA LEU GLY L237 L238 H242 R245 R264 G265 S266 S267 E294 Y298 F330 P335 T336 F337 M342 V346 I347 V351
V358 V359 V360 L361 D362 P363 A366 N389 T393 T397 H398 L399 ALA HIS SER GLN ASN GLU ALA THR THR ASP A410 M416 V420 L437 H445 D456 A471 L472 T473 E480 L484 Q501 R506 I513 L520 Q521 A522 E523 E524 I525 A529
L530 VAL GLU SER GLU SER ALA HIS GLU ARG GLN ARG LEU ALA ASP ALA ASP THR LEU ALA ARG SER ARG GLY ASN GLU ARG PHE ALA ASP LEU LEU MET ASN LYS GLY GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	105.11Å 136.09Å 146.20Å 93.13° 94.43° 108.09°	Depositor
Resolution (Å)	48.10 – 3.50 48.10 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.10-3.50) 97.7 (48.10-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.236 , 0.279 0.238 , 0.281	Depositor DCC
R_{free} test set	1988 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å^2)	90.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	93625	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MG, ADP

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	0.26	0/3938	0.52	0/5312
1	B	0.26	0/3930	0.52	0/5296
1	C	0.26	0/3941	0.53	0/5312
1	D	0.26	0/3975	0.54	0/5361
1	E	0.26	0/3976	0.52	0/5364
1	F	0.26	0/3910	0.52	0/5268
1	G	0.26	0/4057	0.52	0/5474
1	H	0.26	0/3969	0.53	0/5352
1	I	0.25	0/3875	0.52	0/5219
1	J	0.25	0/3961	0.52	0/5344
1	K	0.26	0/3944	0.52	0/5320
1	L	0.26	0/3946	0.53	0/5316
All	All	0.26	0/47422	0.52	0/63938

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	3879	3810	3876	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3875	3812	3871	45	0
1	C	3885	3821	3872	54	0
1	D	3916	3859	3929	63	2
1	E	3916	3862	3900	45	2
1	F	3852	3810	3851	52	0
1	G	3995	3913	4002	47	0
1	H	3910	3887	3917	39	3
1	I	3819	3695	3816	53	0
1	J	3902	3812	3900	47	0
1	K	3884	3822	3872	43	0
1	L	3888	3786	3899	54	1
2	A	54	23	24	1	0
2	B	54	24	24	2	0
2	C	54	23	24	4	0
2	D	54	23	24	1	0
2	E	54	23	24	2	0
2	F	54	23	24	0	0
2	G	54	23	24	3	0
2	H	54	23	24	1	0
2	I	54	23	24	1	0
2	J	54	23	24	0	0
2	K	54	23	24	3	0
2	L	54	23	24	2	0
3	A	2	0	0	0	0
3	B	3	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	1	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	1	0
4	C	7	0	0	4	0
4	D	6	0	0	0	0
4	E	6	0	0	1	0
4	F	6	0	0	1	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	7	0	0	4	0
4	J	5	0	0	0	0
4	K	6	0	0	3	0
4	L	5	0	0	0	0
All	All	47459	46166	46993	507	4

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.

The worst 5 of 507 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:D:520:LEU:HD11	1:K:509:ALA:CB	2.00	0.90
1:C:37:LYS:NZ	2:C:601:ADP:O2B	2.06	0.89
1:E:498:LEU:HD11	1:J:531:VAL:HG21	1.58	0.83
1:C:510:ARG:O	1:C:513:ILE:HG22	1.80	0.81
1:I:245:ARG:NH2	1:I:443:MET:SD	2.54	0.81

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:ARG:HH12	1:L:294:GLU:OE2[1_445]	1.49	0.11
1:E:245:ARG:O	1:H:485:ARG:NH1[1_545]	2.14	0.06
1:E:245:ARG:NH2	1:H:481:GLU:OE2[1_545]	2.15	0.05
1:D:87:LYS:NZ	1:H:51:ASP:OD1[1_435]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/568 (88%)	466 (93%)	31 (6%)	2 (0%)	34	72
1	B	495/568 (87%)	473 (96%)	21 (4%)	1 (0%)	47	81
1	C	498/568 (88%)	472 (95%)	25 (5%)	1 (0%)	47	81
1	D	502/568 (88%)	460 (92%)	36 (7%)	6 (1%)	13	50
1	E	505/568 (89%)	481 (95%)	23 (5%)	1 (0%)	47	81
1	F	492/568 (87%)	463 (94%)	28 (6%)	1 (0%)	47	81
1	G	514/568 (90%)	476 (93%)	34 (7%)	4 (1%)	19	58
1	H	503/568 (89%)	476 (95%)	27 (5%)	0	100	100
1	I	484/568 (85%)	455 (94%)	26 (5%)	3 (1%)	25	64
1	J	504/568 (89%)	472 (94%)	28 (6%)	4 (1%)	19	58
1	K	502/568 (88%)	479 (95%)	19 (4%)	4 (1%)	19	58
1	L	495/568 (87%)	462 (93%)	32 (6%)	1 (0%)	47	81
All	All	5993/6816 (88%)	5635 (94%)	330 (6%)	28 (0%)	29	68

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	95	VAL
1	D	474	GLY
1	J	363	PRO
1	K	232	VAL
1	A	469	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/457 (87%)	392 (98%)	6 (2%)	65	84
1	B	398/457 (87%)	393 (99%)	5 (1%)	69	86
1	C	397/457 (87%)	389 (98%)	8 (2%)	55	79
1	D	403/457 (88%)	402 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	403/457 (88%)	397 (98%)	6 (2%)	65 84
1	F	397/457 (87%)	394 (99%)	3 (1%)	81 91
1	G	415/457 (91%)	412 (99%)	3 (1%)	84 93
1	H	404/457 (88%)	397 (98%)	7 (2%)	60 82
1	I	394/457 (86%)	388 (98%)	6 (2%)	65 84
1	J	401/457 (88%)	395 (98%)	6 (2%)	65 84
1	K	397/457 (87%)	393 (99%)	4 (1%)	76 88
1	L	402/457 (88%)	397 (99%)	5 (1%)	71 87
All	All	4809/5484 (88%)	4749 (99%)	60 (1%)	71 87

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	465	HIS
1	L	64	ARG
1	H	425	ARG
1	K	497	ARG
1	L	456	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	284	HIS
1	F	465	HIS
1	J	445	HIS
1	I	239	HIS
1	E	343	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 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 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	ADP	D	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	5 (17%)
2	ADP	F	603	3	24,29,29	0.92	1 (4%)	29,45,45	1.49	5 (17%)
2	ADP	B	604	3	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	L	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	I	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	C	601	3	24,29,29	0.91	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	H	601	3	24,29,29	0.93	1 (4%)	29,45,45	1.53	5 (17%)
2	ADP	K	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.53	5 (17%)
2	ADP	G	604	3	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	H	603	3	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	D	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)
2	ADP	A	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	5 (17%)
2	ADP	E	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	G	601	3	24,29,29	0.92	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	K	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	F	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	L	602	3	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	B	601	3	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	E	604	3	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	A	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	J	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.46	5 (17%)
2	ADP	J	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.45	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	C	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	5 (17%)
2	ADP	I	604	3,1	24,29,29	0.91	1 (4%)	29,45,45	1.52	5 (17%)

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	ADP	D	604	3	-	5/12/32/32	0/3/3/3
2	ADP	F	603	3	-	5/12/32/32	0/3/3/3
2	ADP	B	604	3	-	5/12/32/32	0/3/3/3
2	ADP	L	601	-	-	0/12/32/32	0/3/3/3
2	ADP	I	601	-	-	6/12/32/32	0/3/3/3
2	ADP	C	601	3	-	5/12/32/32	0/3/3/3
2	ADP	H	601	3	-	7/12/32/32	0/3/3/3
2	ADP	K	604	3	-	2/12/32/32	0/3/3/3
2	ADP	G	604	3	-	4/12/32/32	0/3/3/3
2	ADP	H	603	3	-	4/12/32/32	0/3/3/3
2	ADP	D	601	-	-	5/12/32/32	0/3/3/3
2	ADP	A	601	-	-	6/12/32/32	0/3/3/3
2	ADP	E	601	-	-	2/12/32/32	0/3/3/3
2	ADP	G	601	3	-	4/12/32/32	0/3/3/3
2	ADP	K	601	-	-	6/12/32/32	0/3/3/3
2	ADP	F	601	-	-	0/12/32/32	0/3/3/3
2	ADP	L	602	3	-	4/12/32/32	0/3/3/3
2	ADP	B	601	3	-	4/12/32/32	0/3/3/3
2	ADP	E	604	3	-	1/12/32/32	0/3/3/3
2	ADP	A	604	3	-	4/12/32/32	0/3/3/3
2	ADP	J	604	3	-	3/12/32/32	0/3/3/3
2	ADP	J	601	-	-	5/12/32/32	0/3/3/3
2	ADP	C	604	3	-	5/12/32/32	0/3/3/3
2	ADP	I	604	3,1	-	5/12/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	ADP	C5-C4	2.43	1.47	1.40
2	D	601	ADP	C5-C4	2.41	1.47	1.40
2	A	601	ADP	C5-C4	2.41	1.47	1.40
2	B	601	ADP	C5-C4	2.40	1.47	1.40
2	J	604	ADP	C5-C4	2.39	1.47	1.40

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	ADP	PA-O3A-PB	-3.89	119.47	132.83
2	A	601	ADP	PA-O3A-PB	-3.78	119.86	132.83
2	H	601	ADP	PA-O3A-PB	-3.77	119.88	132.83
2	I	604	ADP	N3-C2-N1	-3.73	122.85	128.68
2	A	604	ADP	N3-C2-N1	-3.70	122.90	128.68

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	C5'-O5'-PA-O3A
2	A	604	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	604	ADP	1	0
2	B	604	ADP	2	0
2	L	601	ADP	2	0
2	I	601	ADP	1	0
2	C	601	ADP	2	0
2	H	601	ADP	1	0
2	K	604	ADP	1	0
2	G	604	ADP	2	0
2	E	601	ADP	1	0
2	G	601	ADP	1	0
2	K	601	ADP	2	0
2	E	604	ADP	1	0
2	A	604	ADP	1	0

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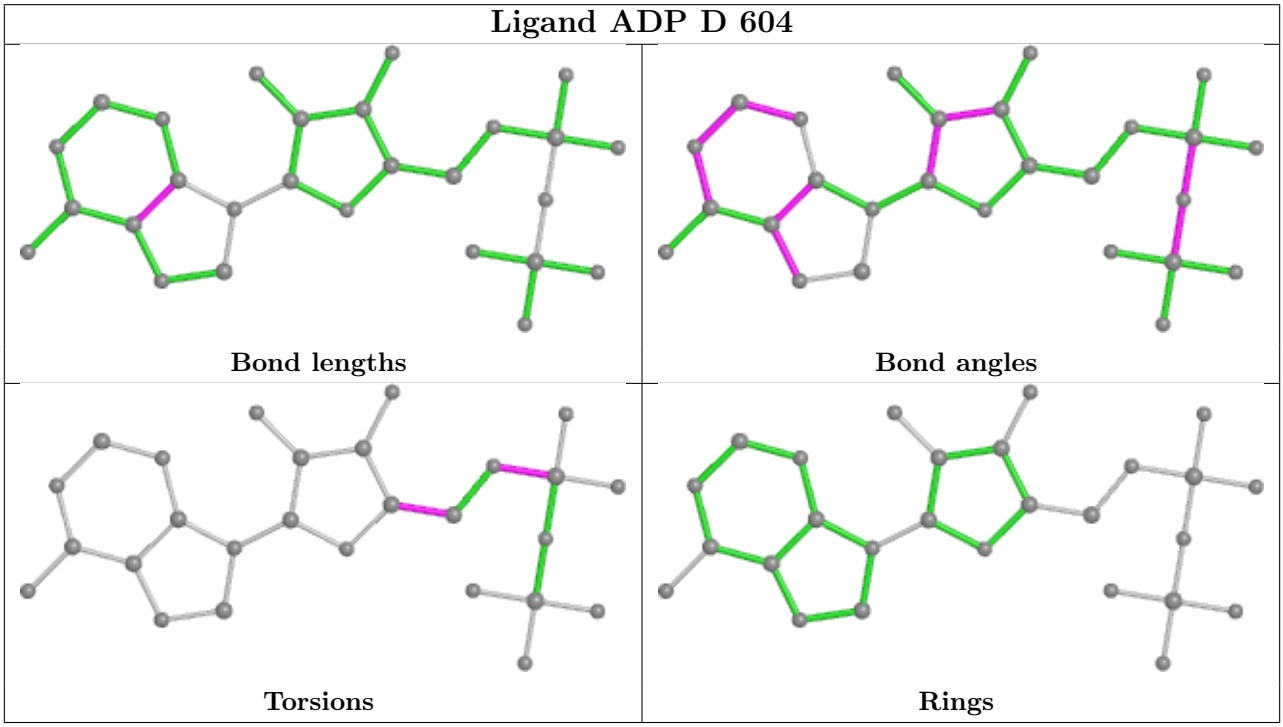
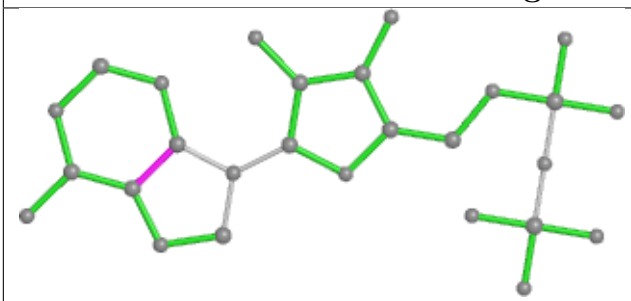
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	604	ADP	2	0

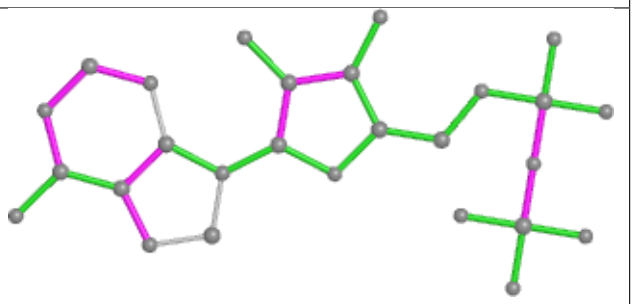
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



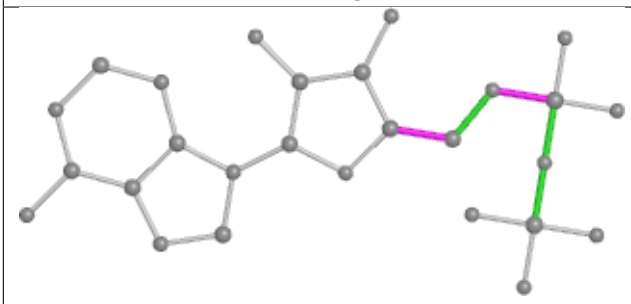
Ligand ADP F 603



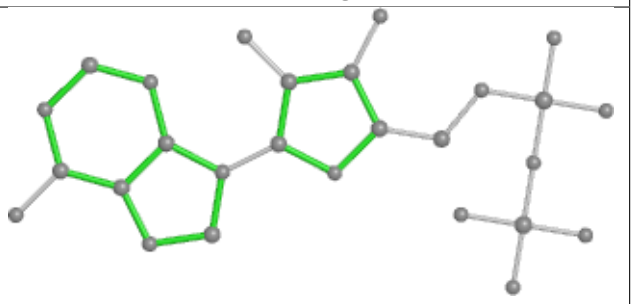
Bond lengths



Bond angles

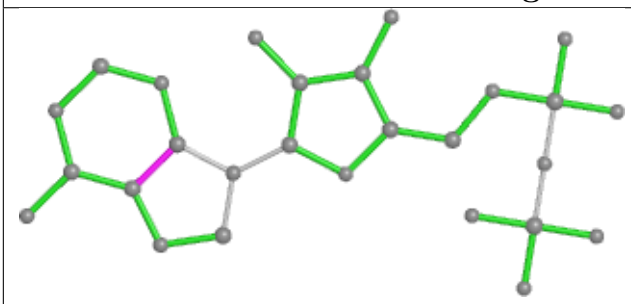


Torsions

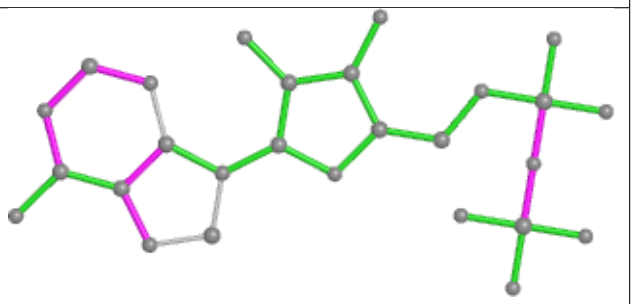


Rings

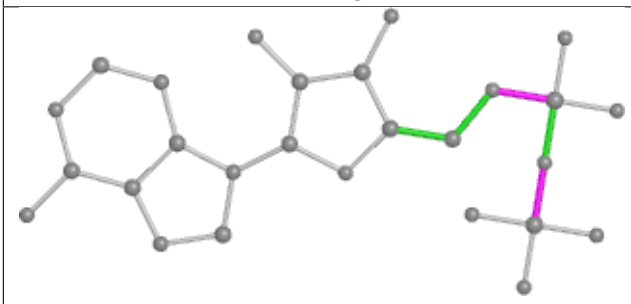
Ligand ADP B 604



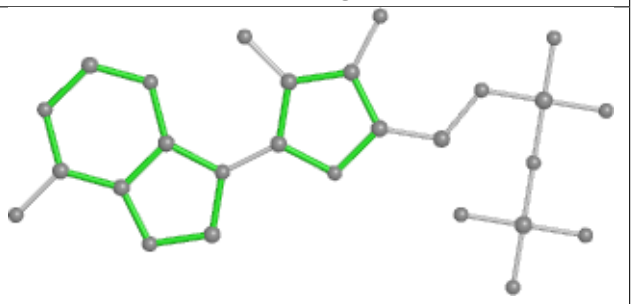
Bond lengths



Bond angles

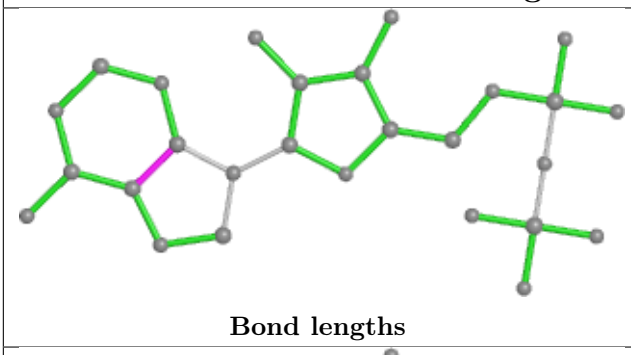


Torsions

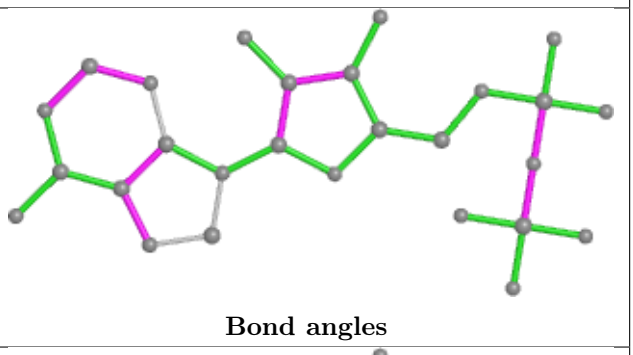


Rings

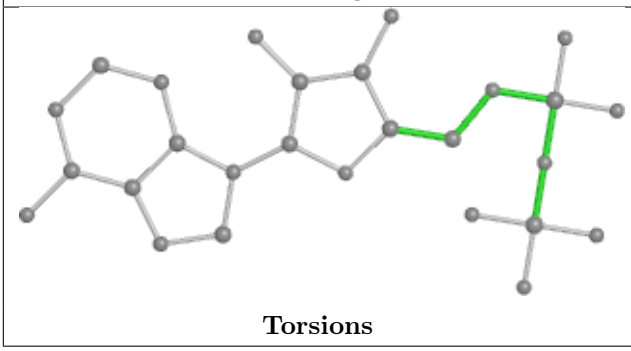
Ligand ADP L 601



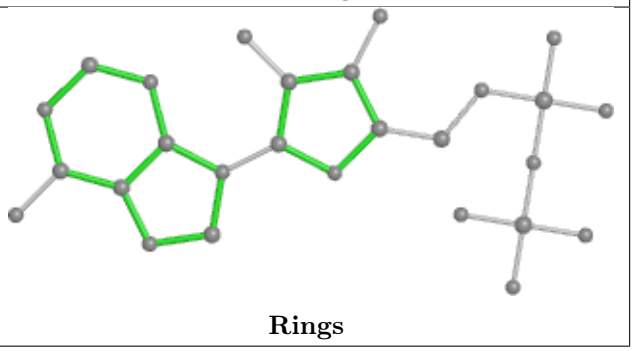
Bond lengths



Bond angles

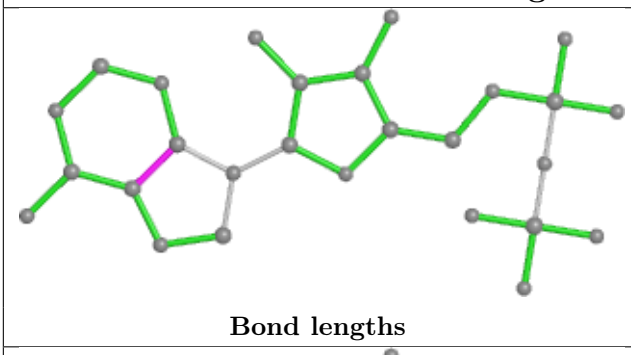


Torsions

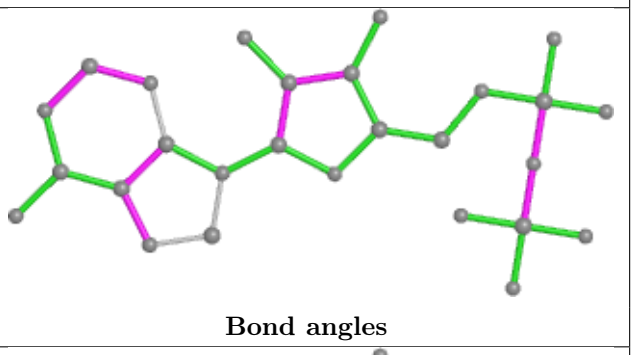


Rings

Ligand ADP I 601



Bond lengths



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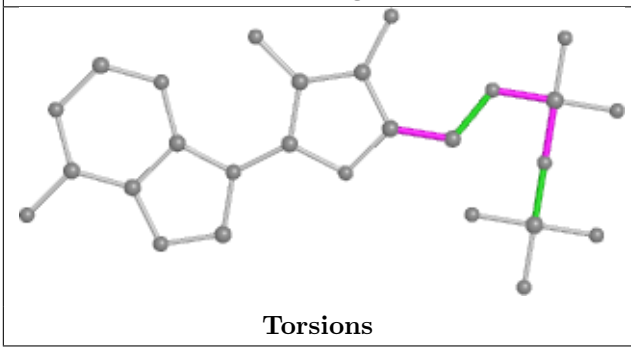

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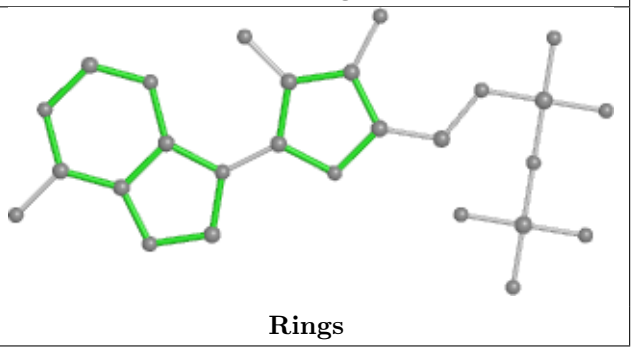
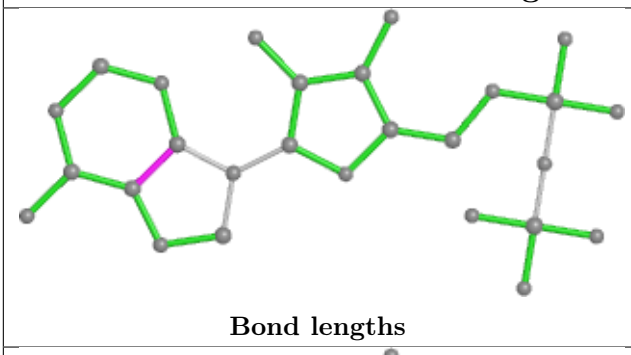


Rings

Ligand ADP C 601



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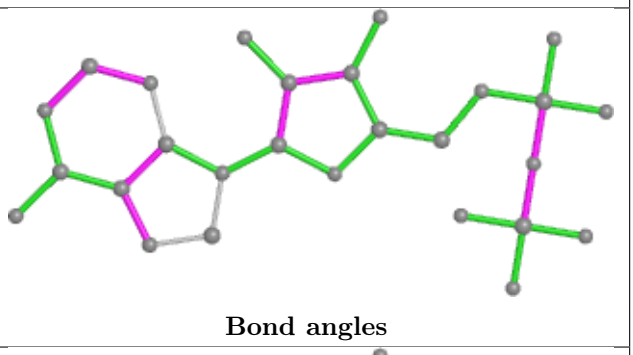

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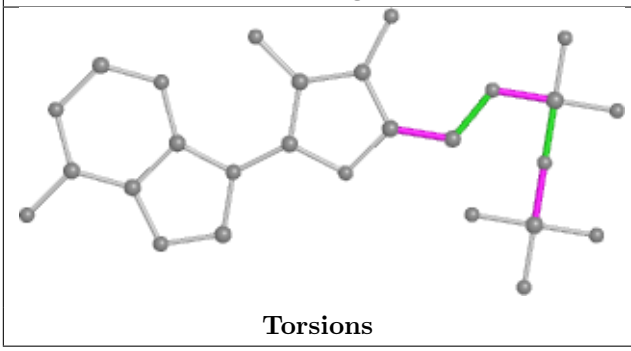

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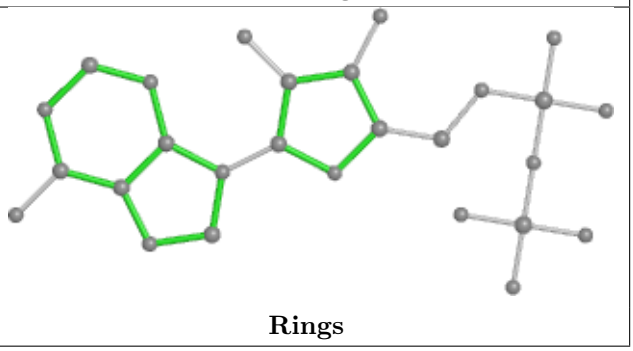

Rings

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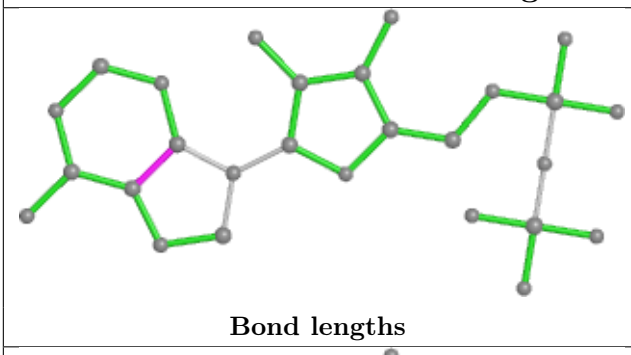

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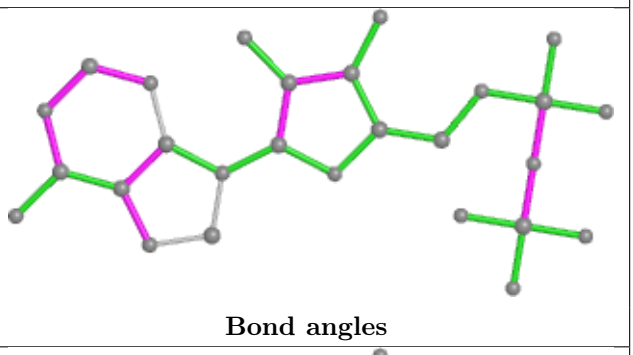

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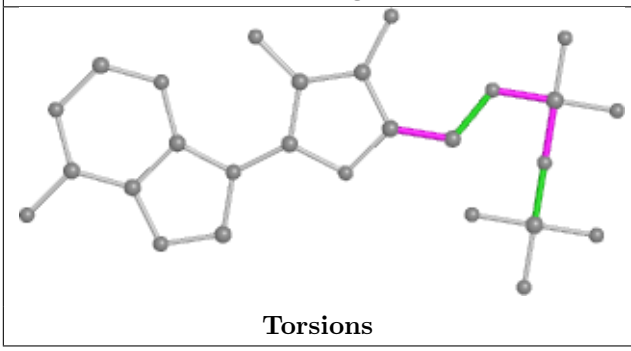

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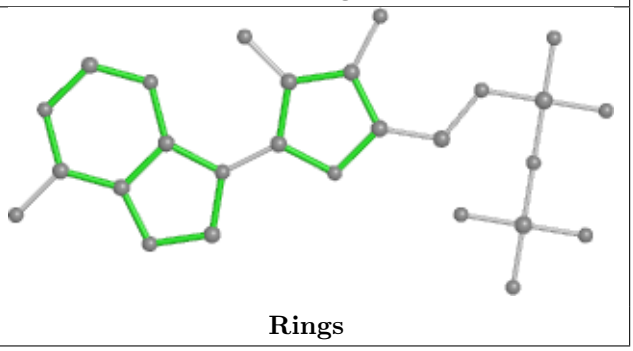
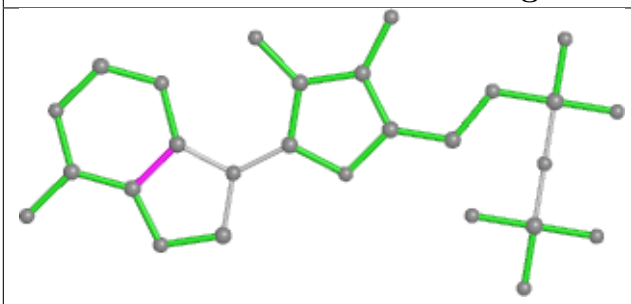


Rings

Ligand ADP K 604



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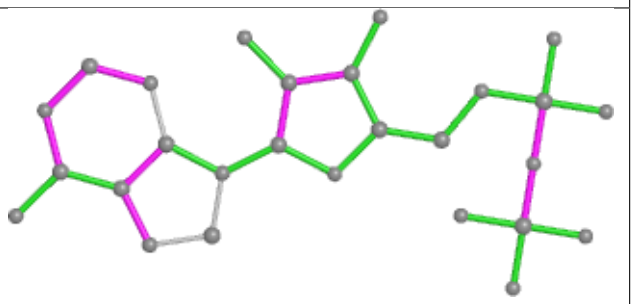

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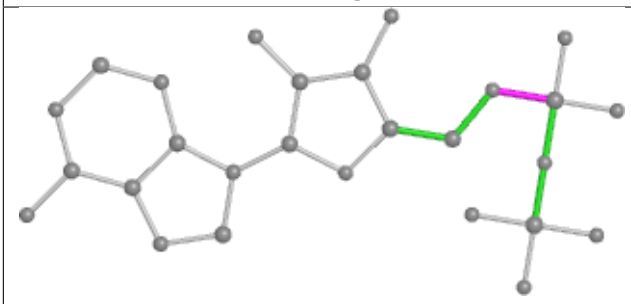

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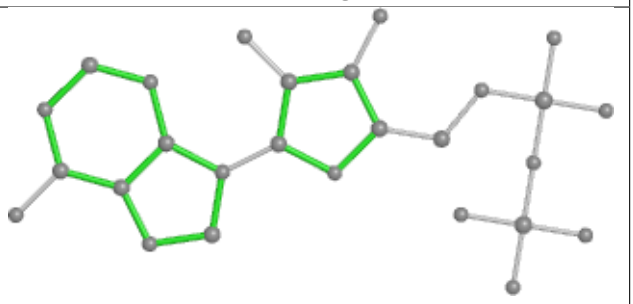

Rings

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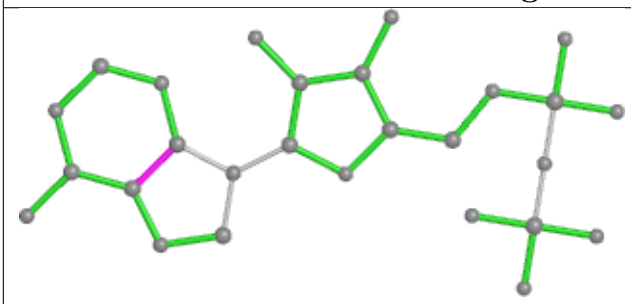

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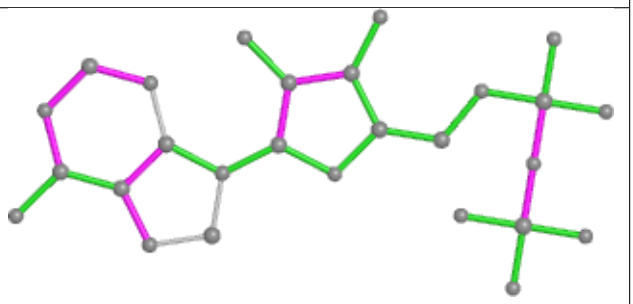

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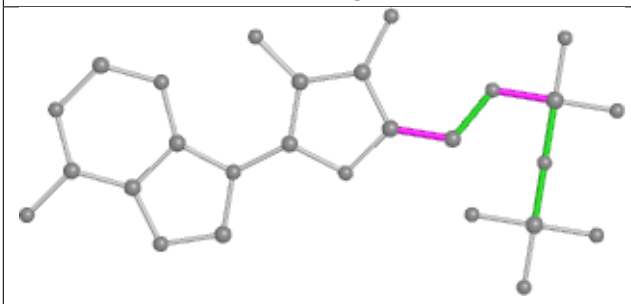

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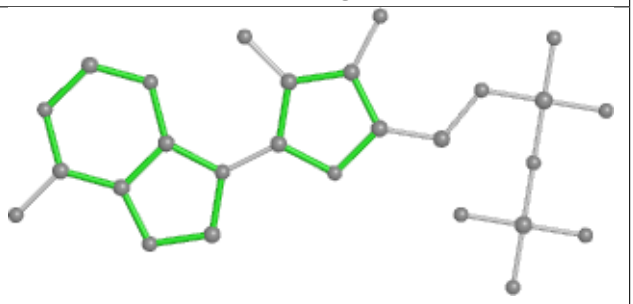
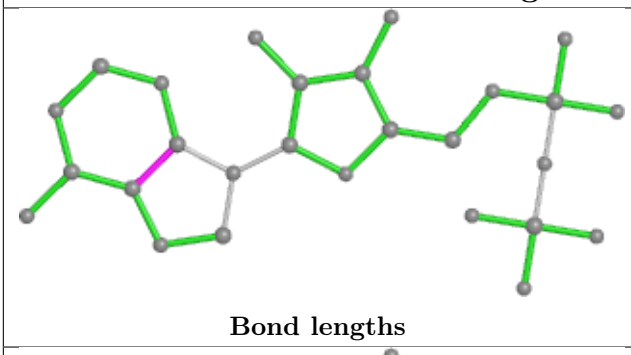


Rings

Ligand ADP H 603



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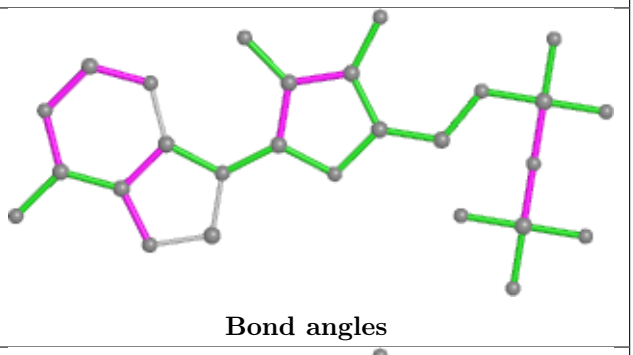

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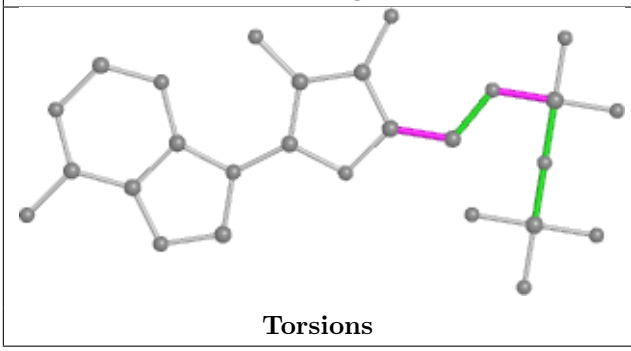

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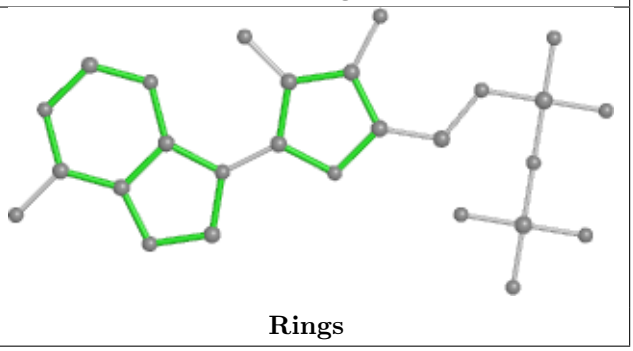
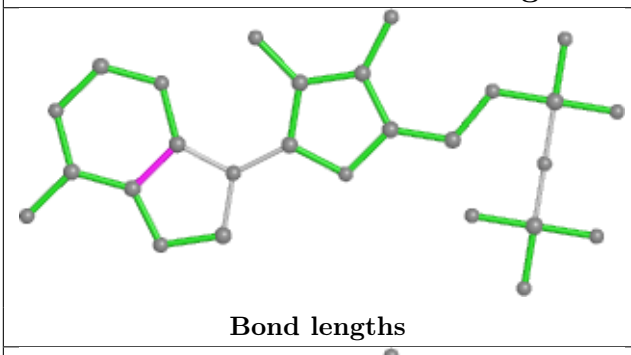


Rings

Ligand ADP D 601



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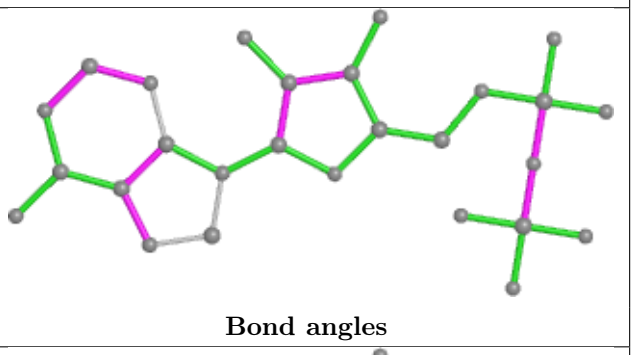

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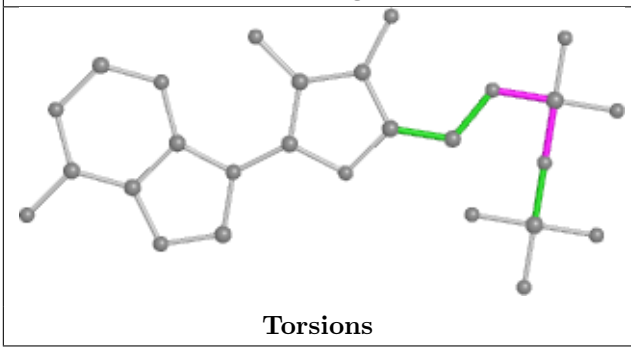

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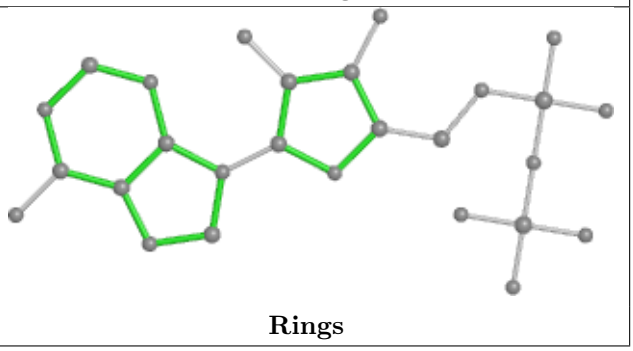
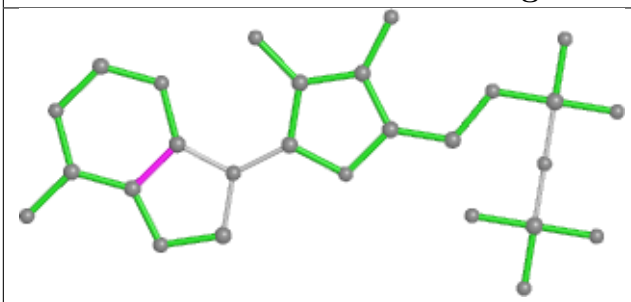


Rings

Ligand ADP A 601



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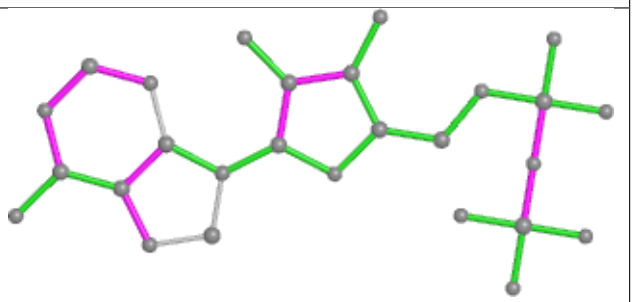

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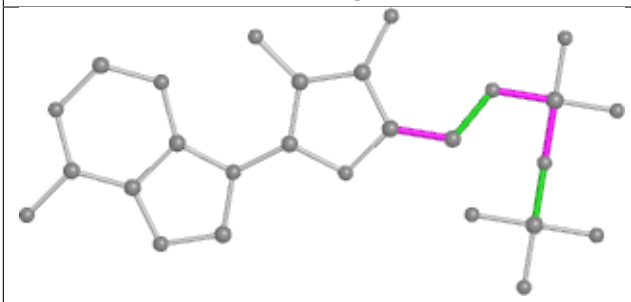

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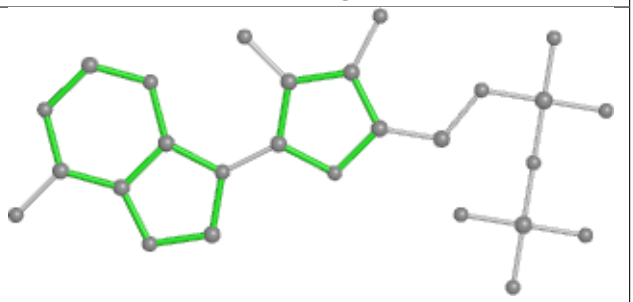
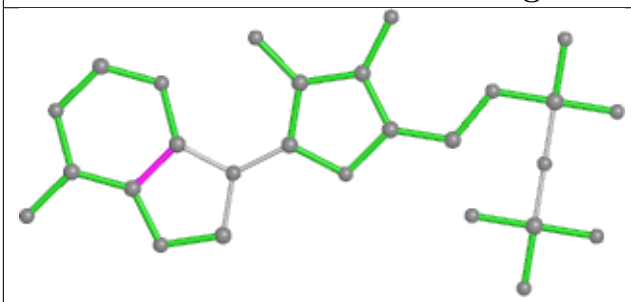


Rings

Ligand ADP E 601



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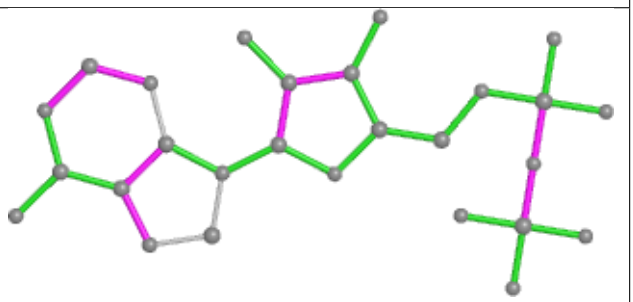

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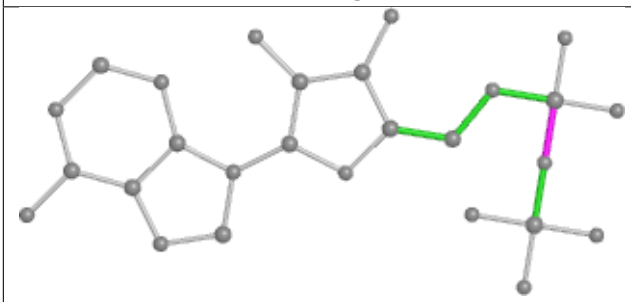

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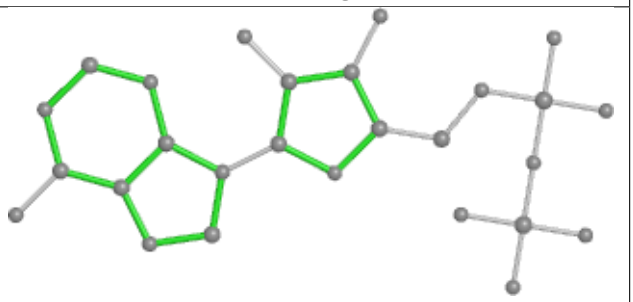

Rings

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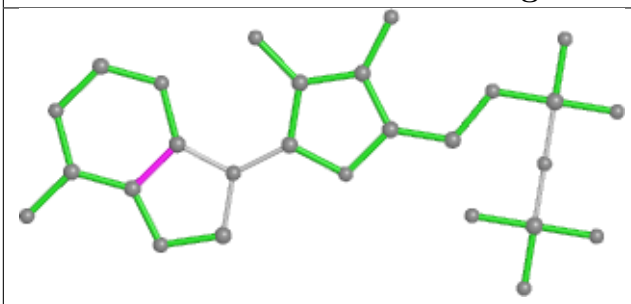

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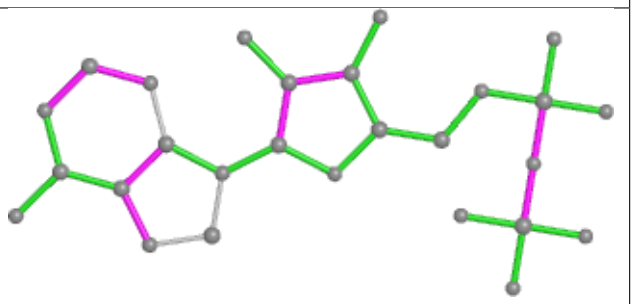

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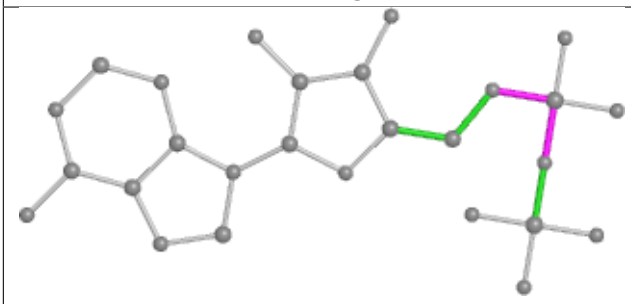

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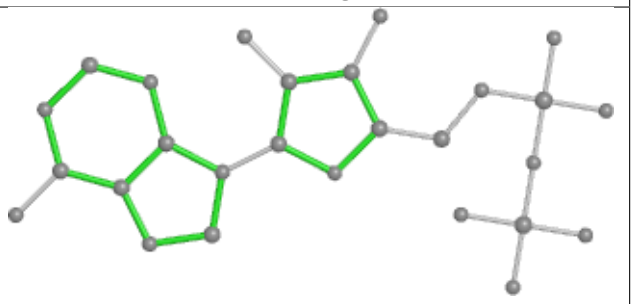

Rings

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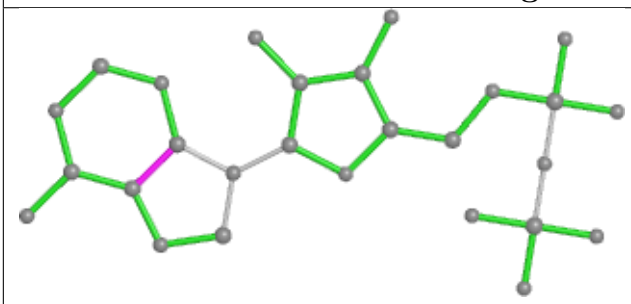

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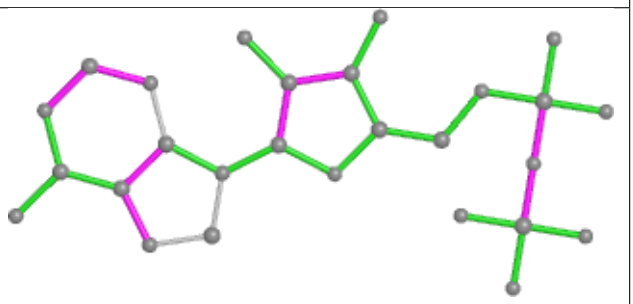

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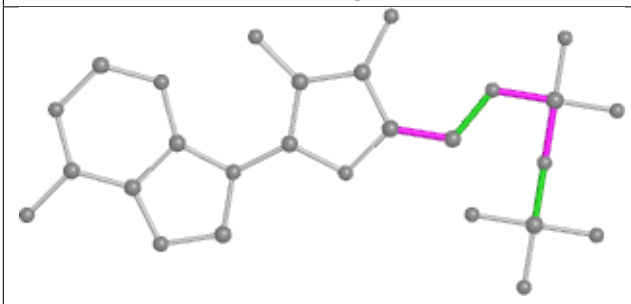

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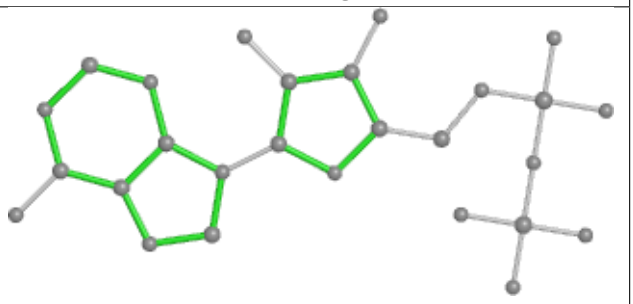

Rings

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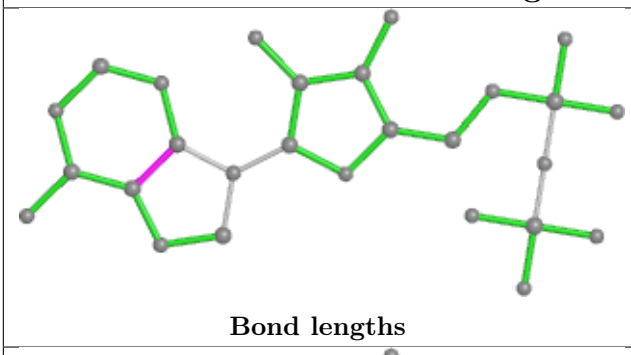

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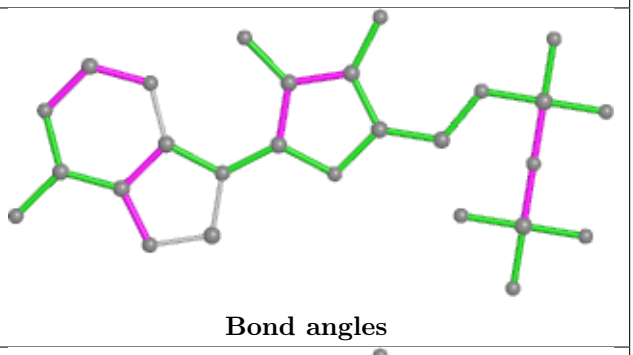
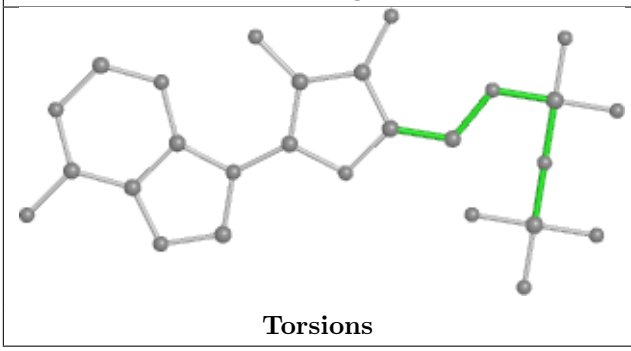


Bond angles



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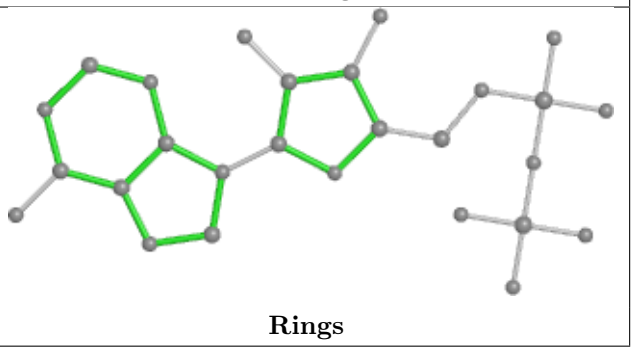

Rings

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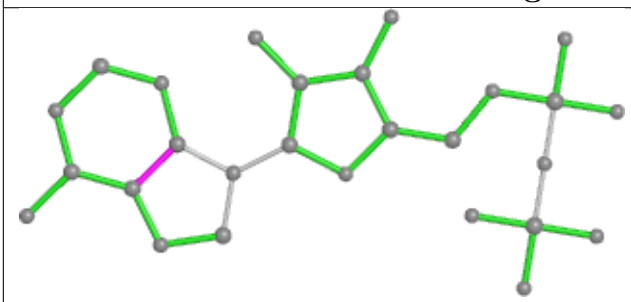

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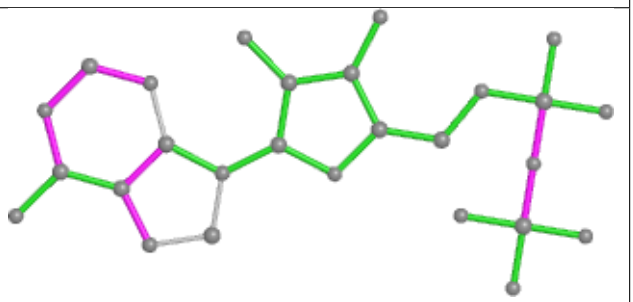
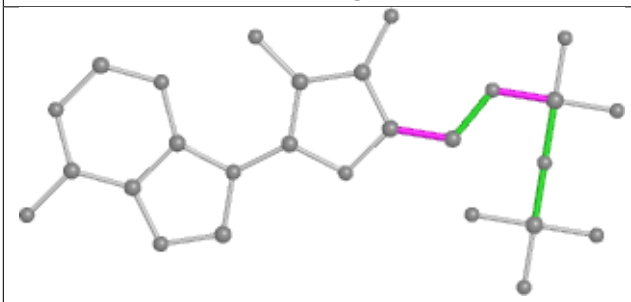


Bond angles



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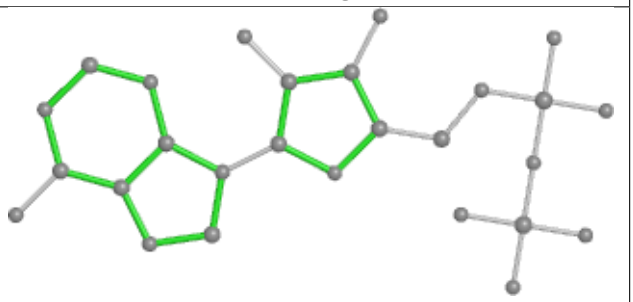

Rings

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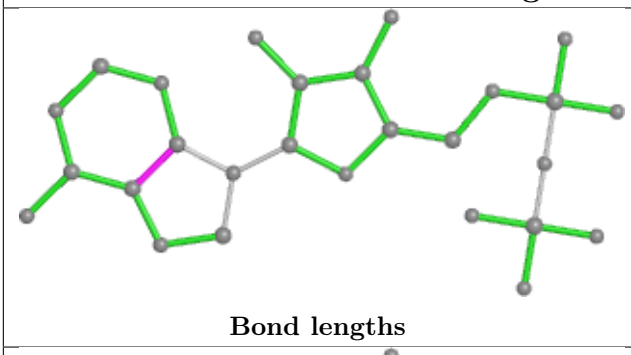
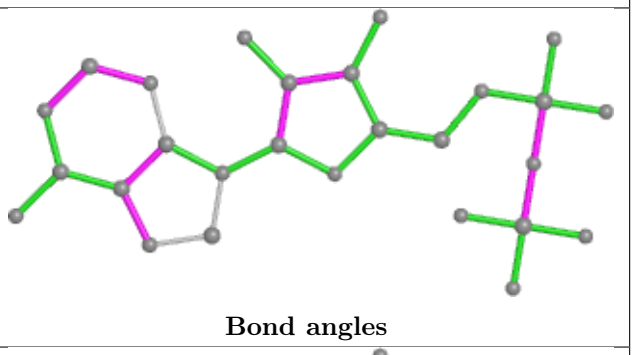
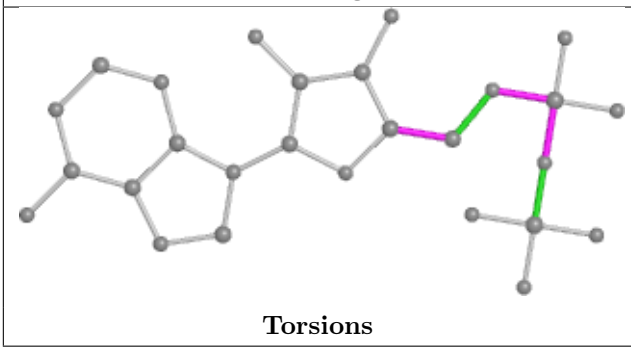


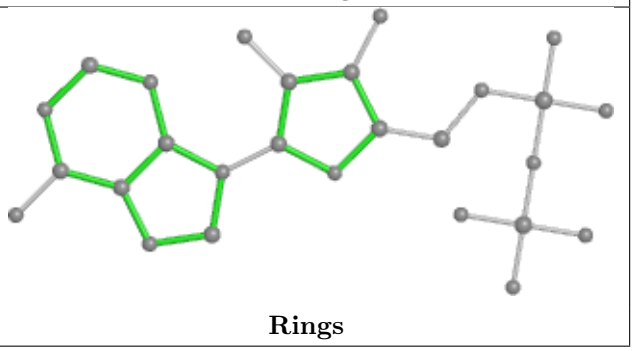
Bond lengths



Bond angles

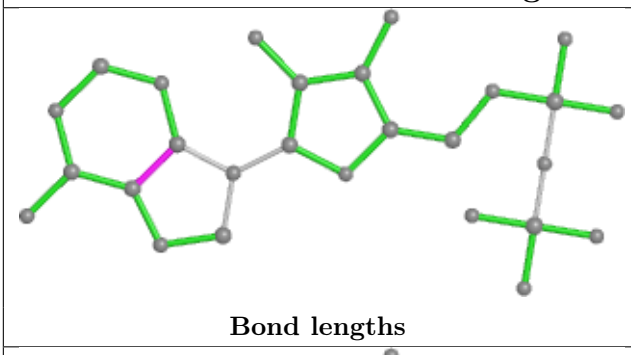


Torsions

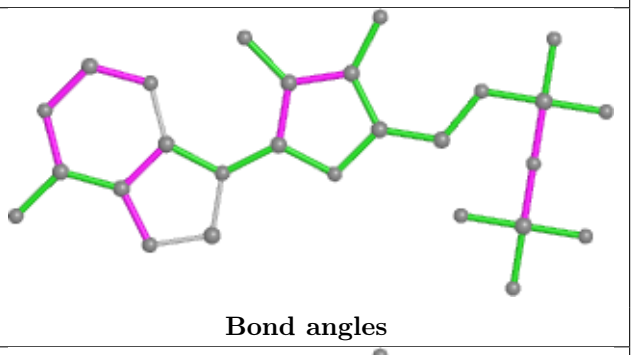


Rings

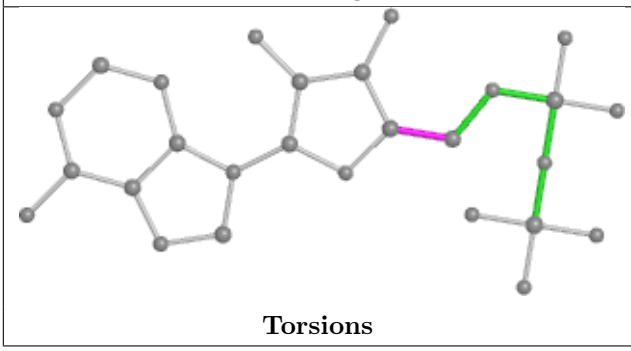
Ligand ADP E 604



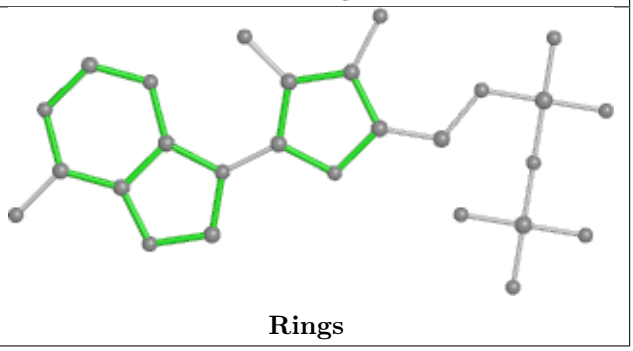
Bond lengths



Bond angles

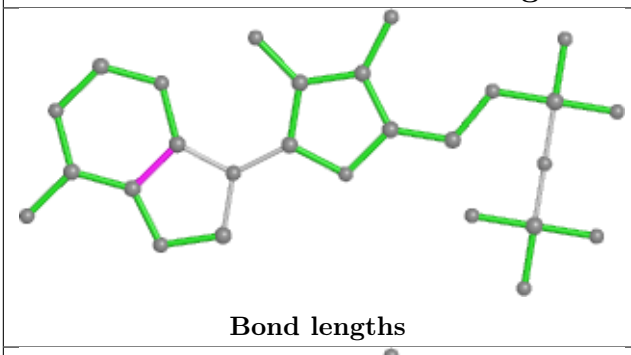


Torsions

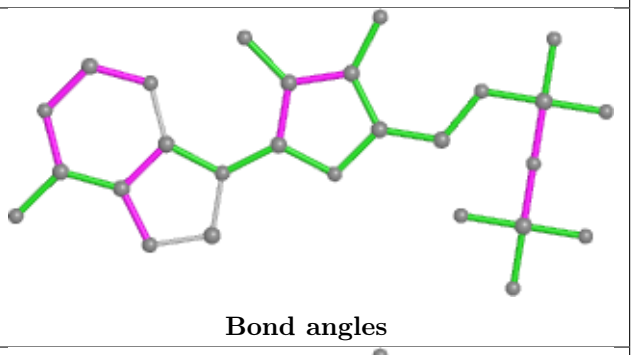


Rings

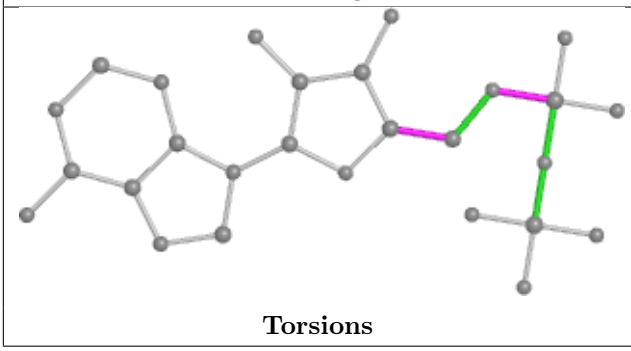
Ligand ADP A 604



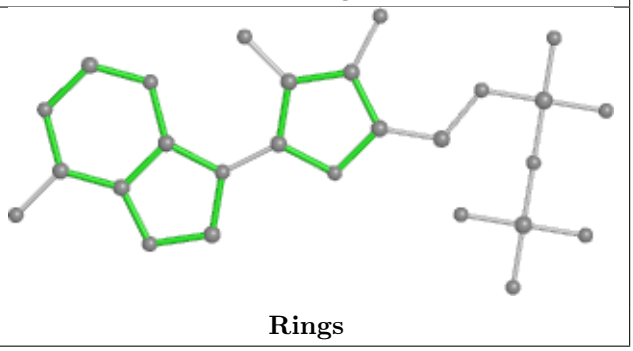
Bond lengths



Bond angles

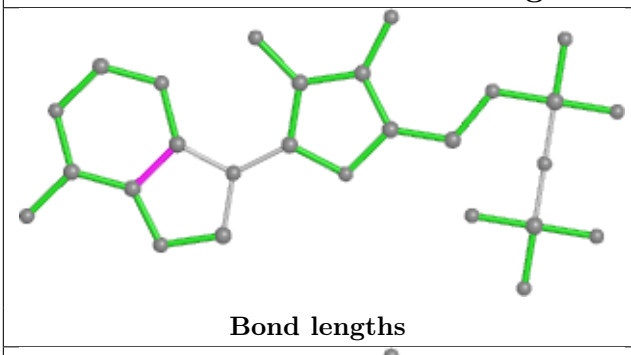


Torsions

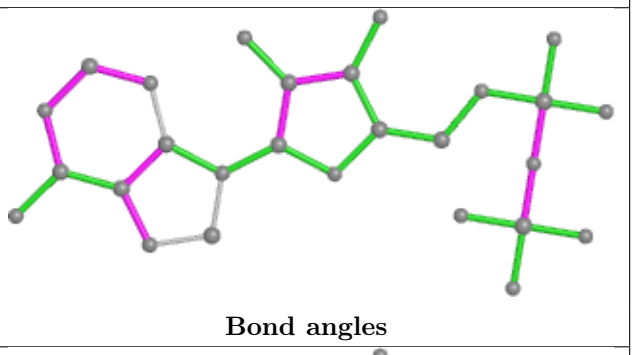


Rings

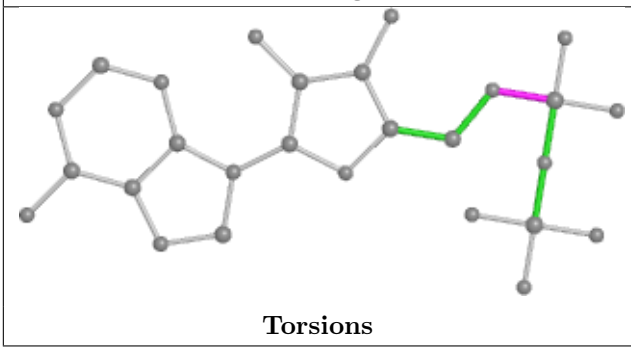
Ligand ADP J 604



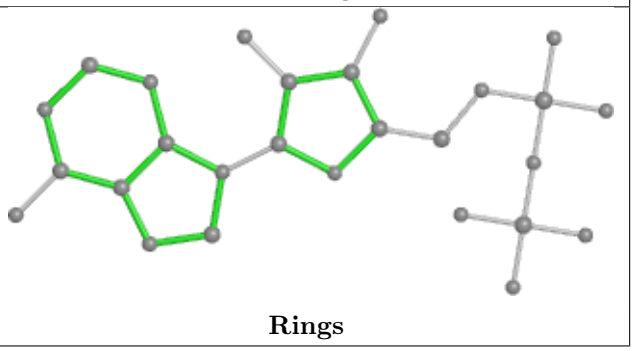
Bond lengths



Bond angles

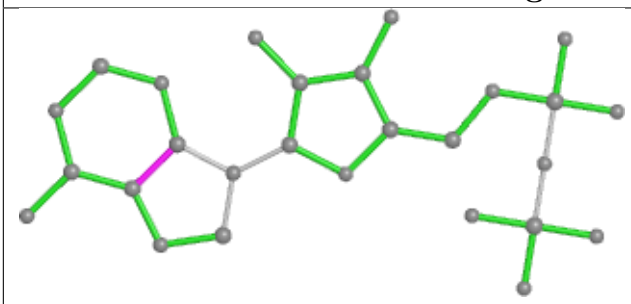


Torsions

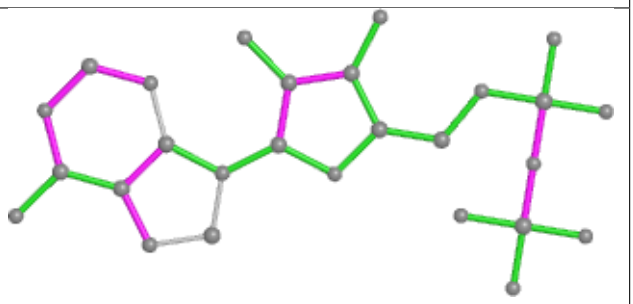


Rings

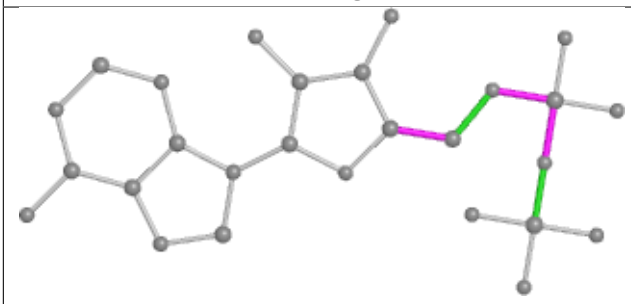
Ligand ADP J 601



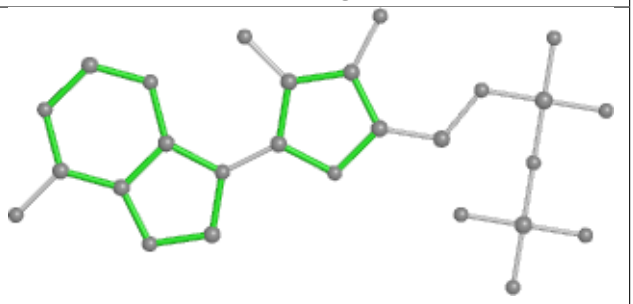
Bond lengths



Bond angles

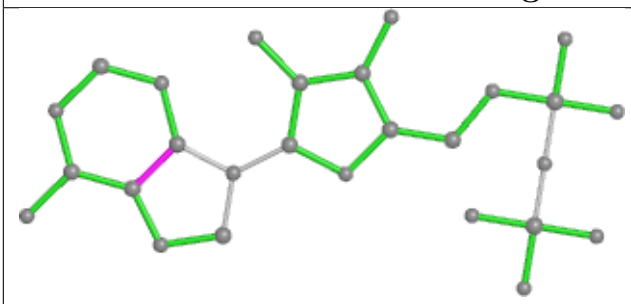


Torsions

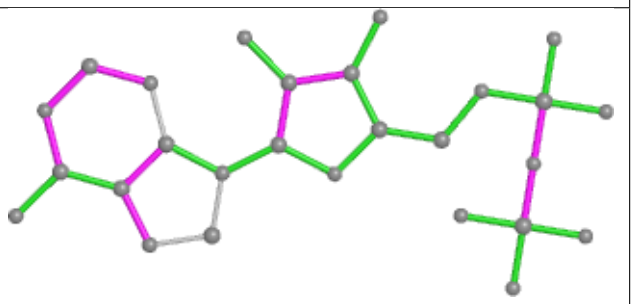


Rings

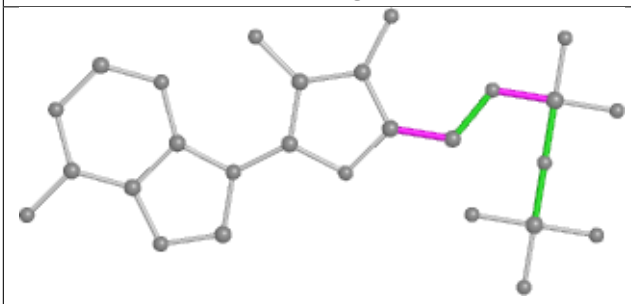
Ligand ADP C 604



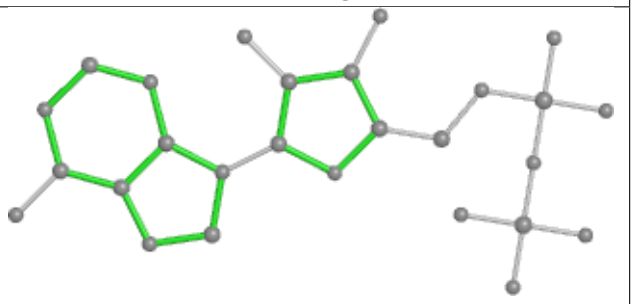
Bond lengths



Bond angles

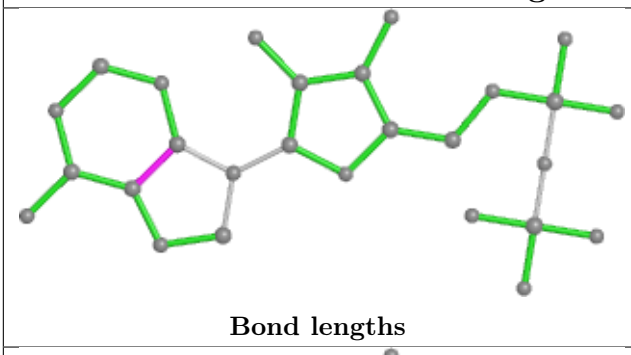


Torsions

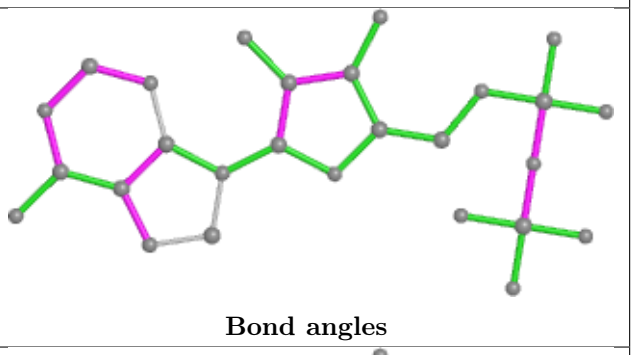


Rings

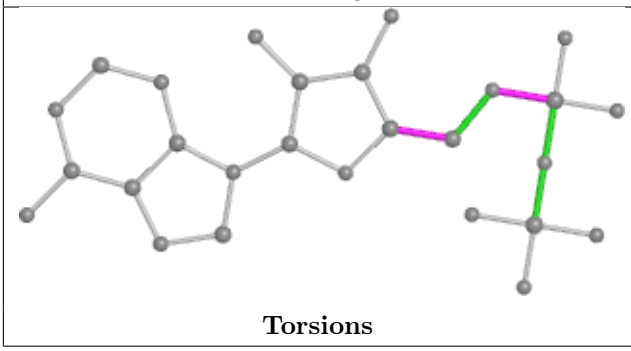
Ligand ADP I 604



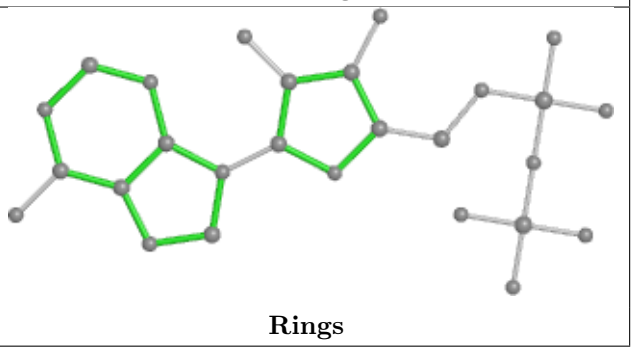
Bond lengths



Bond angles



Torsions



Rings

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	507/568 (89%)	0.12	13 (2%)	56	49	55, 98, 161, 204	0
1	B	505/568 (88%)	-0.03	9 (1%)	68	62	51, 99, 142, 165	0
1	C	508/568 (89%)	-0.03	7 (1%)	75	69	54, 98, 150, 186	0
1	D	510/568 (89%)	0.00	11 (2%)	62	56	57, 90, 146, 211	0
1	E	511/568 (89%)	-0.17	3 (0%)	89	86	51, 89, 139, 177	0
1	F	500/568 (88%)	-0.14	4 (0%)	86	81	42, 94, 138, 200	0
1	G	518/568 (91%)	-0.01	10 (1%)	66	61	53, 99, 161, 216	0
1	H	509/568 (89%)	0.05	13 (2%)	56	49	41, 92, 149, 206	0
1	I	494/568 (86%)	0.02	7 (1%)	75	69	58, 101, 149, 175	0
1	J	510/568 (89%)	0.09	19 (3%)	41	37	65, 121, 171, 202	0
1	K	508/568 (89%)	0.25	16 (3%)	49	43	63, 115, 165, 195	0
1	L	503/568 (88%)	-0.02	10 (1%)	65	60	47, 106, 165, 180	0
All	All	6083/6816 (89%)	0.01	122 (2%)	65	60	41, 99, 157, 216	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	87	LYS	6.6
1	H	143	ALA	5.9
1	K	91	GLU	4.6
1	B	468	GLU	4.5
1	L	88	ILE	4.2

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 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
3	MG	I	603	1/1	0.67	0.28	79,79,79,79	0
3	MG	C	603	1/1	0.71	0.26	98,98,98,98	0
2	ADP	L	601	27/27	0.81	0.27	94,126,152,158	0
2	ADP	J	601	27/27	0.84	0.29	105,136,162,167	0
2	ADP	F	601	27/27	0.87	0.29	72,117,146,151	0
3	MG	J	603	1/1	0.88	0.29	104,104,104,104	0
2	ADP	G	604	27/27	0.89	0.27	47,77,119,137	0
2	ADP	C	601	27/27	0.89	0.27	73,95,115,117	0
2	ADP	B	601	27/27	0.90	0.27	87,114,141,141	0
2	ADP	G	601	27/27	0.90	0.30	89,114,139,143	0
3	MG	B	605	1/1	0.91	0.24	84,84,84,84	0
2	ADP	I	604	27/27	0.91	0.21	69,104,130,139	0
3	MG	K	603	1/1	0.91	0.23	85,85,85,85	0
2	ADP	K	604	27/27	0.92	0.23	77,106,129,131	0
2	ADP	A	604	27/27	0.92	0.29	69,88,114,127	0
3	MG	K	602	1/1	0.92	0.23	70,70,70,70	0
3	MG	I	602	1/1	0.92	0.13	53,53,53,53	0
2	ADP	A	601	27/27	0.93	0.24	95,112,137,158	0
2	ADP	I	601	27/27	0.93	0.27	100,123,156,158	0
2	ADP	K	601	27/27	0.93	0.22	108,131,158,171	0
2	ADP	D	601	27/27	0.94	0.27	72,97,132,137	0
2	ADP	H	603	27/27	0.94	0.28	65,93,117,137	0
3	MG	C	602	1/1	0.94	0.35	63,63,63,63	0
2	ADP	E	601	27/27	0.94	0.22	60,91,112,122	0
3	MG	D	602	1/1	0.94	0.28	85,85,85,85	0
3	MG	G	603	1/1	0.94	0.25	98,98,98,98	0
3	MG	H	604	1/1	0.94	0.16	77,77,77,77	0
2	ADP	E	604	27/27	0.94	0.26	51,78,112,113	0
2	ADP	B	604	27/27	0.94	0.23	58,75,91,106	0
2	ADP	J	604	27/27	0.94	0.29	64,84,108,124	0
2	ADP	F	603	27/27	0.94	0.25	58,94,119,126	0
2	ADP	C	604	27/27	0.94	0.26	72,87,114,123	0

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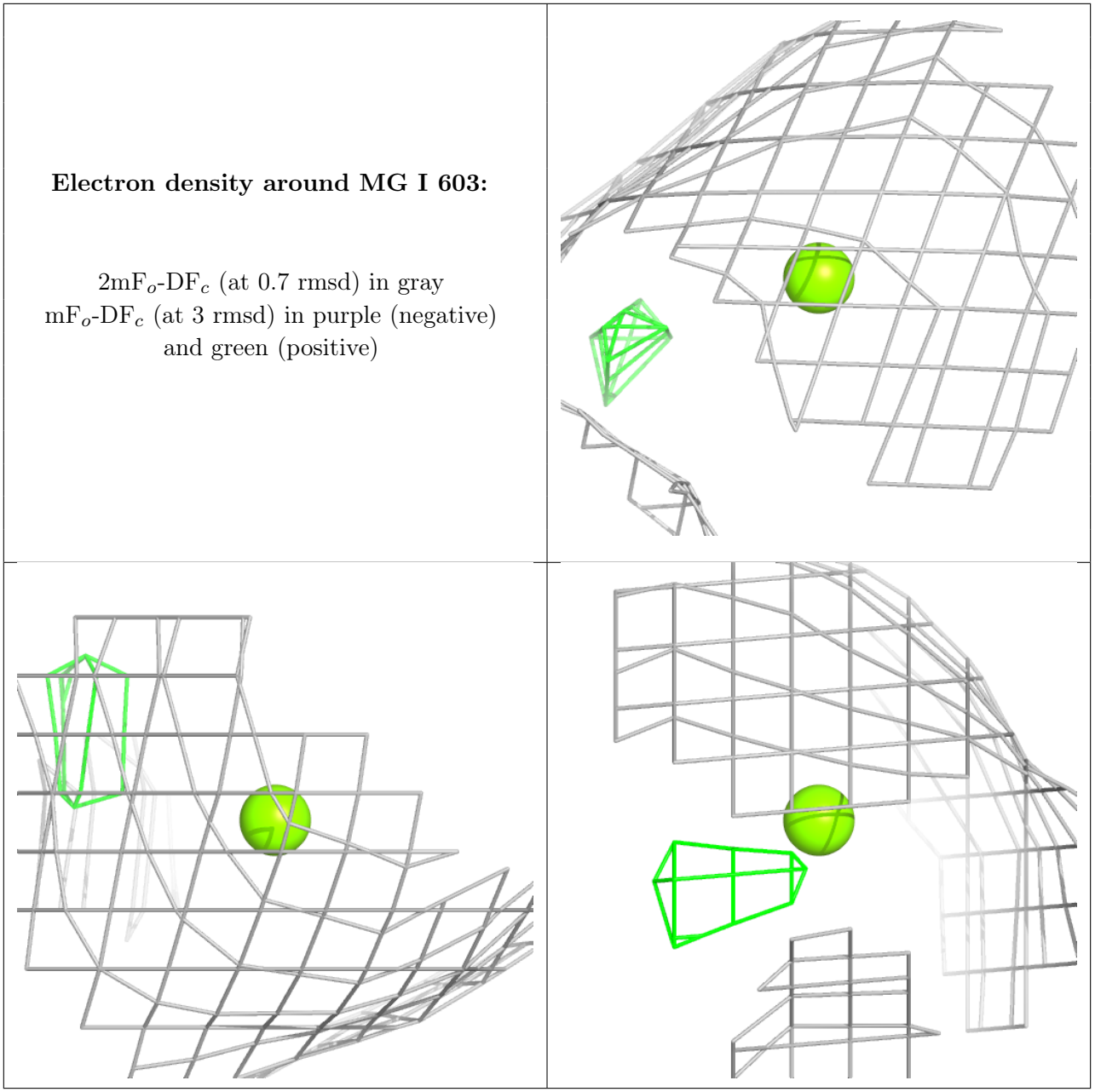
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	602	1/1	0.95	0.13	36,36,36,36	0
2	ADP	D	604	27/27	0.95	0.27	57,77,98,106	0
2	ADP	H	601	27/27	0.95	0.23	68,95,134,137	0
2	ADP	L	602	27/27	0.96	0.18	41,78,99,103	0
3	MG	H	602	1/1	0.96	0.24	77,77,77,77	0
3	MG	A	602	1/1	0.97	0.17	76,76,76,76	0
3	MG	E	603	1/1	0.97	0.42	66,66,66,66	0
3	MG	F	602	1/1	0.97	0.24	82,82,82,82	0
3	MG	G	602	1/1	0.97	0.33	46,46,46,46	0
3	MG	G	605	1/1	0.98	0.23	58,58,58,58	0
3	MG	J	602	1/1	0.98	0.34	62,62,62,62	0
3	MG	B	603	1/1	0.98	0.19	65,65,65,65	0
3	MG	E	602	1/1	0.98	0.21	46,46,46,46	0
3	MG	A	603	1/1	0.98	0.17	98,98,98,98	0
3	MG	D	603	1/1	0.99	0.29	68,68,68,68	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.

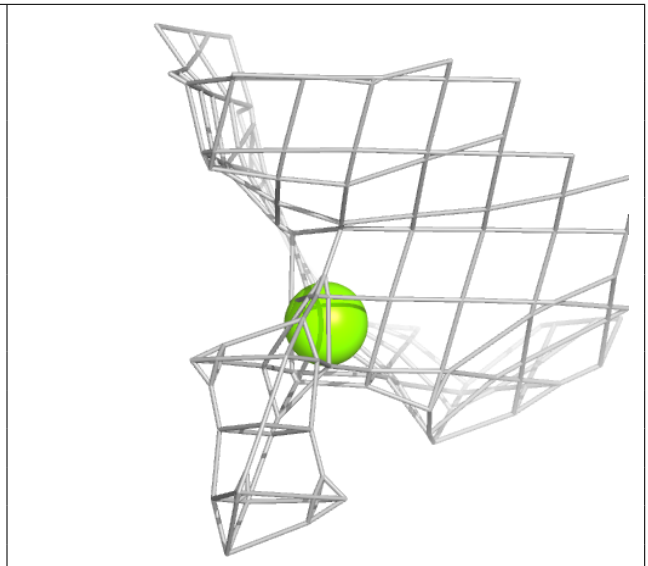
Electron density around MG I 603:

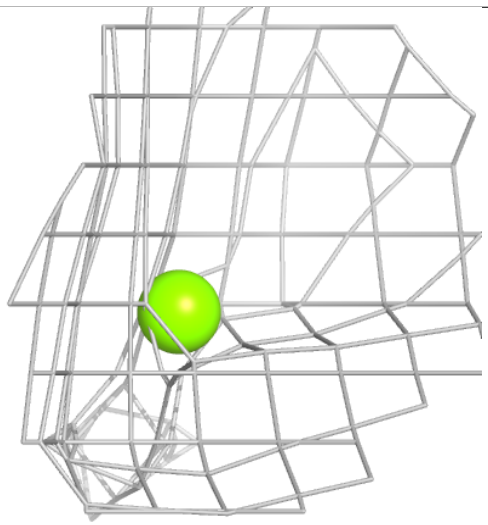
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

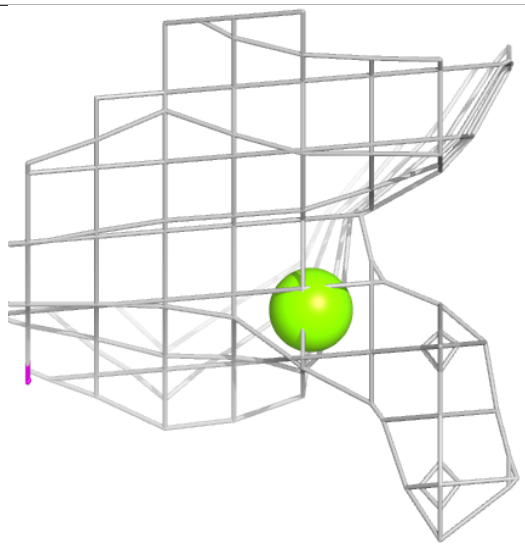


Electron density around MG C 603:

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

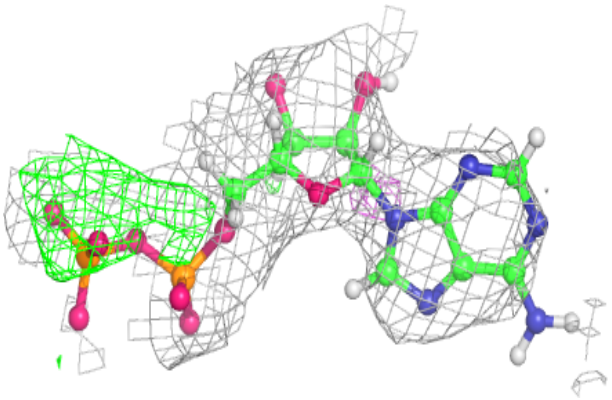


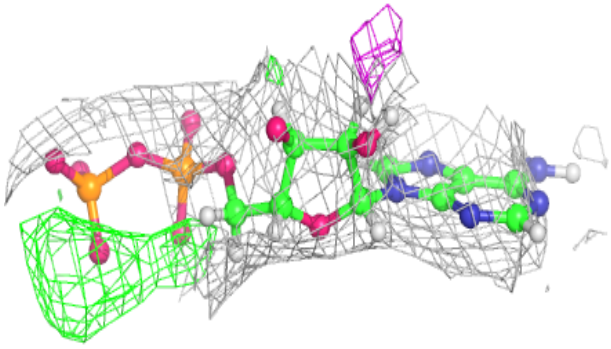


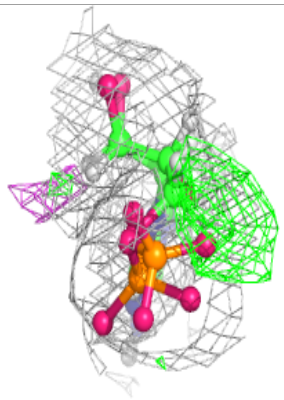


Electron density around ADP L 601:

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

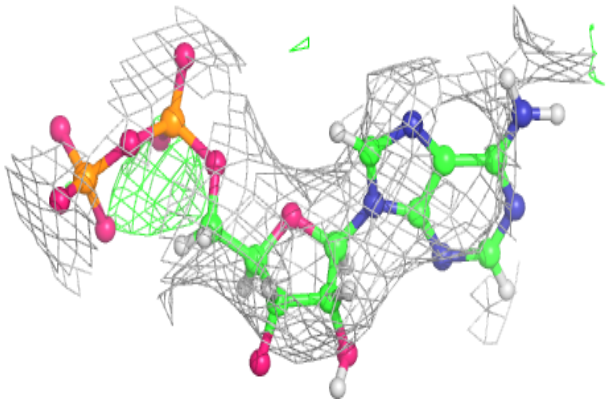


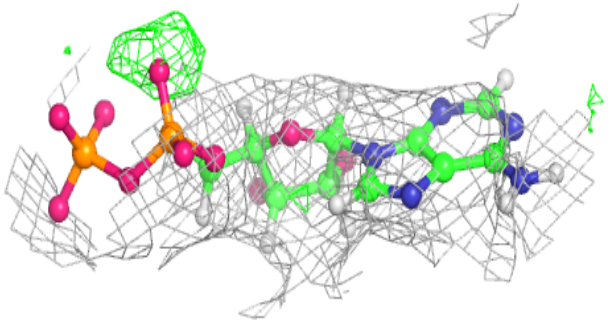


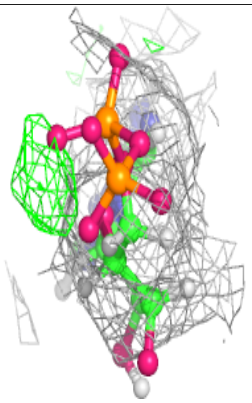


Electron density around ADP J 601:

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

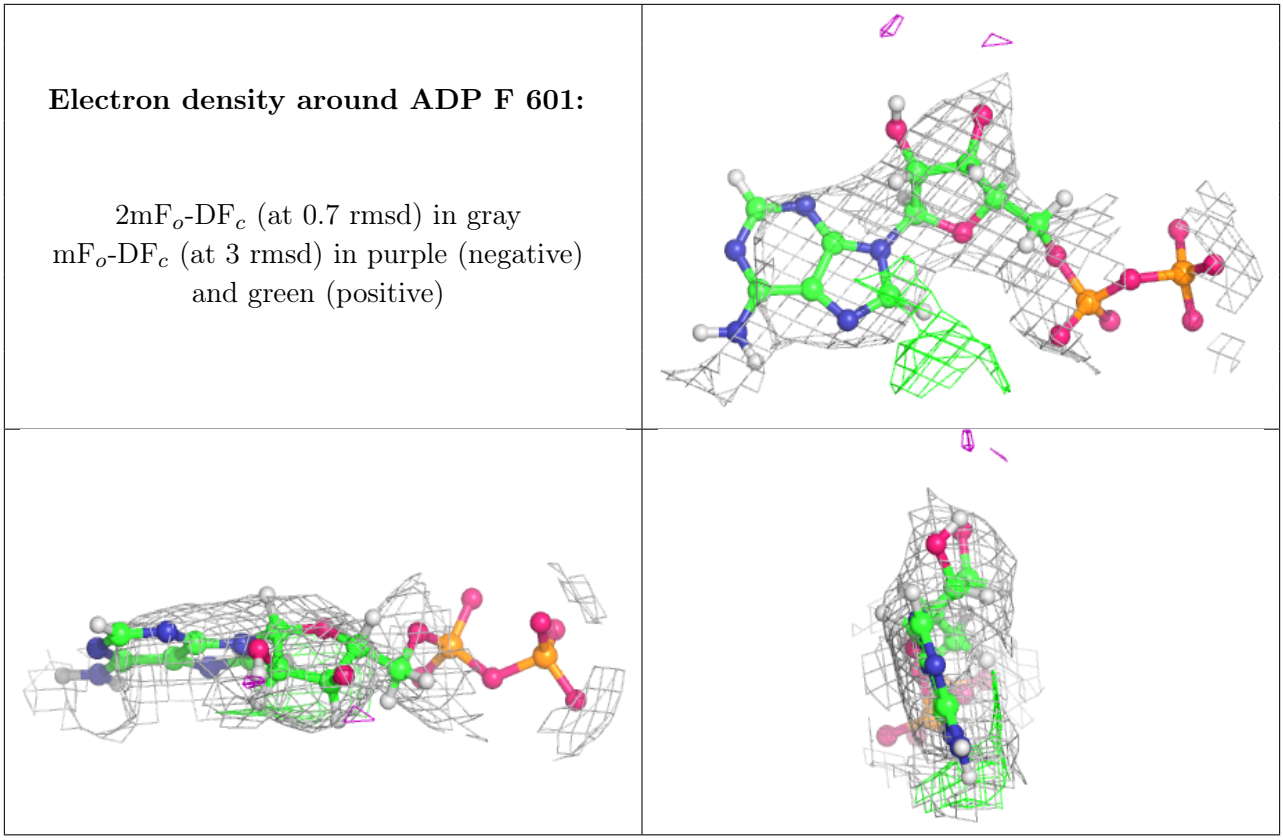






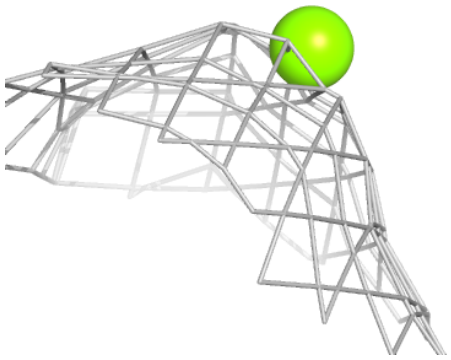
Electron density around ADP F 601:

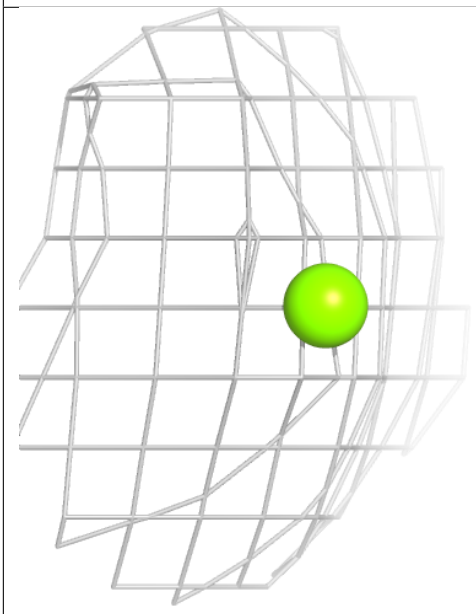
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

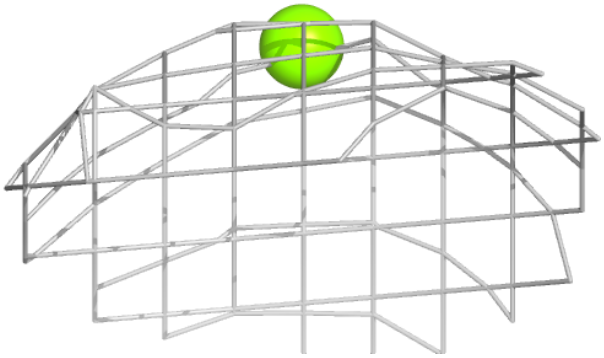


Electron density around MG J 603:

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

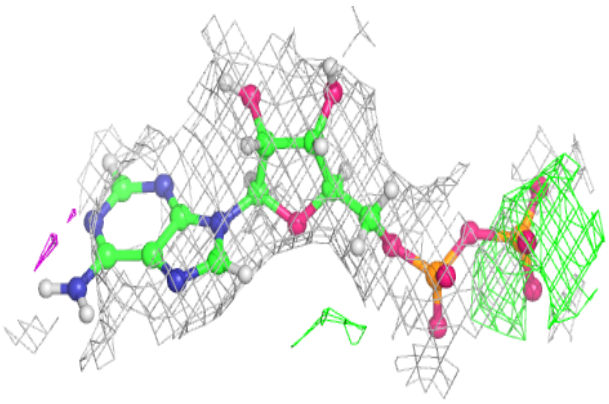


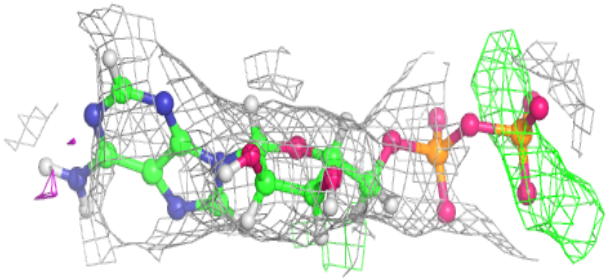


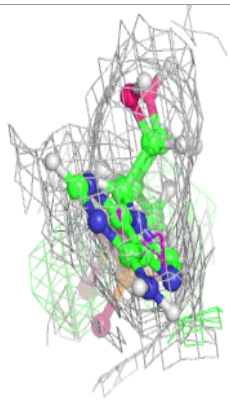


Electron density around ADP G 604:

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

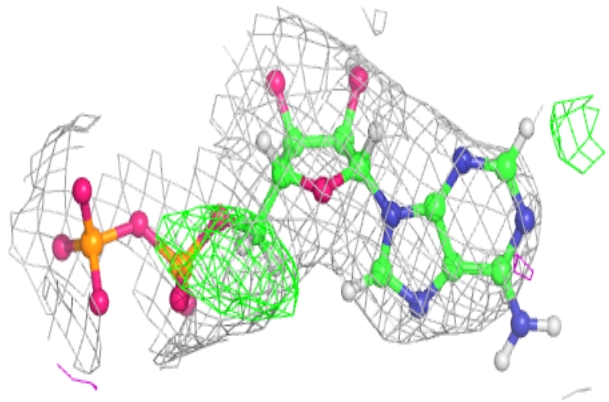


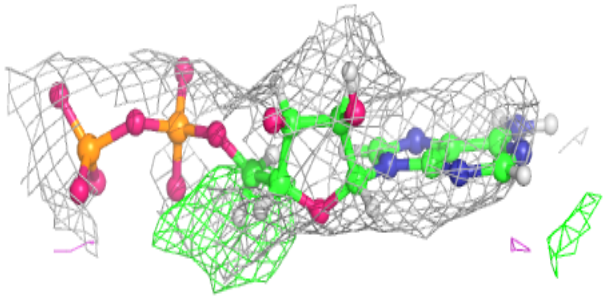


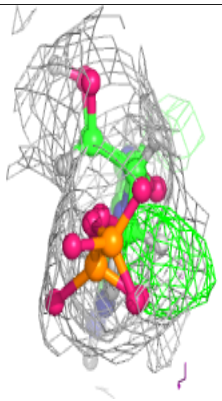


Electron density around ADP C 601:

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

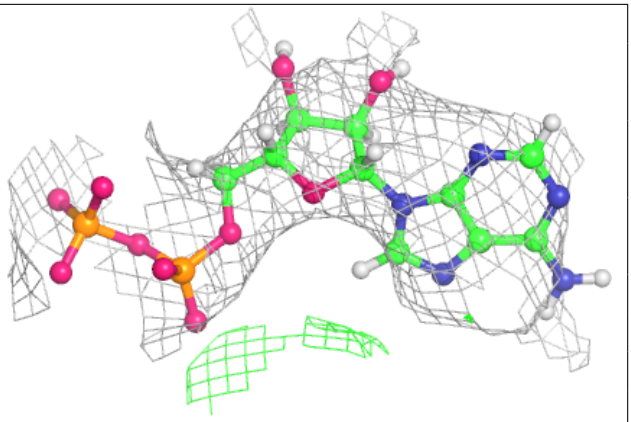


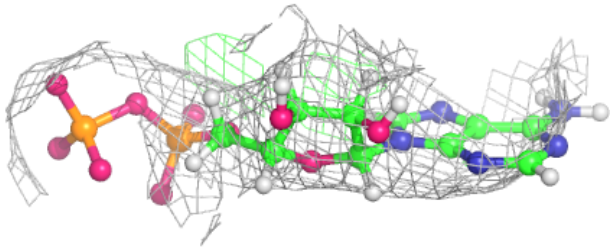


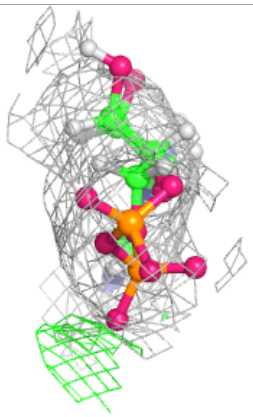


Electron density around ADP B 601:

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

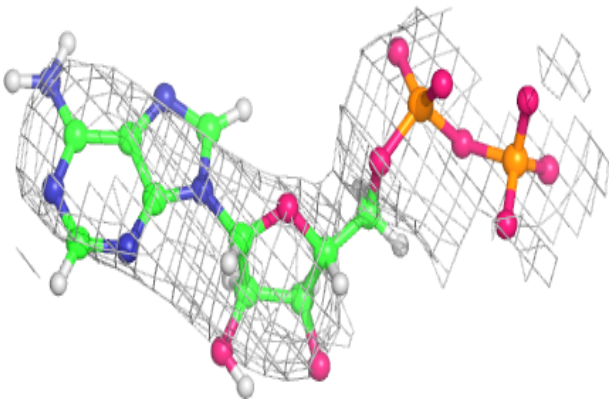


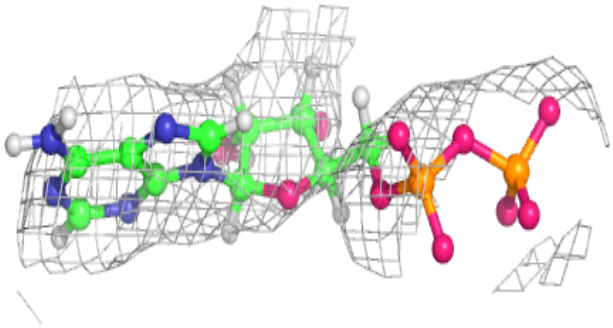


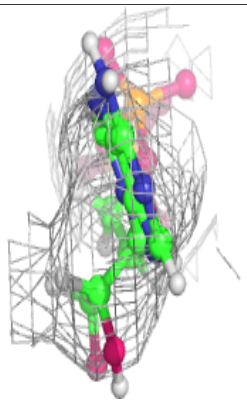


Electron density around ADP G 601:

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

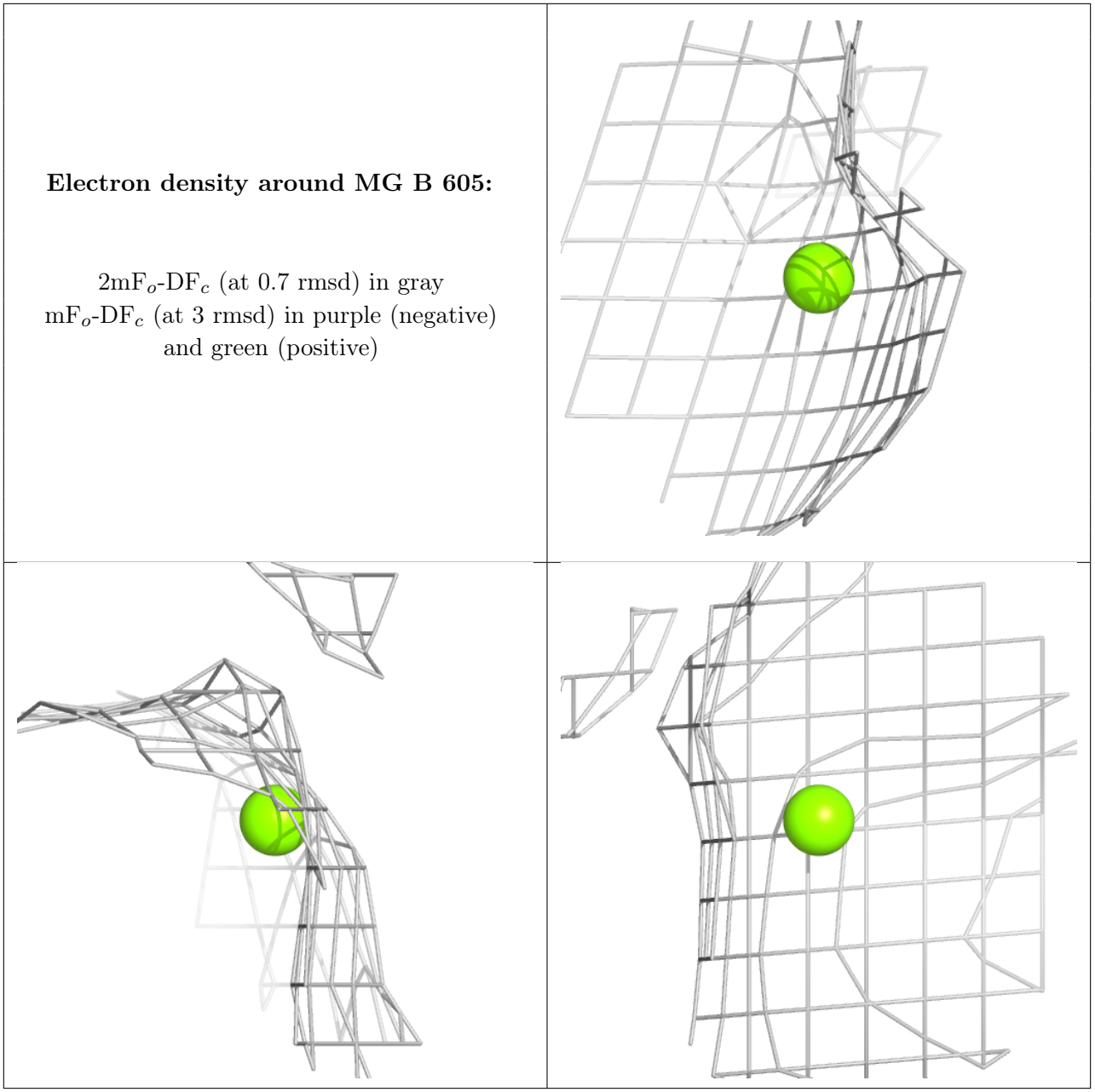






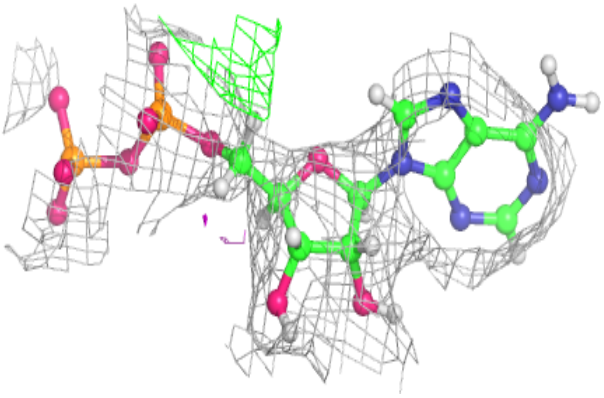
Electron density around MG B 605:

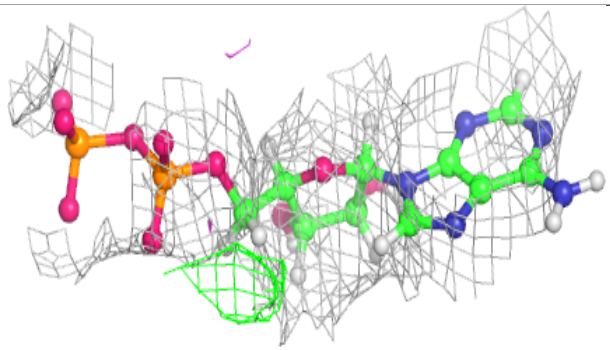
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

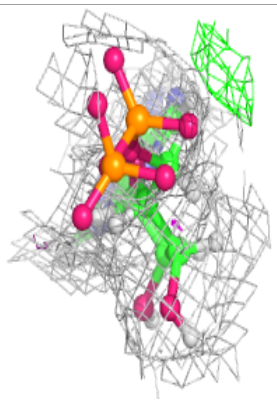


Electron density around ADP I 604:

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

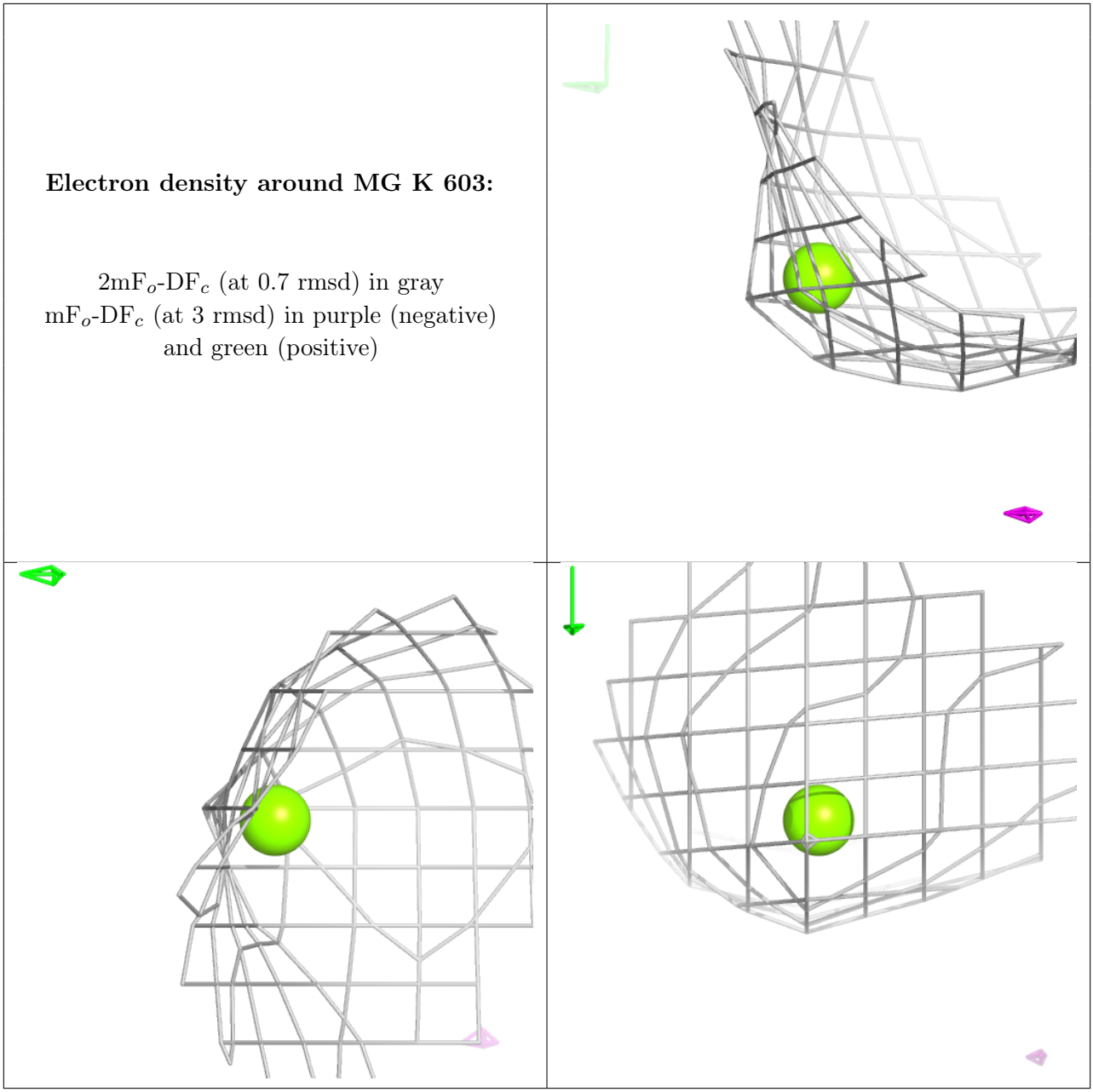






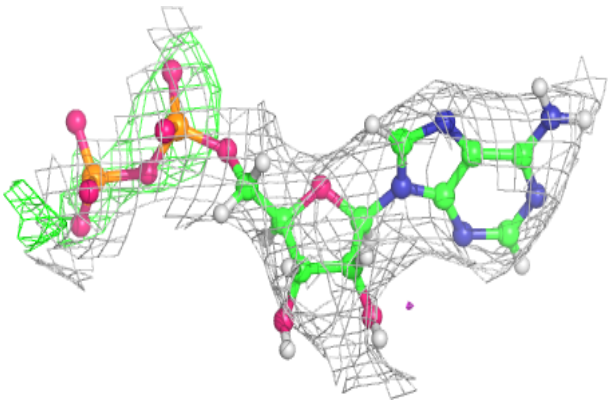
Electron density around MG K 603:

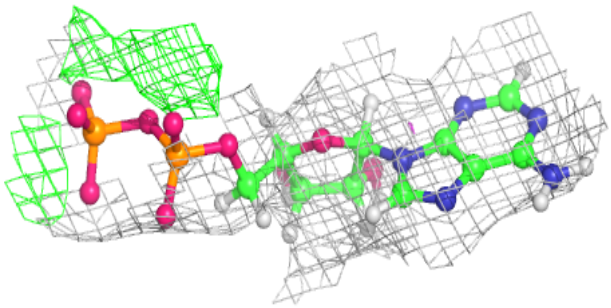
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

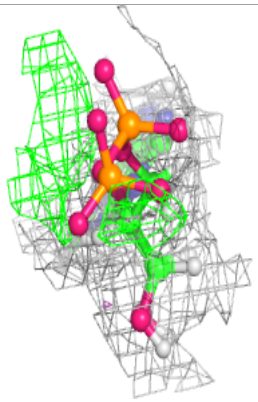


Electron density around ADP K 604:

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

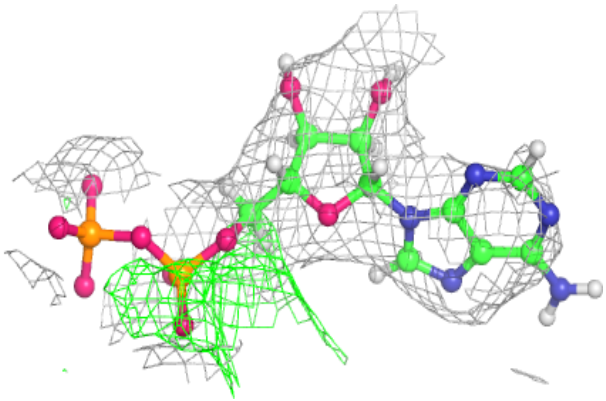


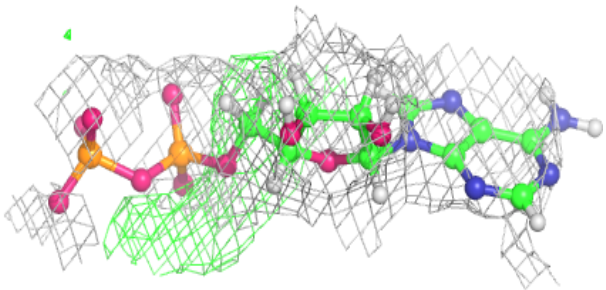


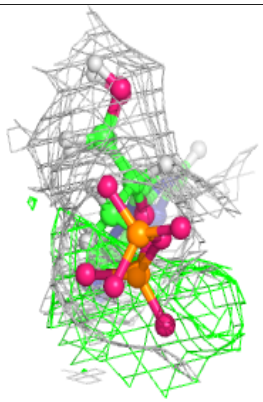


Electron density around ADP A 604:

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

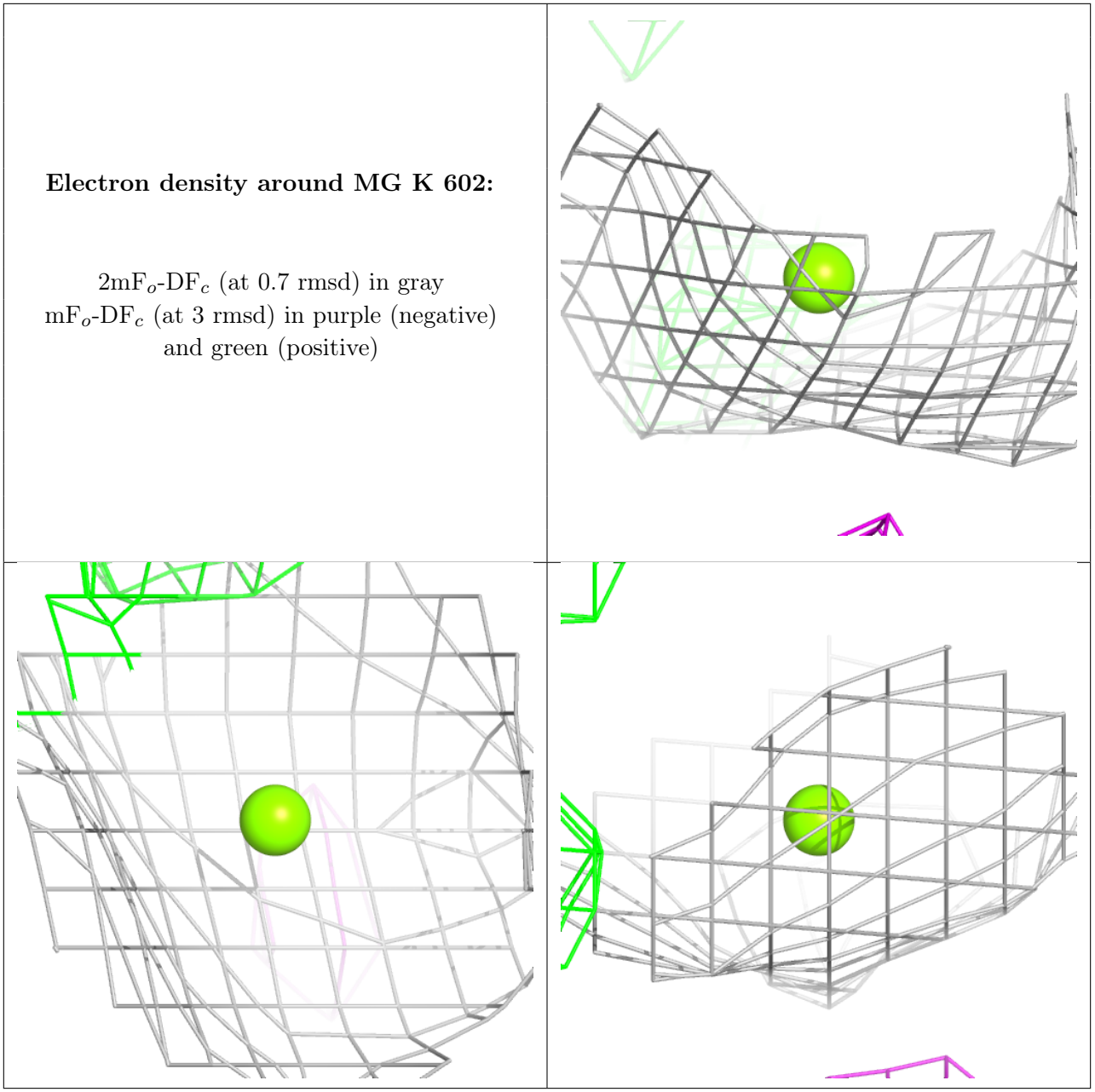






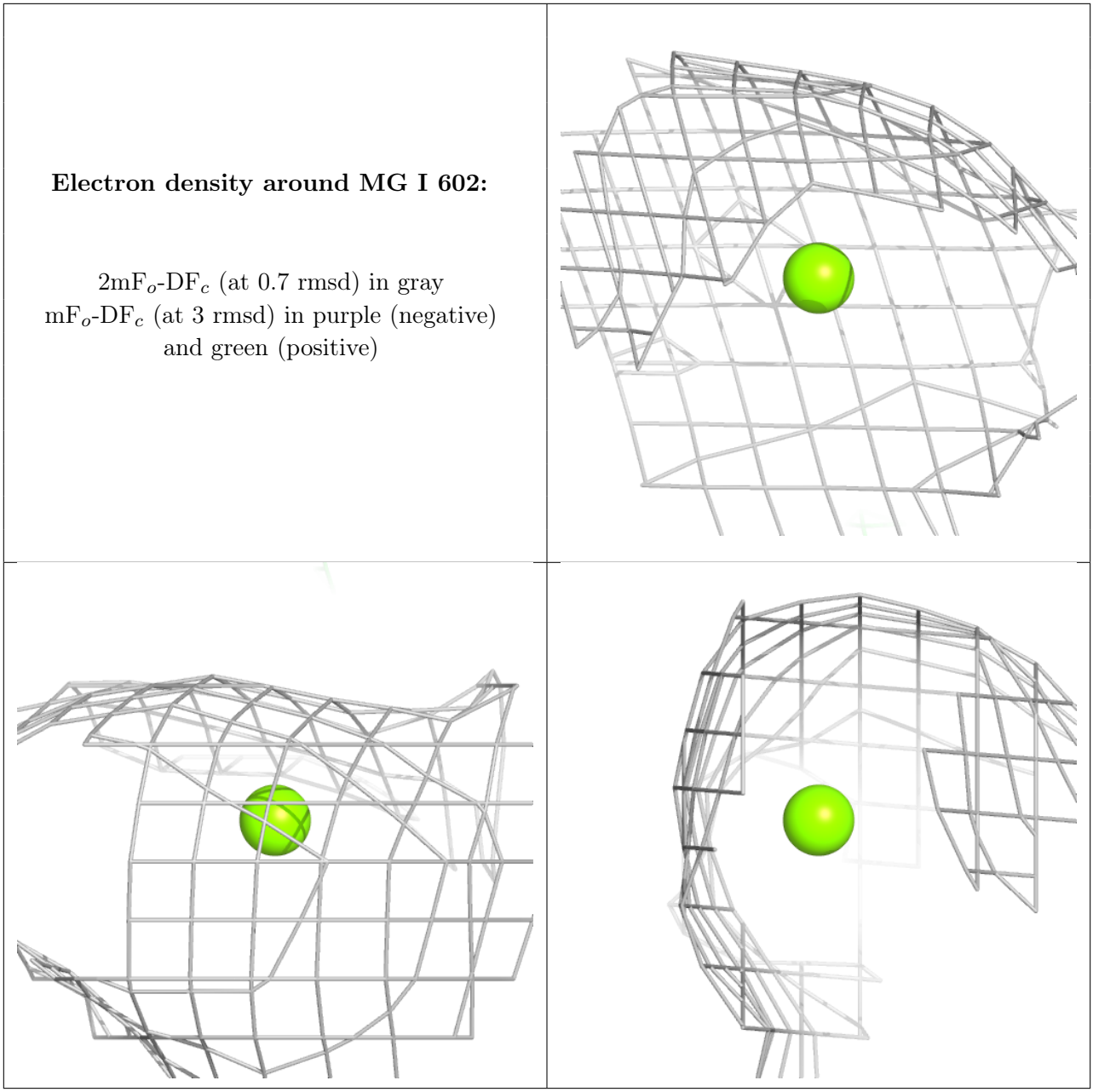
Electron density around MG K 602:

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



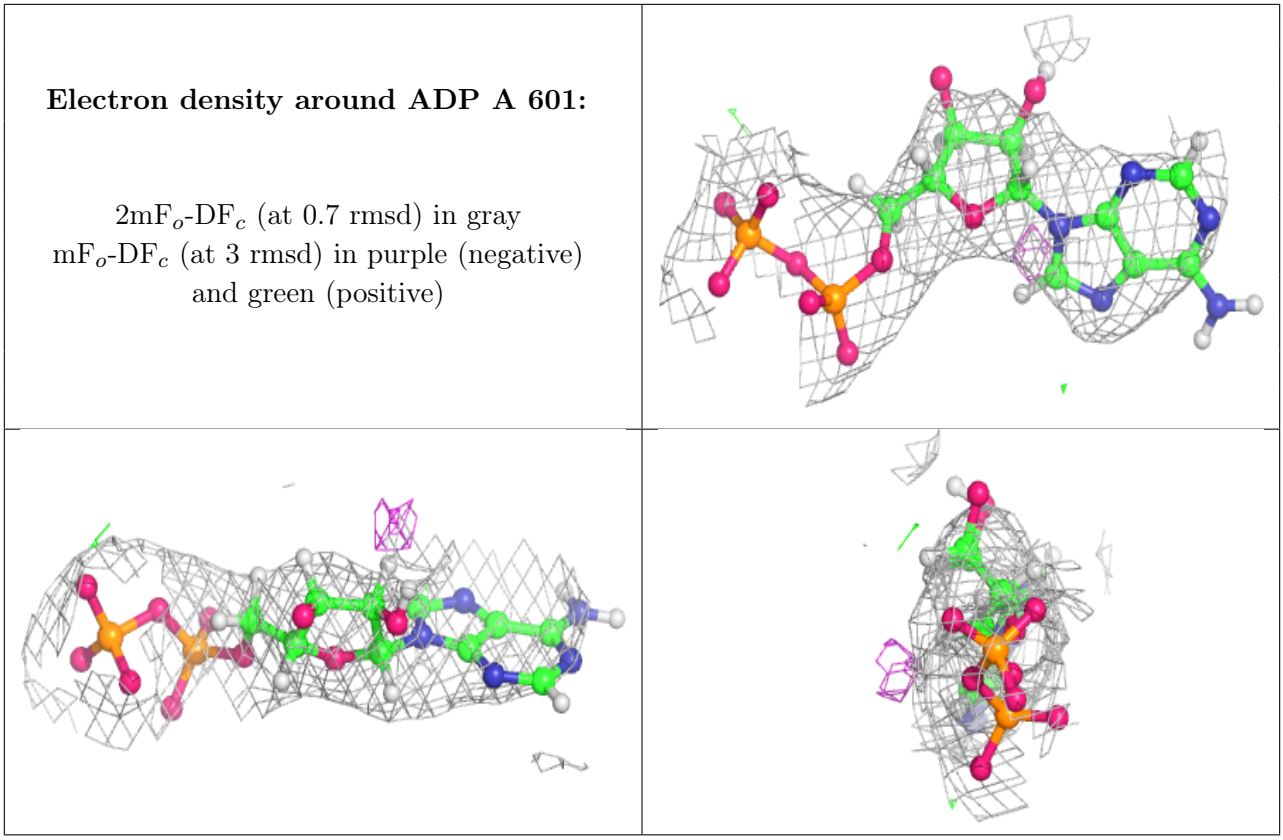
Electron density around MG I 602:

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



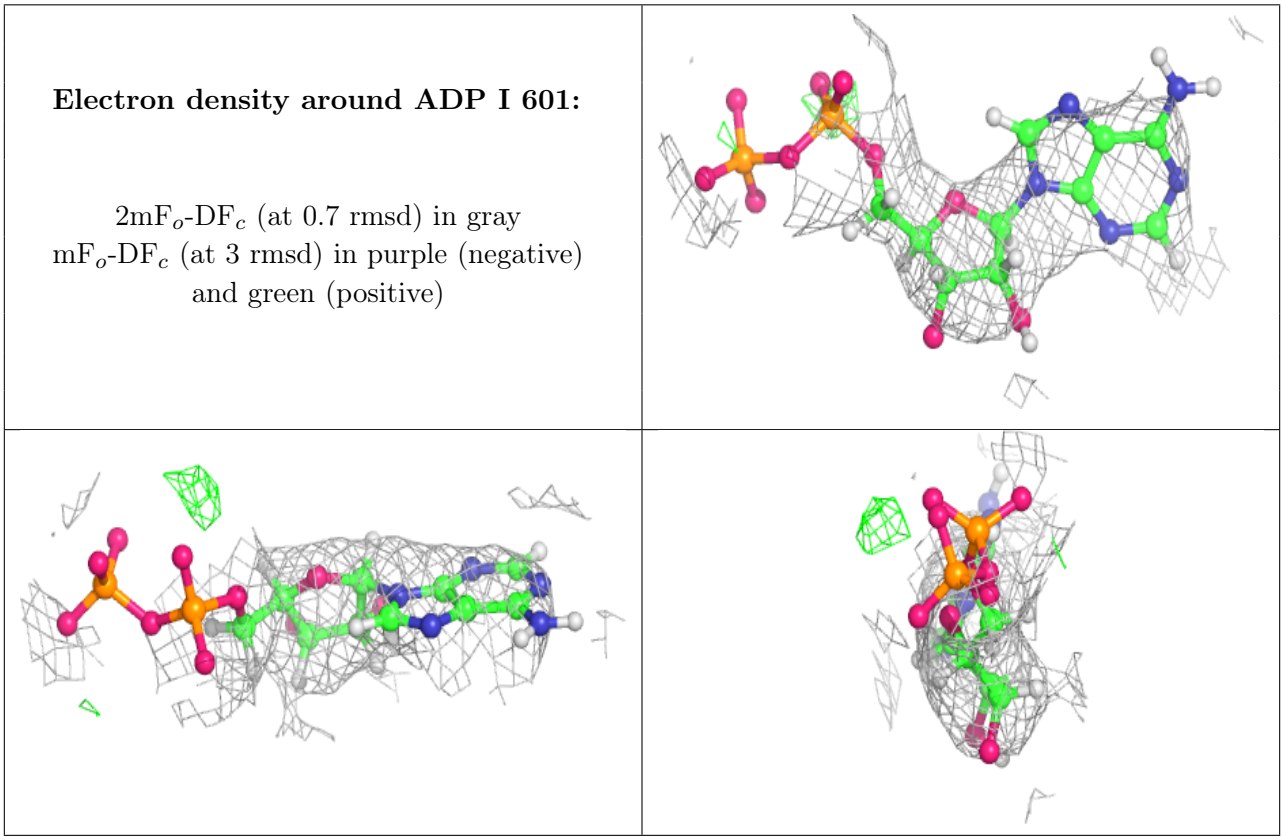
Electron density around ADP A 601:

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



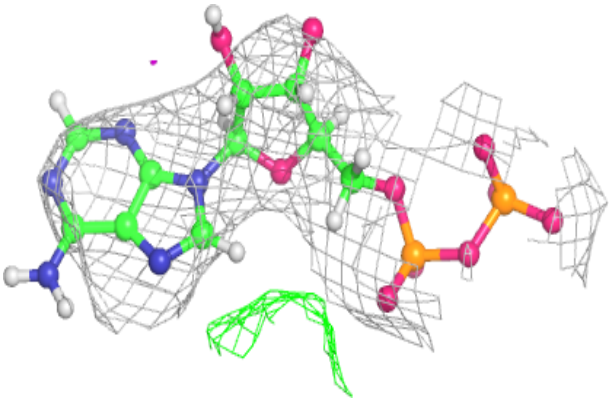
Electron density around ADP I 601:

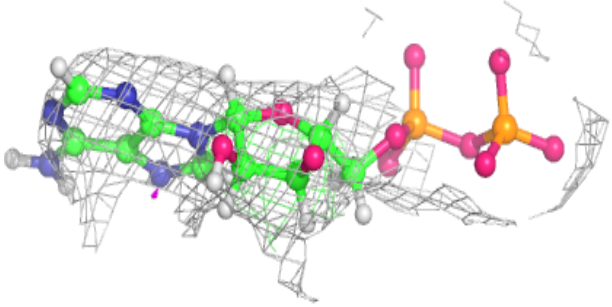
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

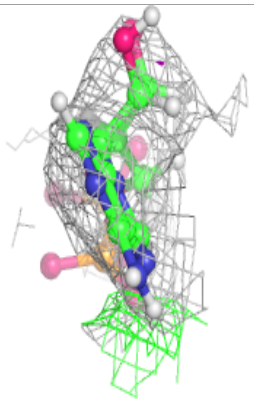


Electron density around ADP K 601:

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

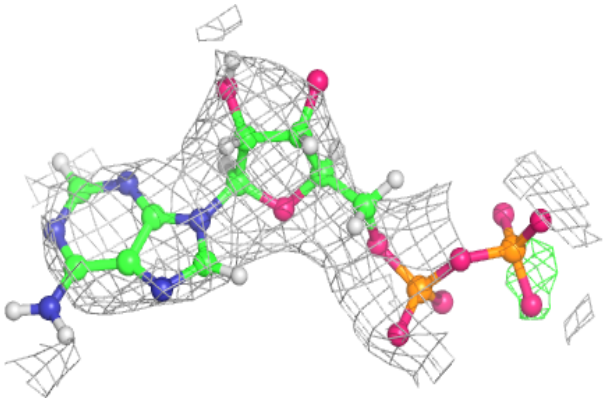


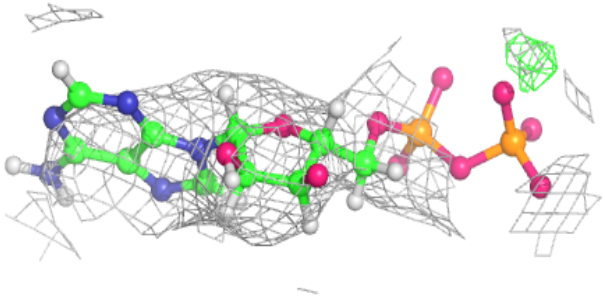


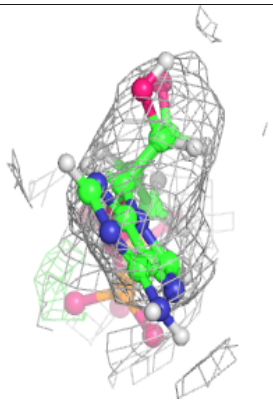


Electron density around ADP D 601:

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

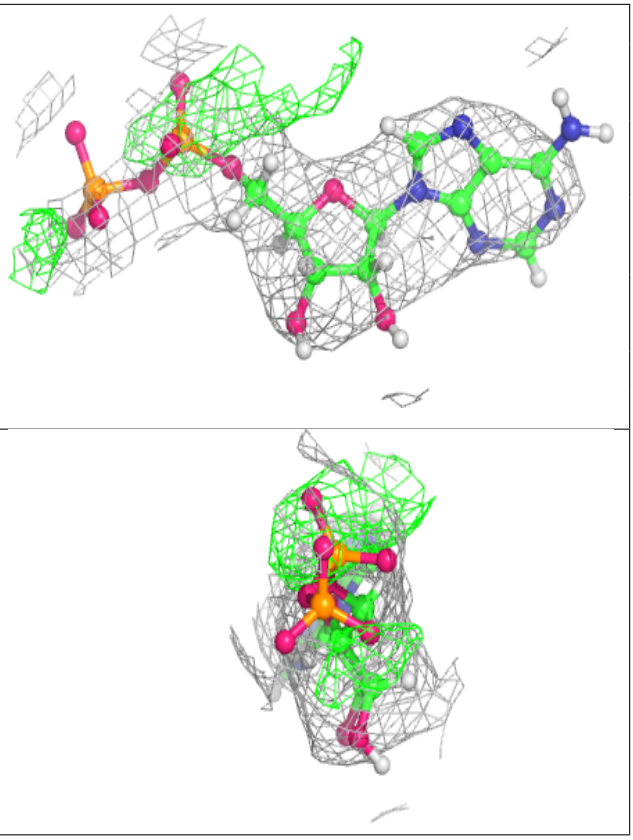


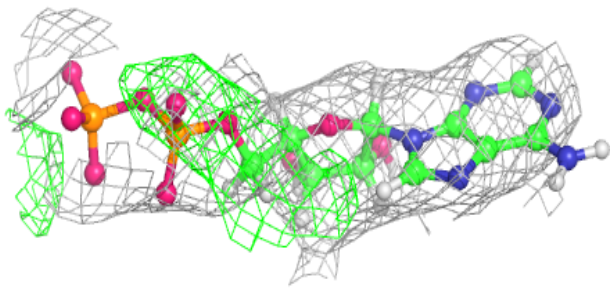




Electron density around ADP H 603:

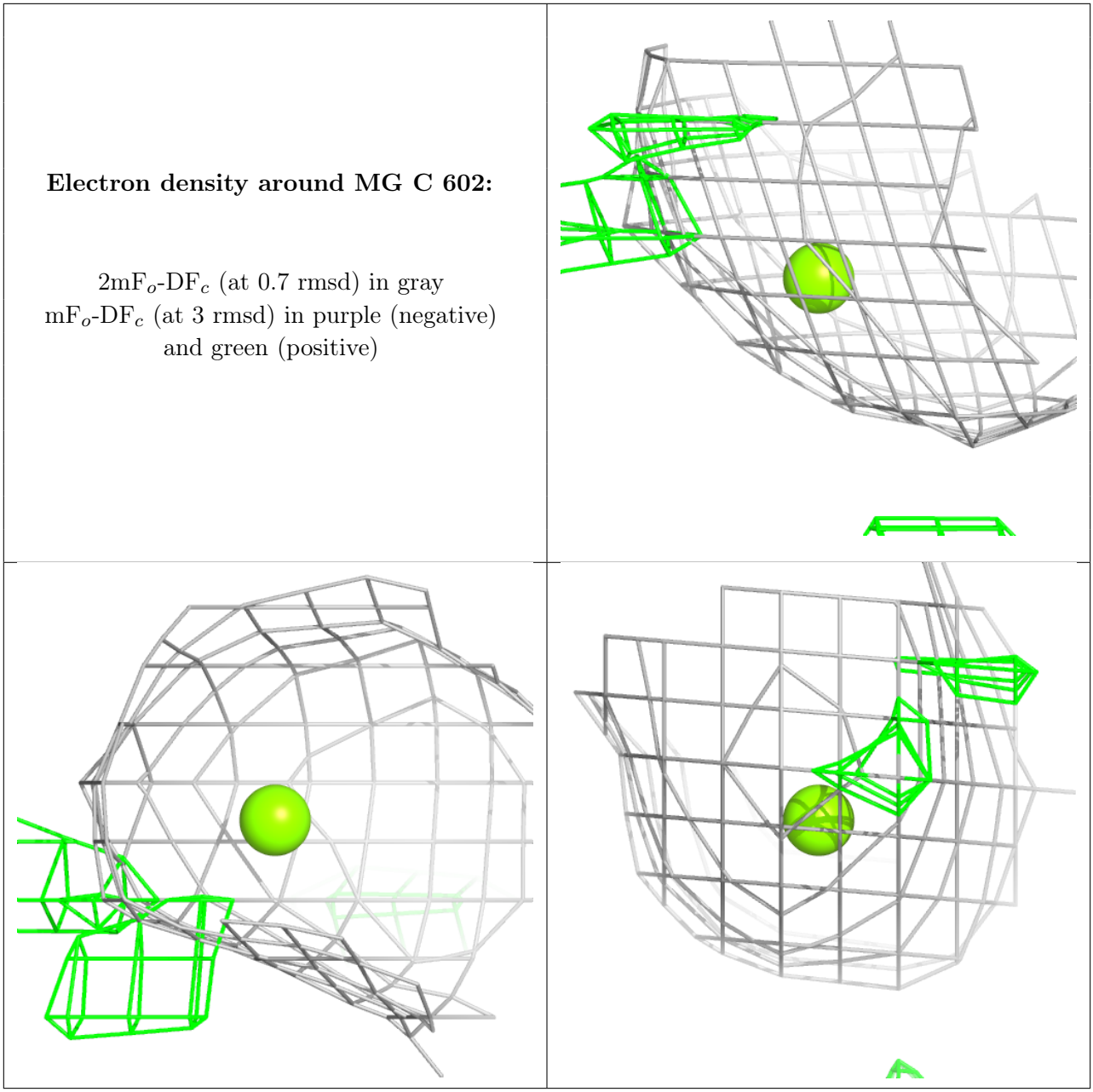
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





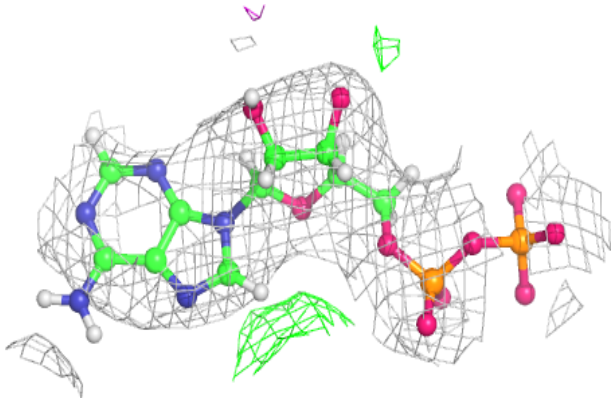
Electron density around MG C 602:

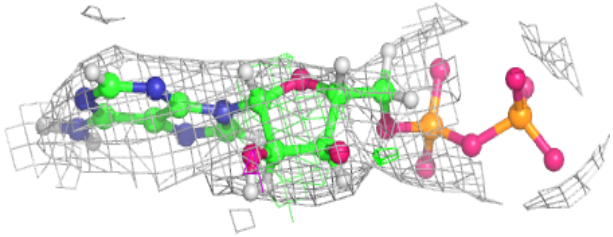
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

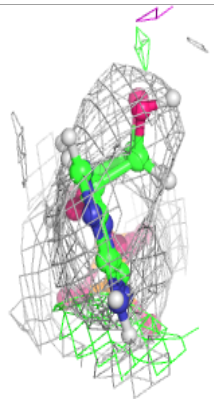


Electron density around ADP E 601:

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

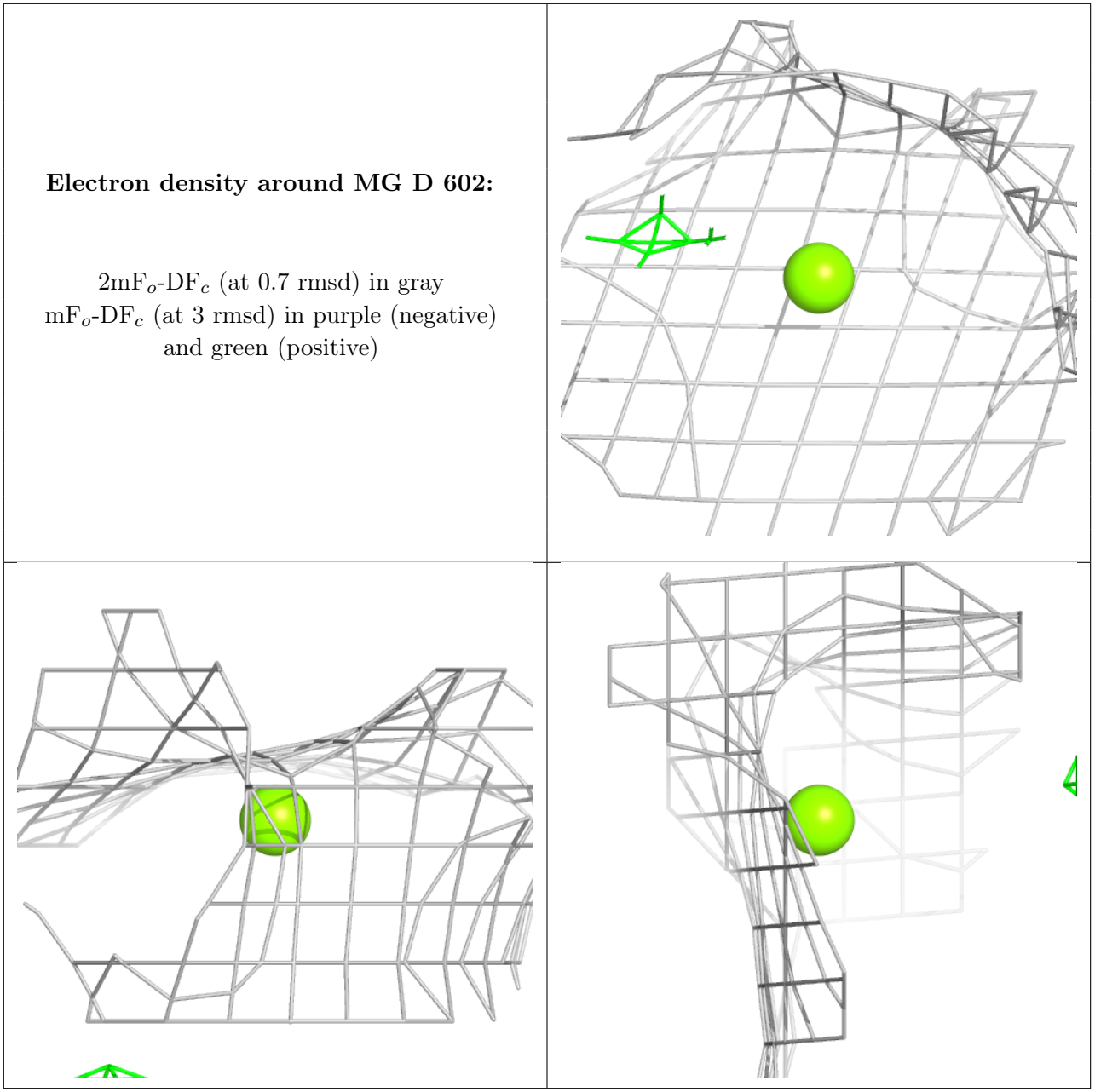






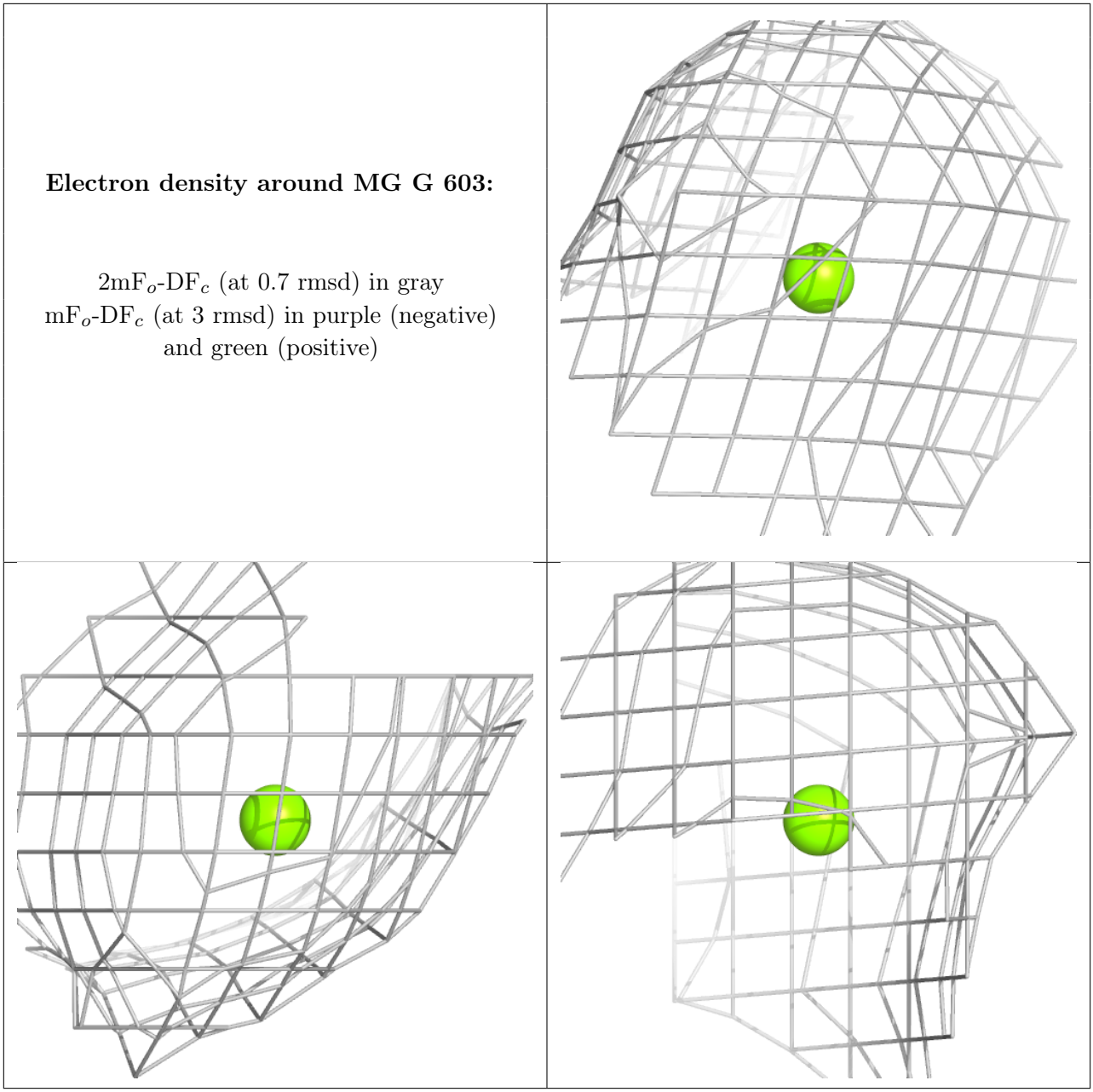
Electron density around MG D 602:

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



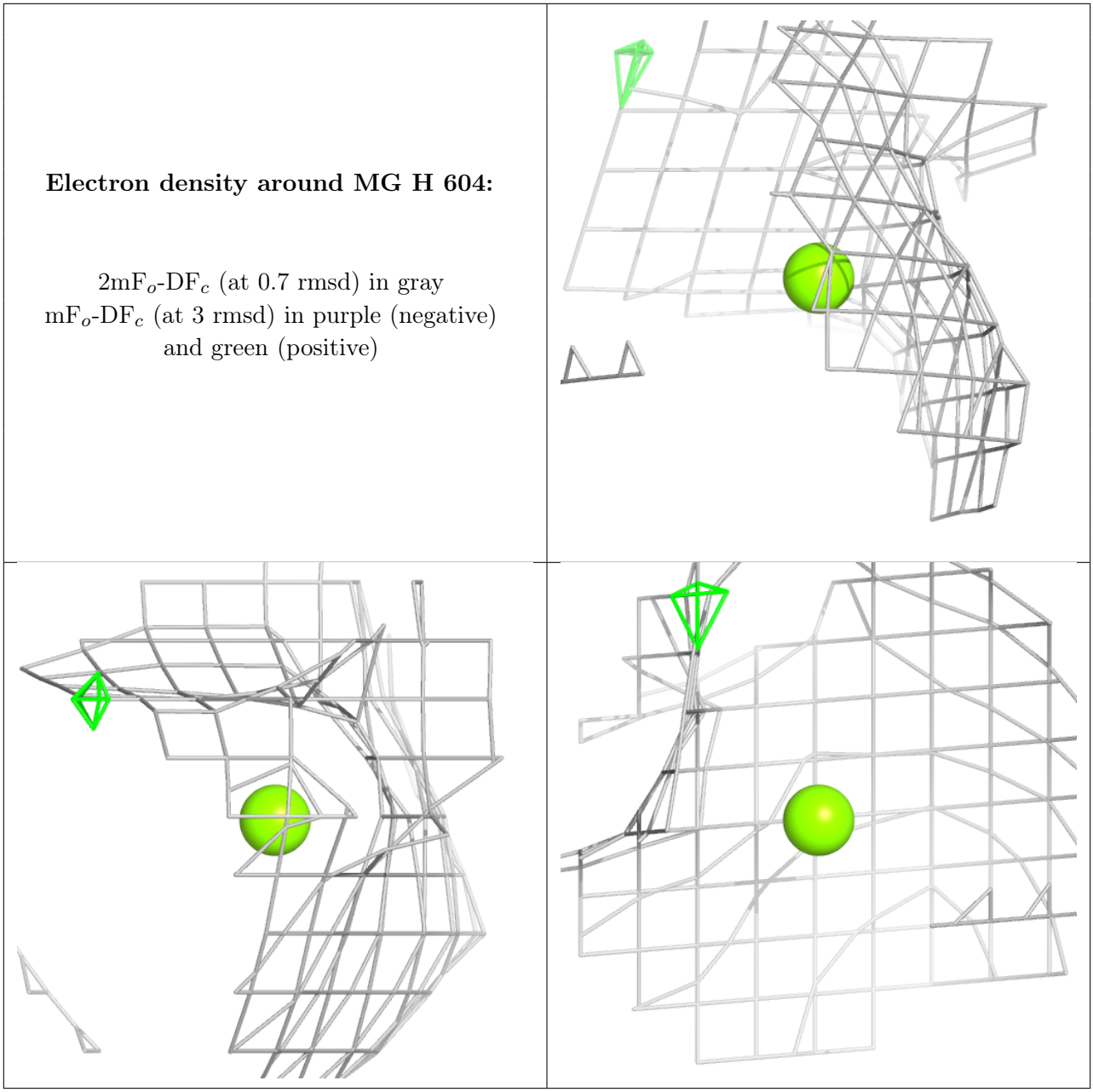
Electron density around MG G 603:

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



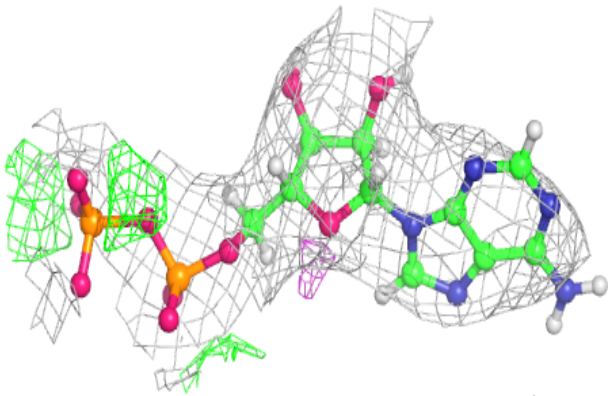
Electron density around MG H 604:

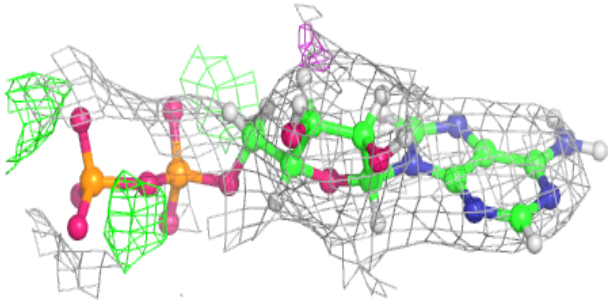
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

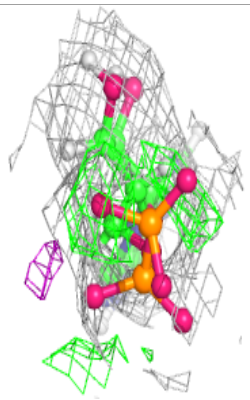


Electron density around ADP E 604:

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

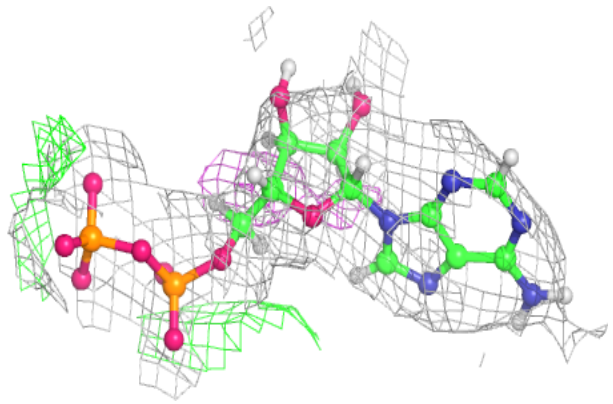


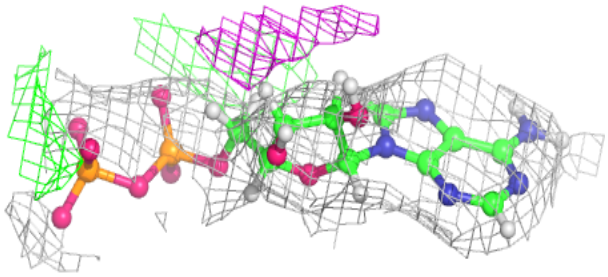


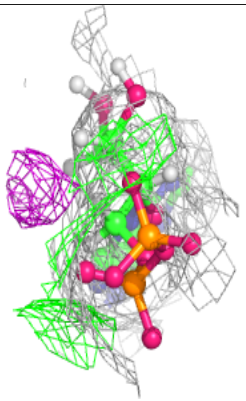


Electron density around ADP B 604:

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

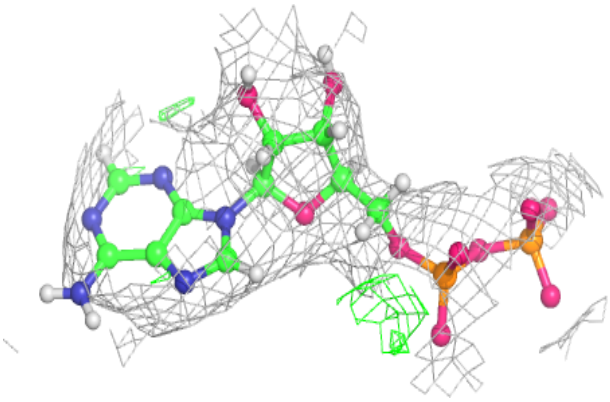


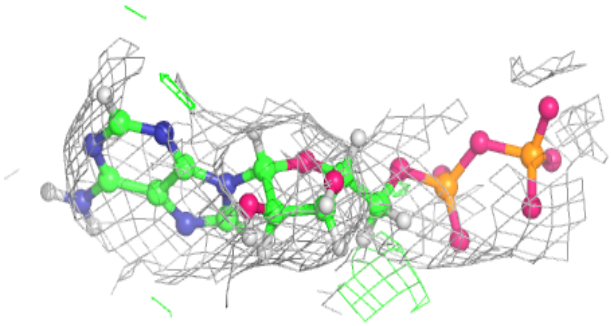


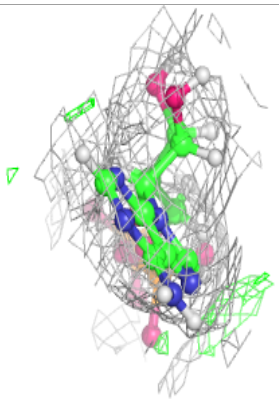


Electron density around ADP J 604:

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

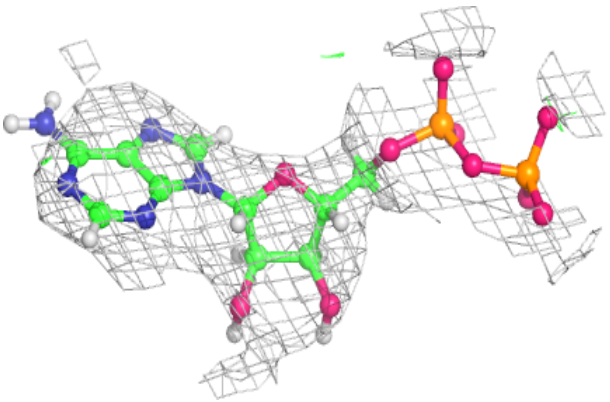


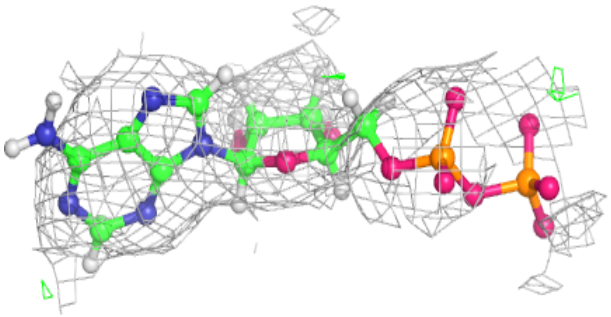


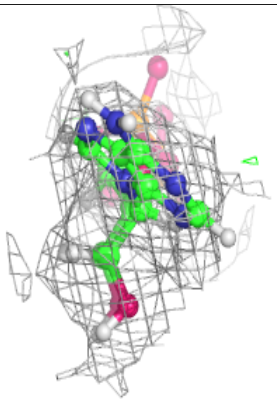


Electron density around ADP F 603:

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

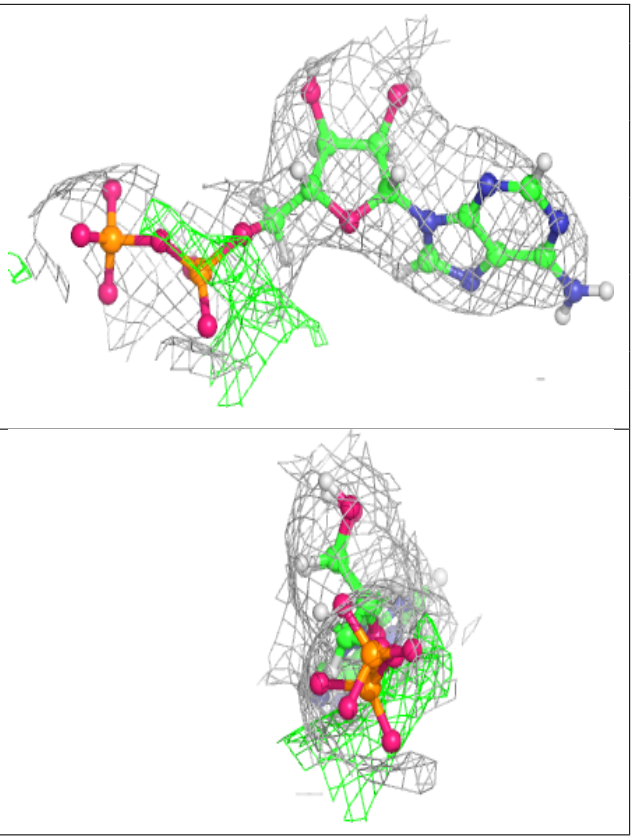


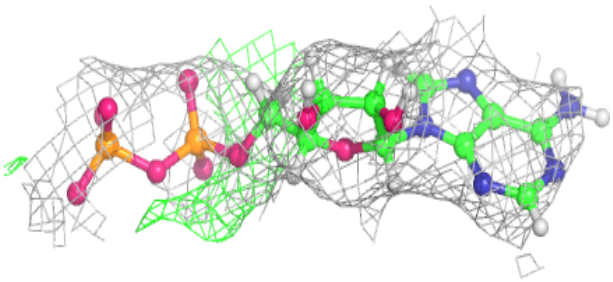




Electron density around ADP C 604:

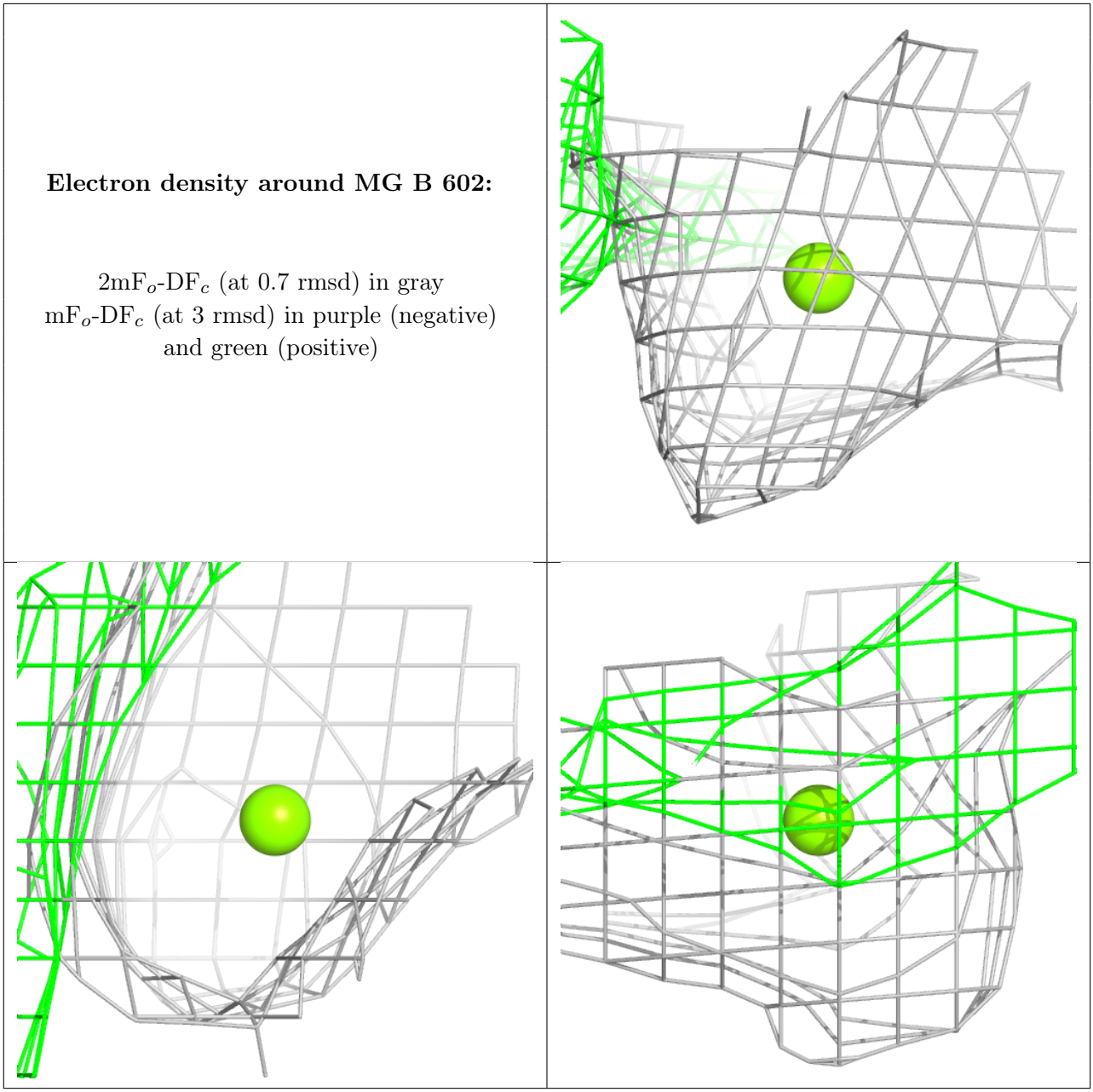
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





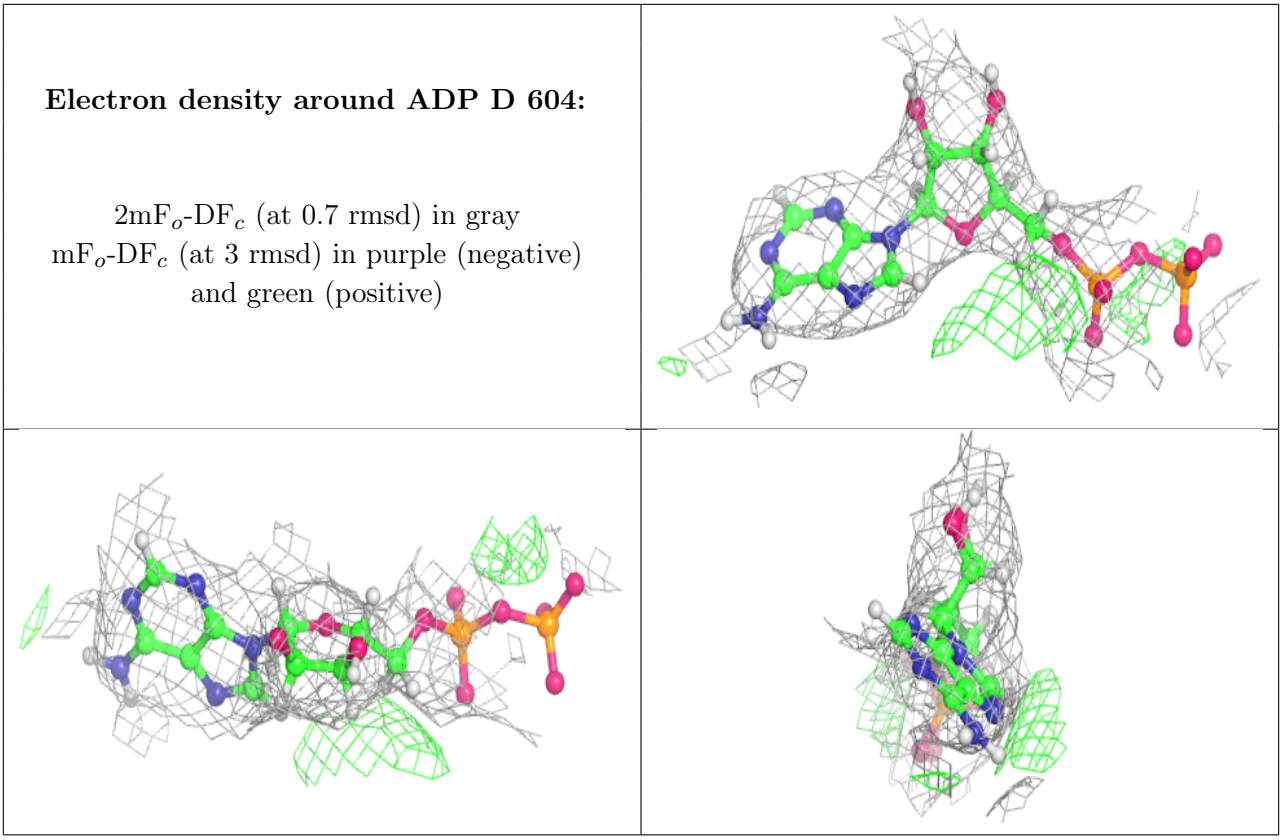
Electron density around MG B 602:

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



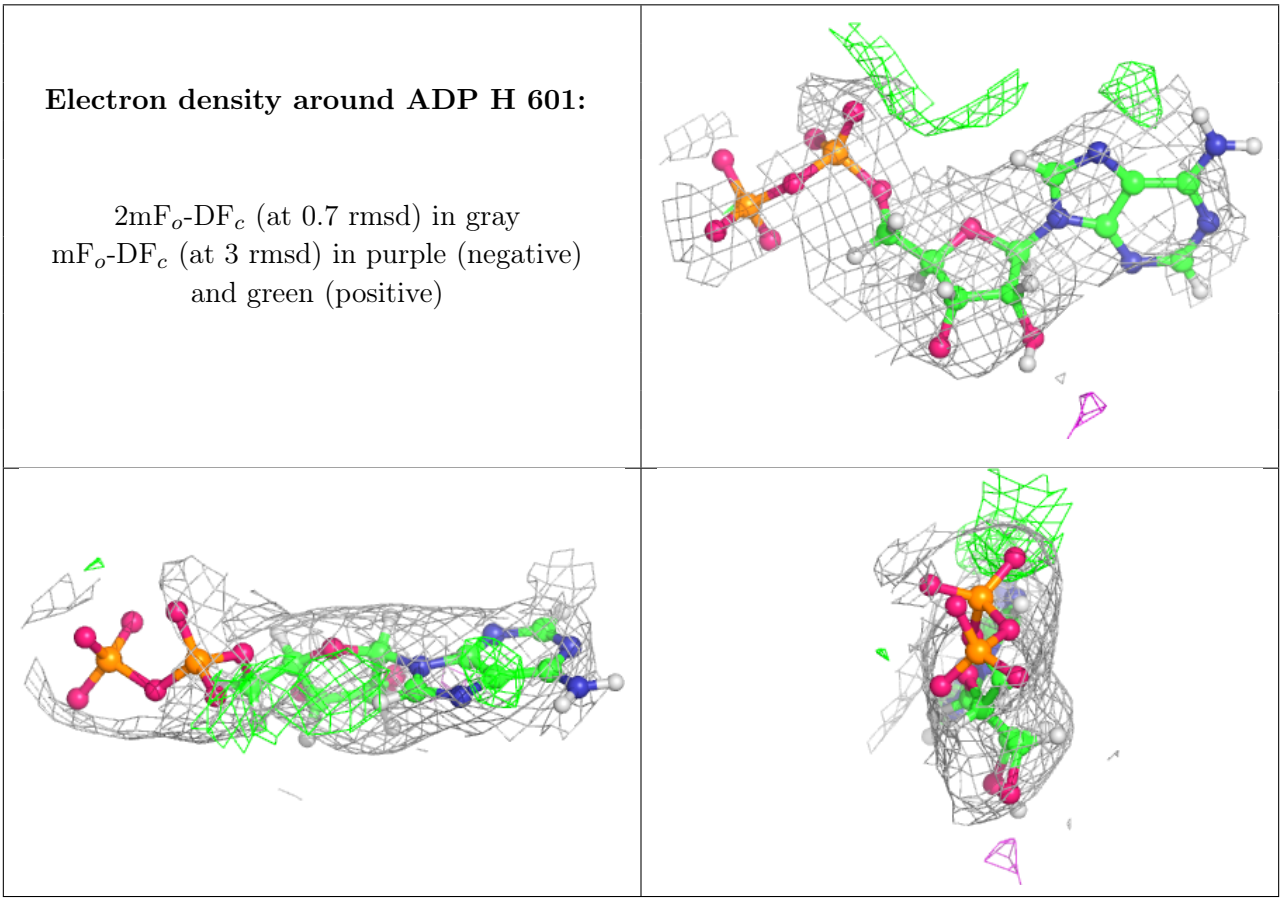
Electron density around ADP D 604:

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



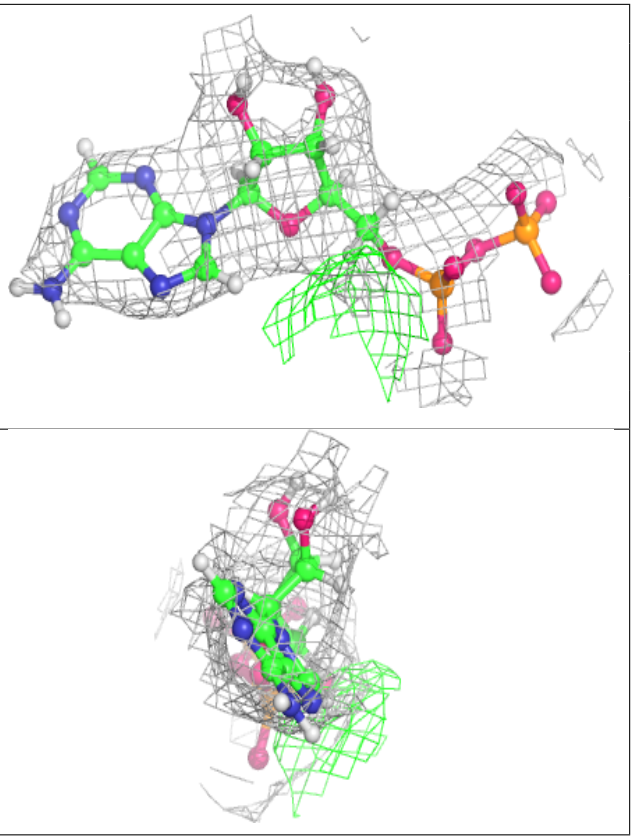
Electron density around ADP H 601:

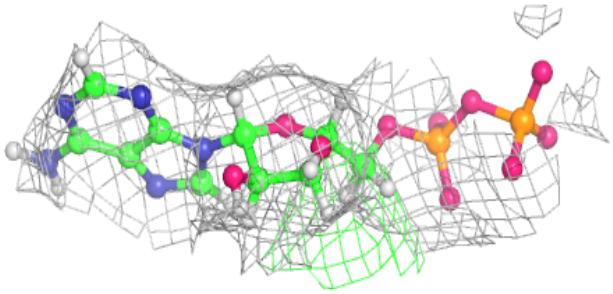
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP L 602:

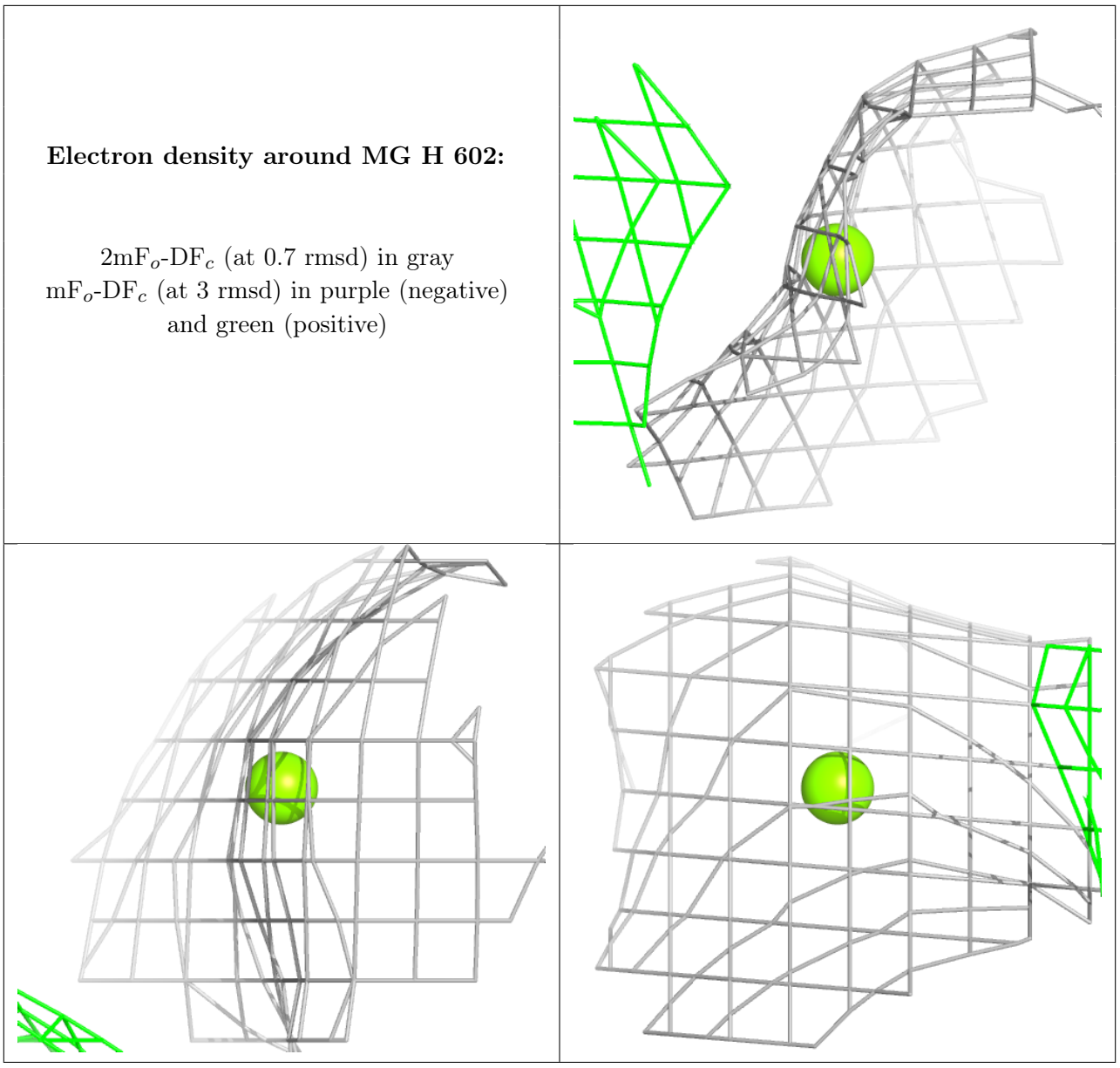
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





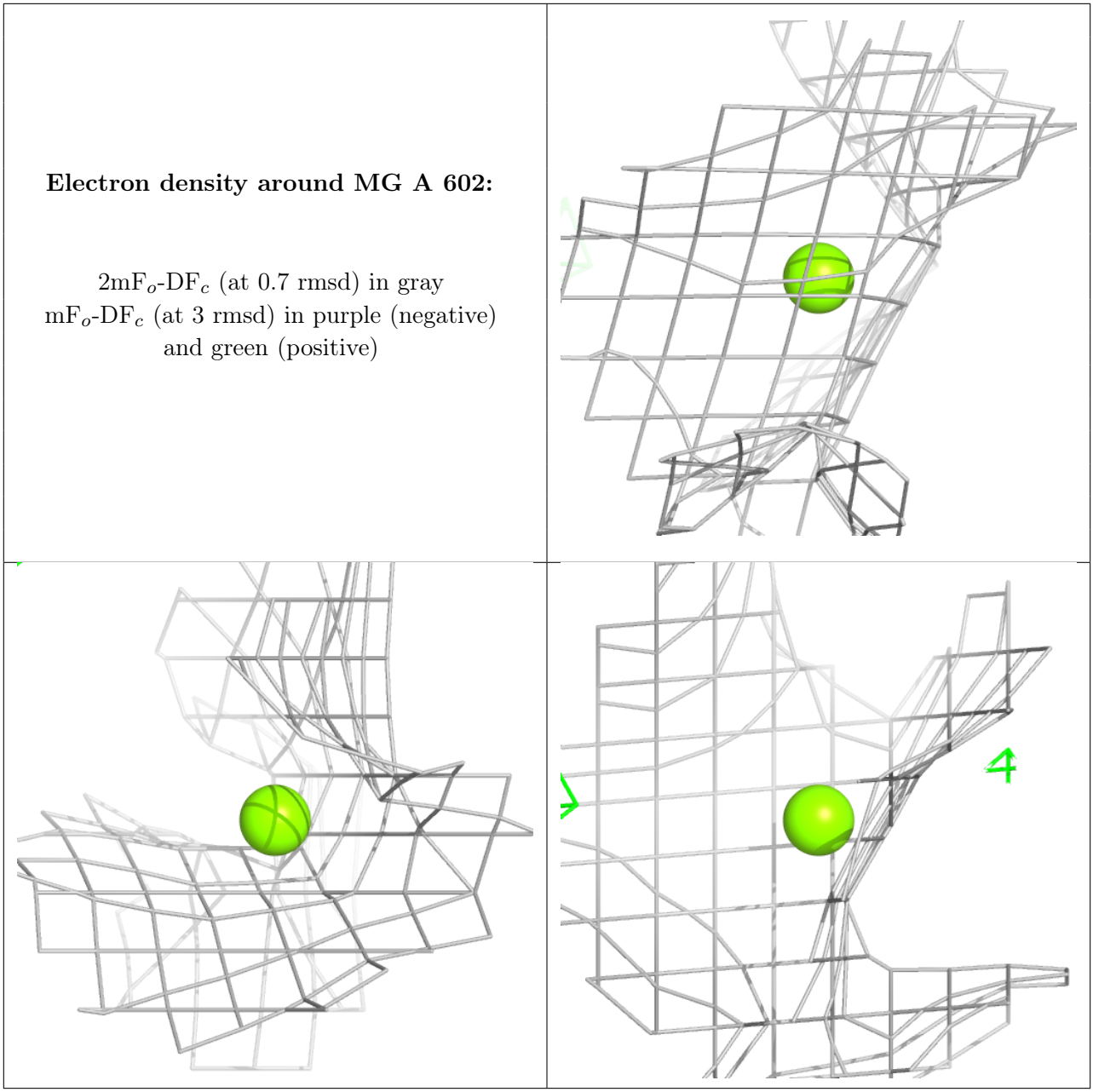
Electron density around MG H 602:

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



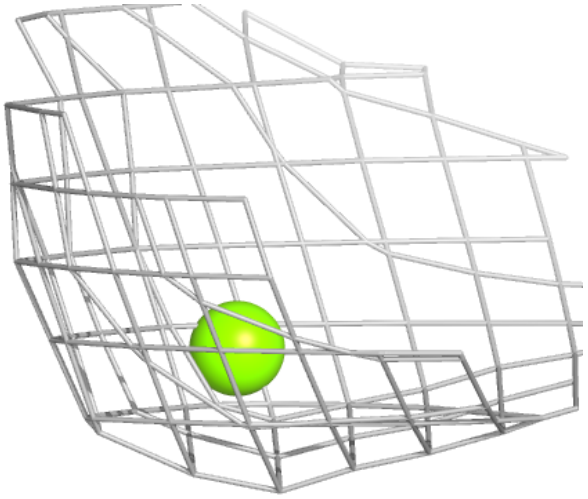
Electron density around MG A 602:

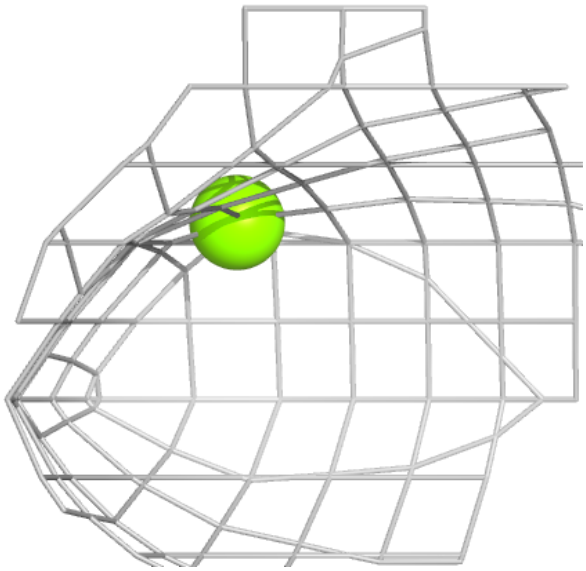
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

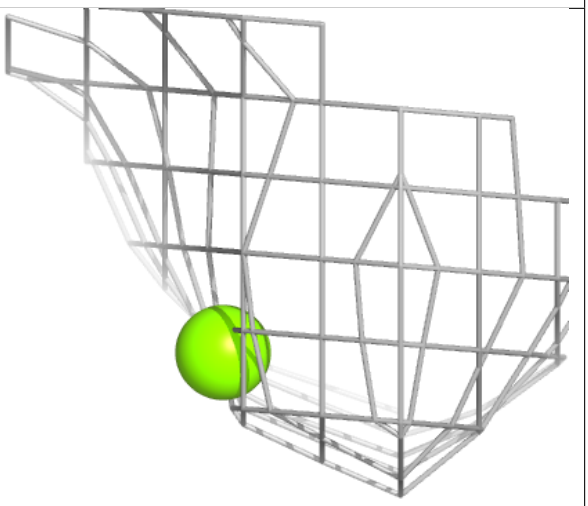


Electron density around MG E 603:

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

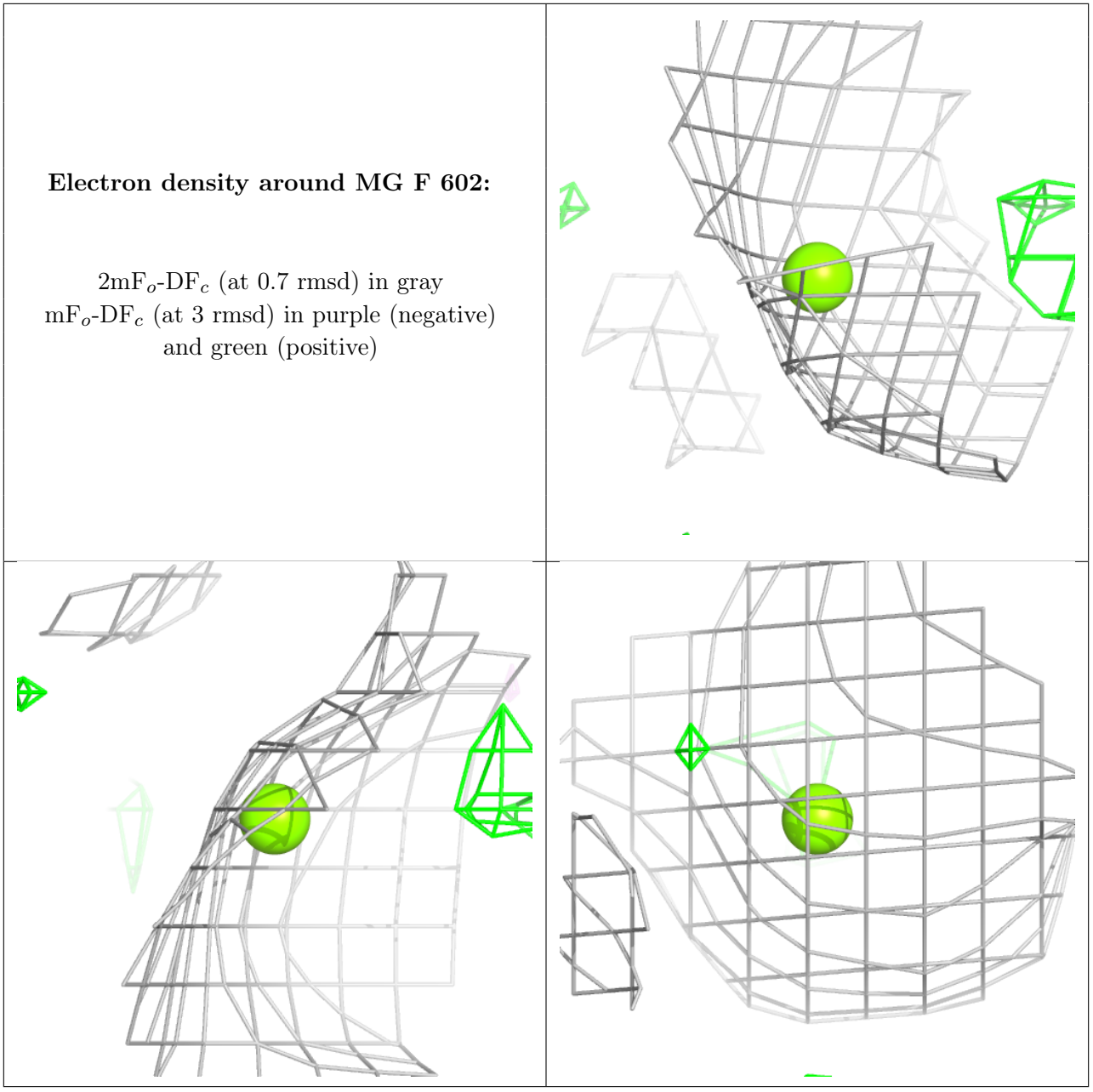






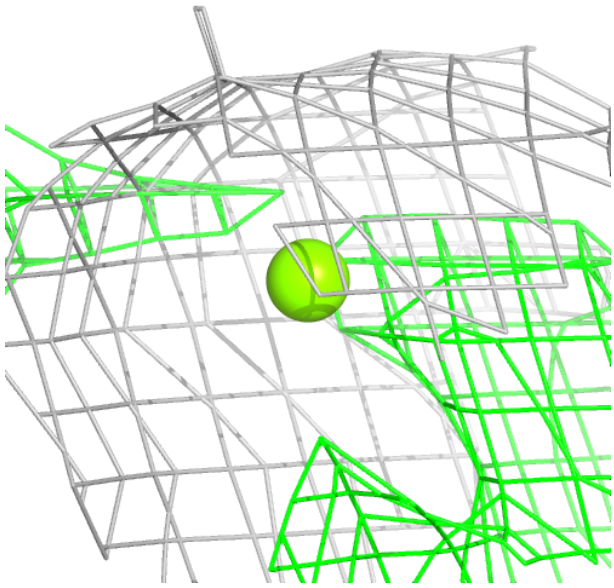
Electron density around MG F 602:

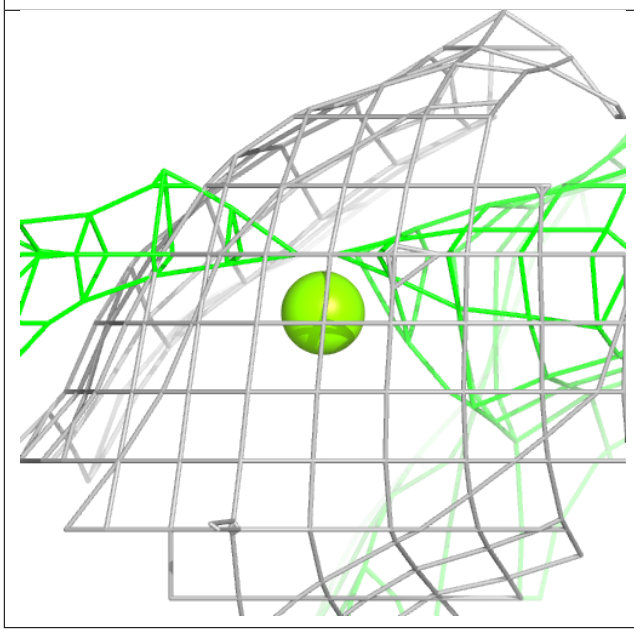
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

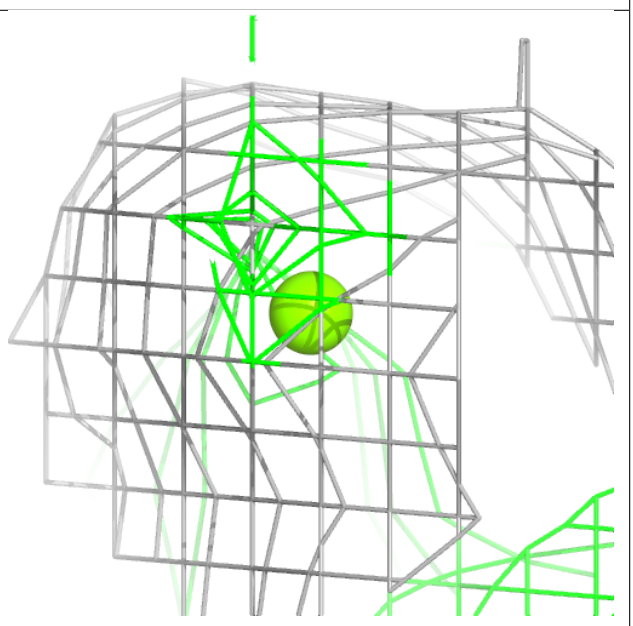


Electron density around MG G 602:

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

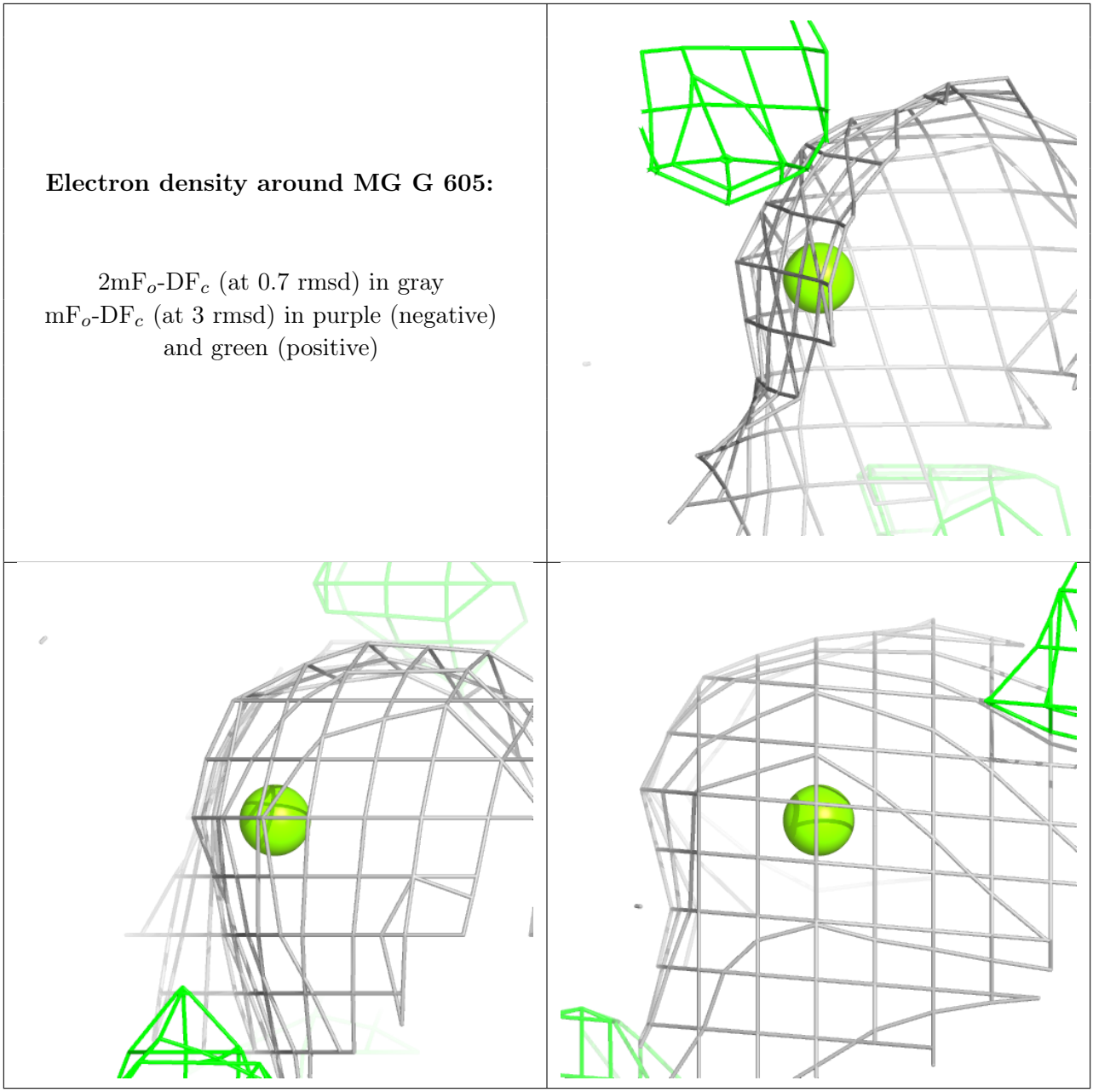






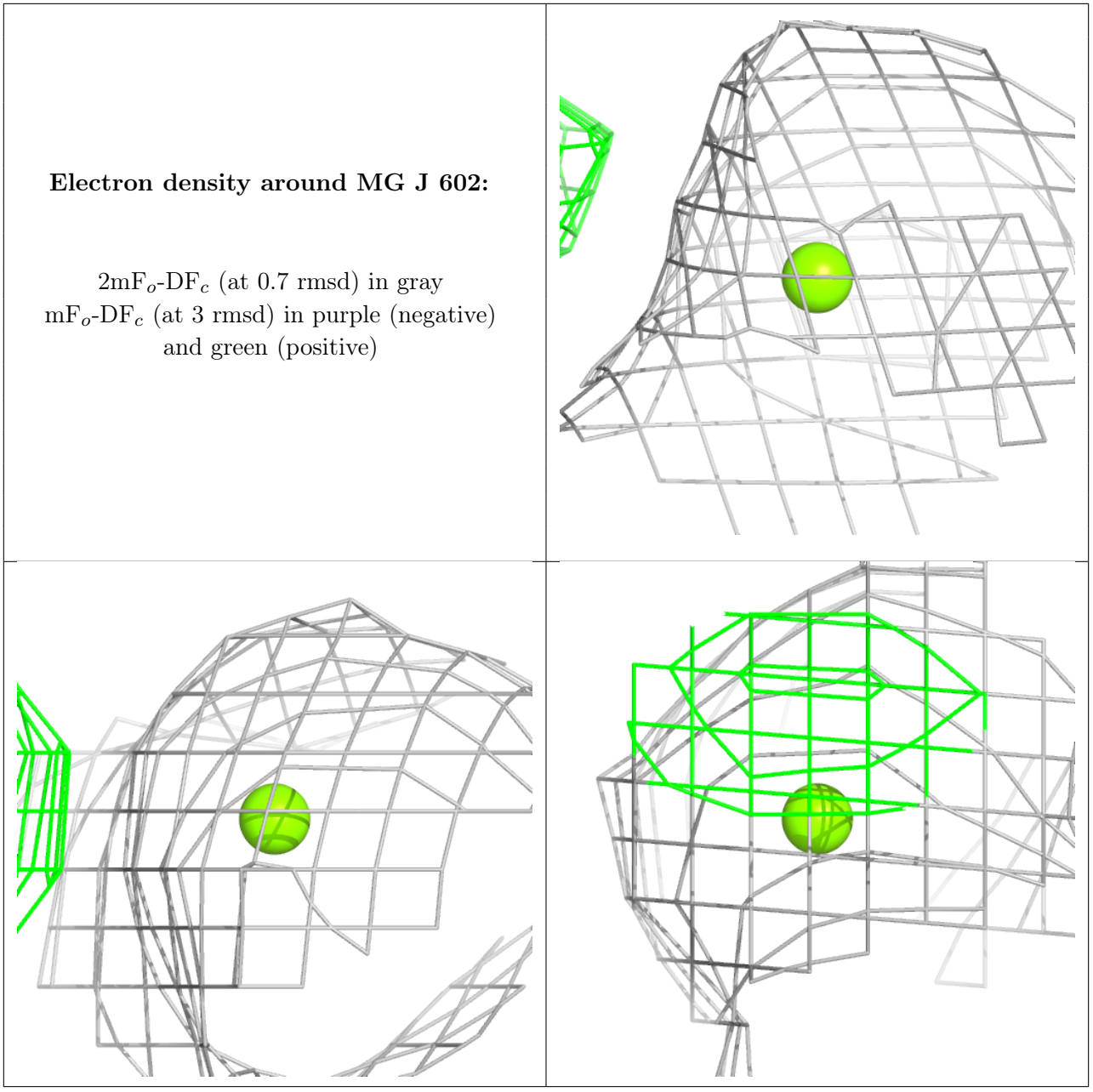
Electron density around MG G 605:

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



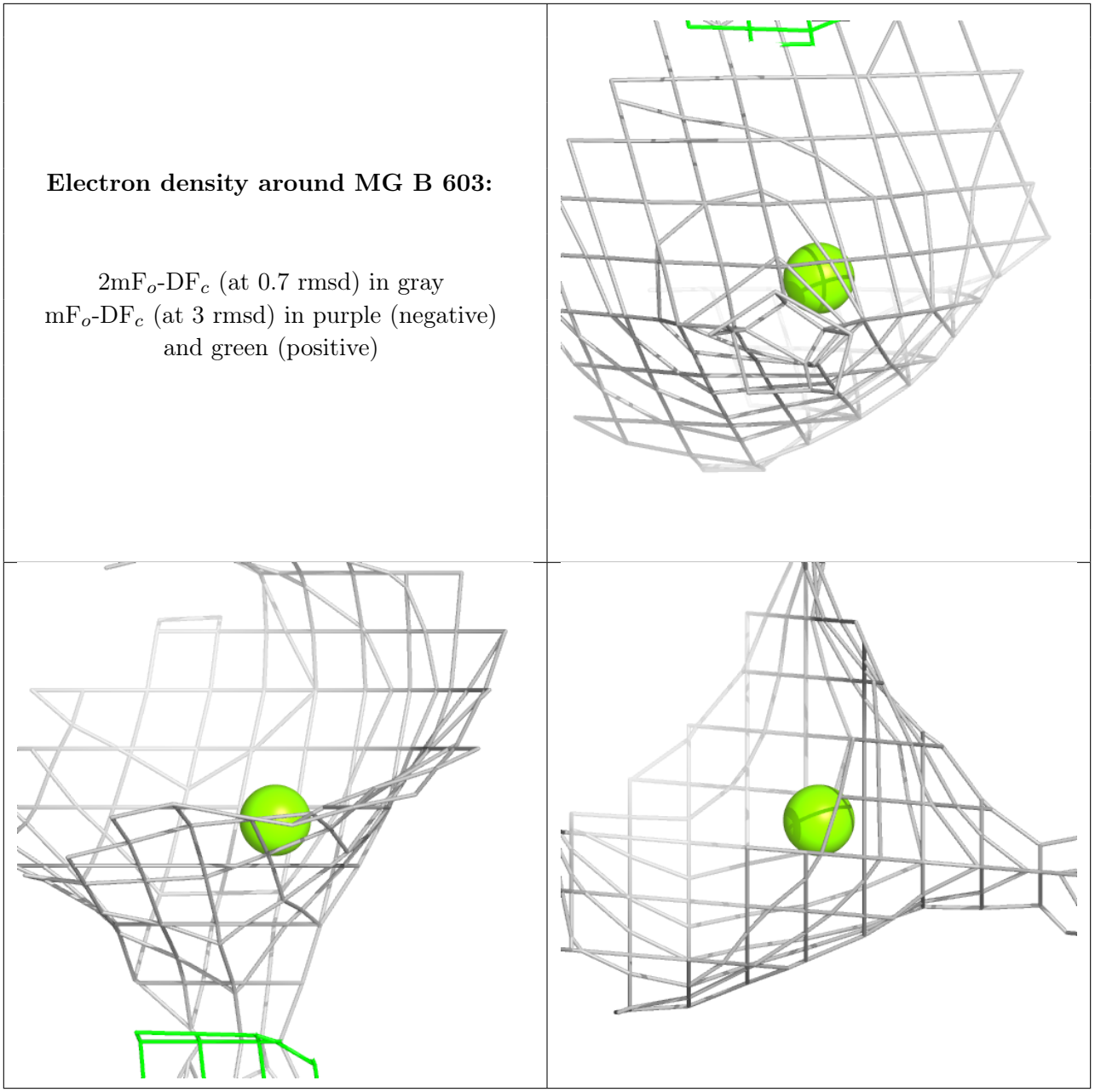
Electron density around MG J 602:

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



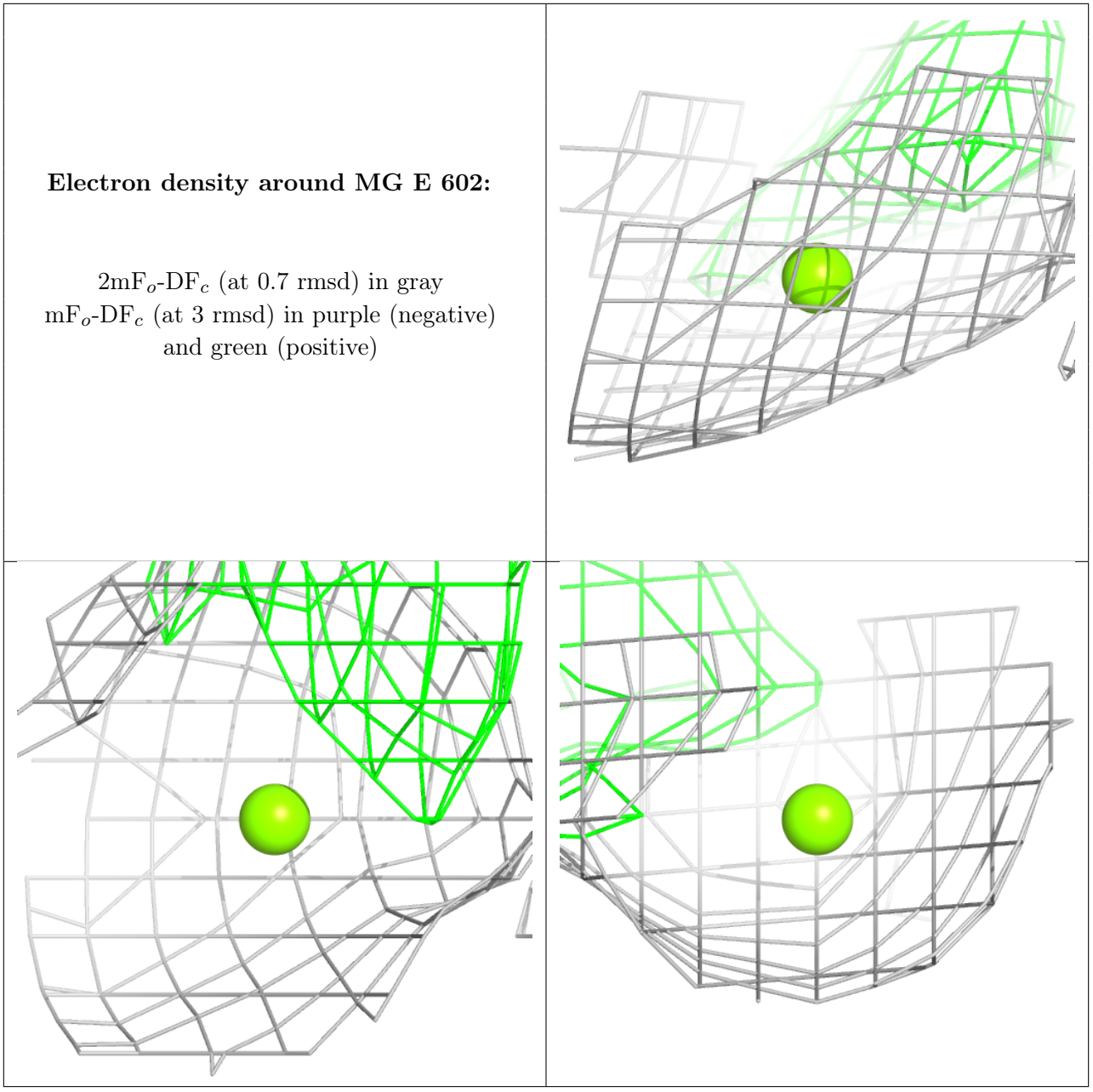
Electron density around MG B 603:

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



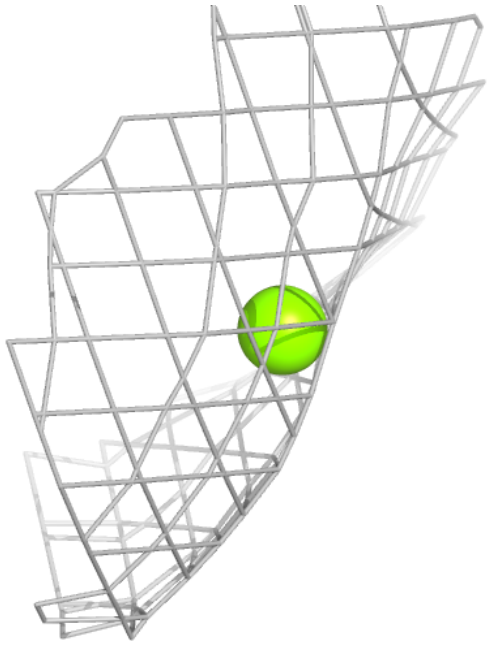
Electron density around MG E 602:

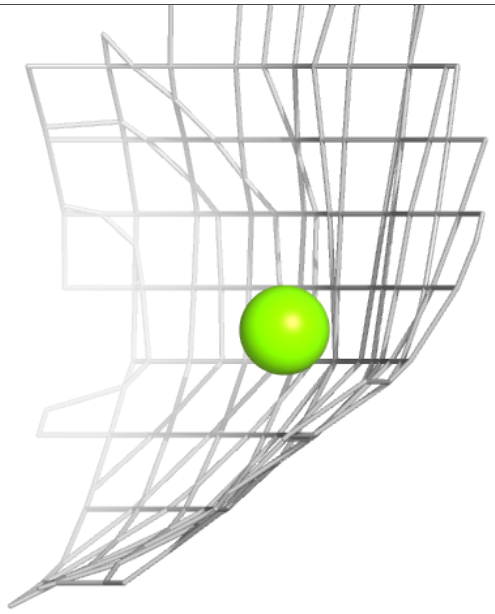
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

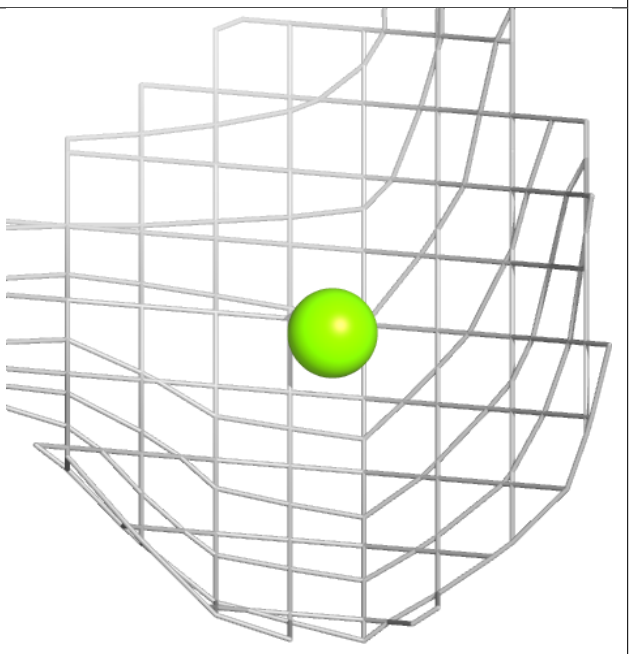


Electron density around MG A 603:

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

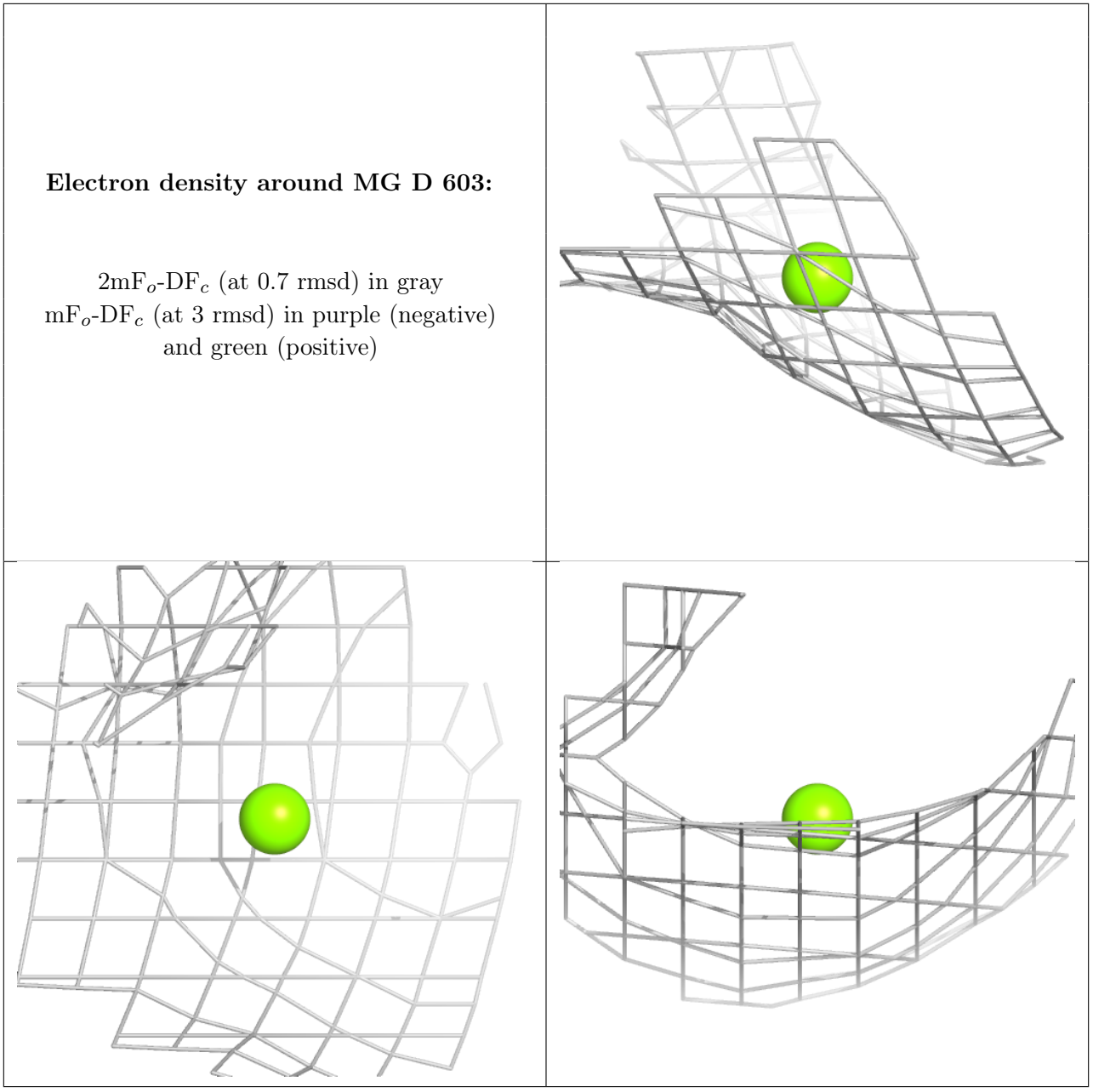






Electron density around MG D 603:

$2mF_o$-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.