



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 08:16 PM UTC

PDB ID : 8DBA / pdb_00008dba
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

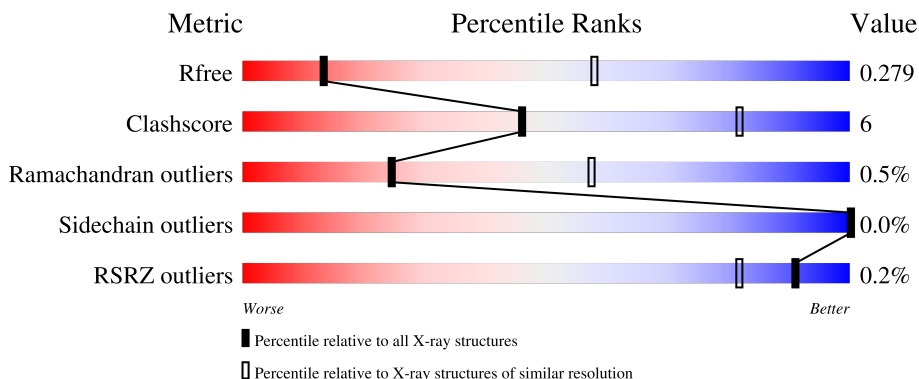
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	 80% 10% 11%
1	B	568	 77% 12% 11%
1	C	568	 76% 13% 11%
1	D	568	 76% 13% 10%
1	E	568	 81% 9% 10%

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Mol	Chain	Length	Quality of chain
1	F	568	 75% 13% 12%
1	G	568	 80% 11% 9%
1	H	568	 80% 10% 10%
1	I	568	 76% 10% 13%
1	J	568	 % 77% 12% 10%
1	K	568	 % 80% 9% 11%
1	L	568	 76% 13% 11%

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

There are 24 discrepancies between the modelled and reference sequences:

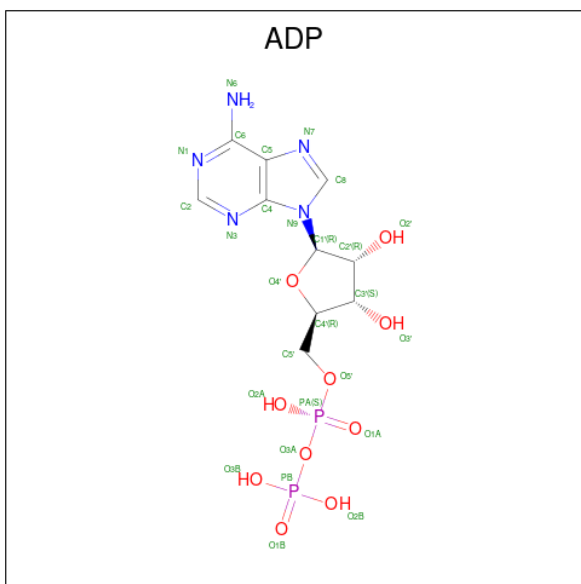
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B9KWX8
A	0	ALA	-	expression tag	UNP B9KWX8
B	-1	GLY	-	expression tag	UNP B9KWX8
B	0	ALA	-	expression tag	UNP B9KWX8
C	-1	GLY	-	expression tag	UNP B9KWX8

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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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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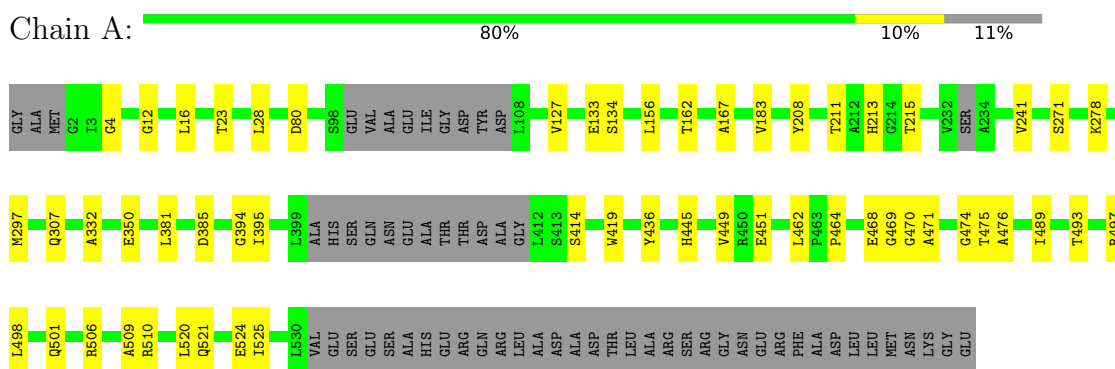
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	6	Total O 6 6	0	0
4	F	6	Total O 6 6	0	0
4	G	5	Total O 5 5	0	0
4	H	5	Total O 5 5	0	0
4	I	7	Total O 7 7	0	0
4	J	5	Total O 5 5	0	0
4	K	6	Total O 6 6	0	0
4	L	5	Total O 5 5	0	0

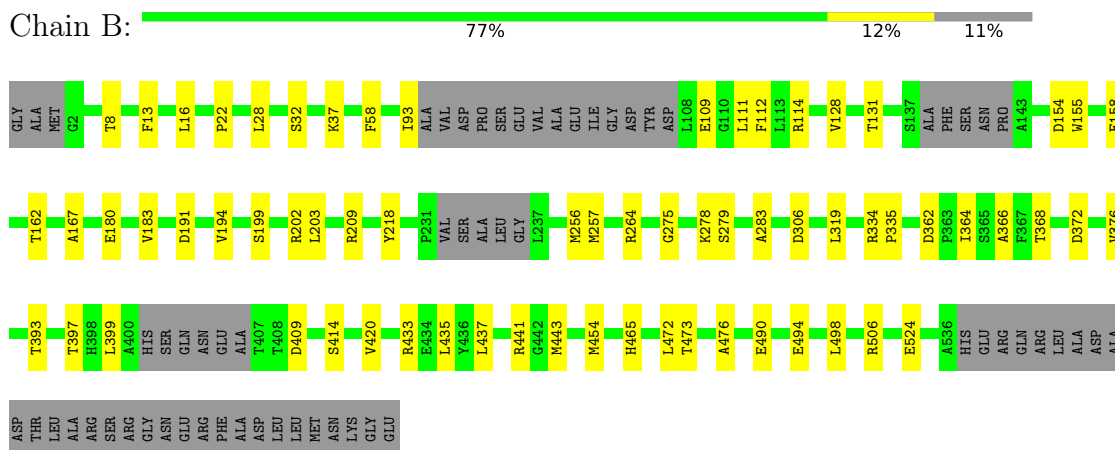
3 Residue-property plots [i](#)

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.

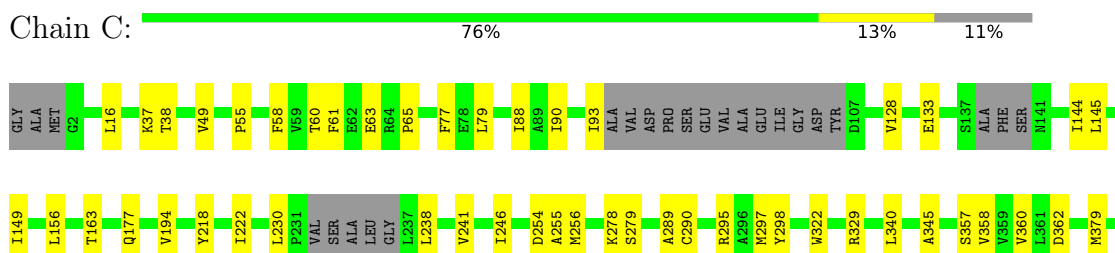
- Molecule 1: Circadian clock protein KaiC

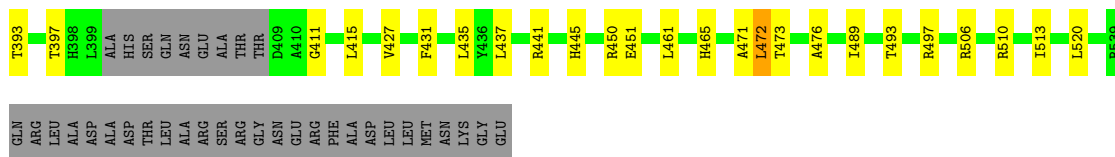


- Molecule 1: Circadian clock protein KaiC

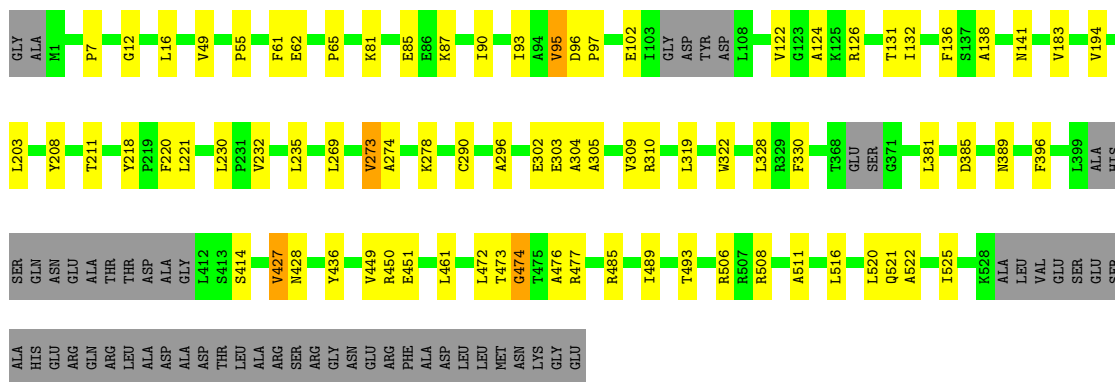
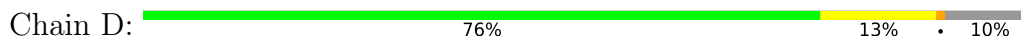


- Molecule 1: Circadian clock protein KaiC

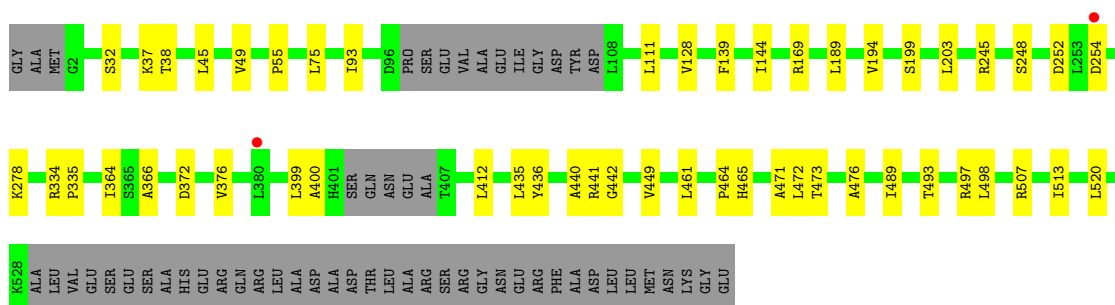
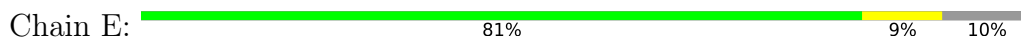




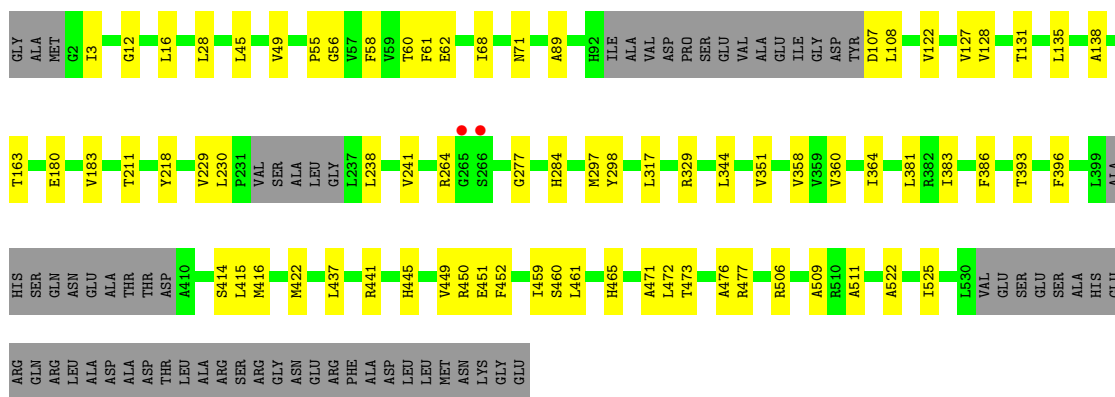
• Molecule 1: Circadian clock protein KaiC



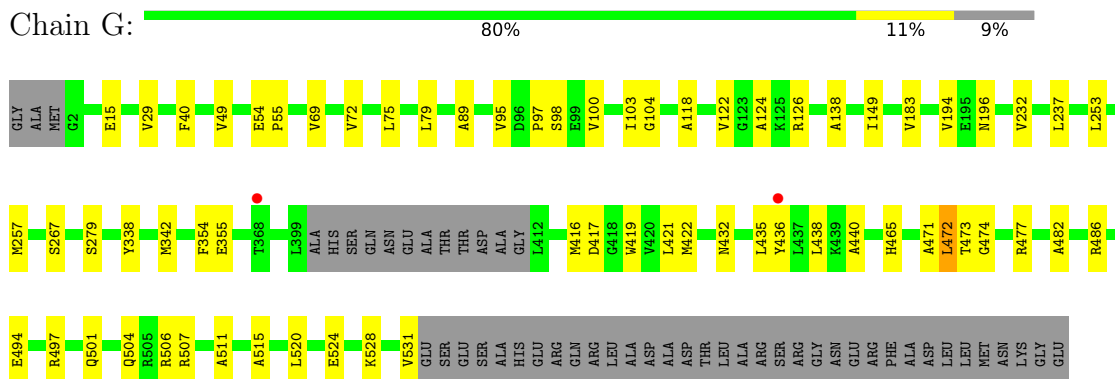
• Molecule 1: Circadian clock protein KaiC



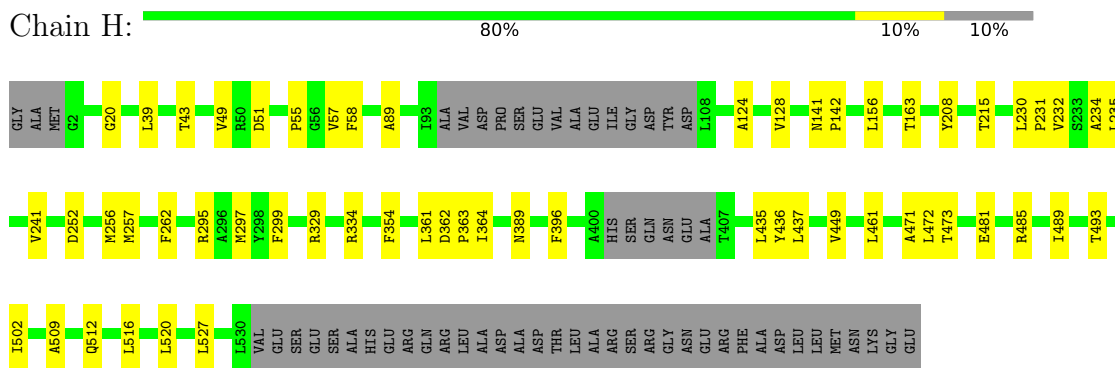
• Molecule 1: Circadian clock protein KaiC



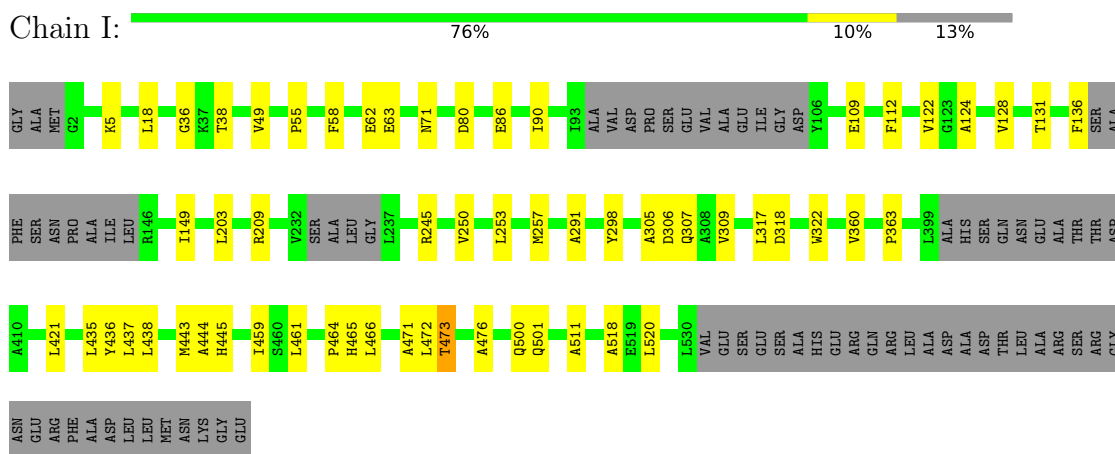
- Molecule 1: Circadian clock protein KaiC



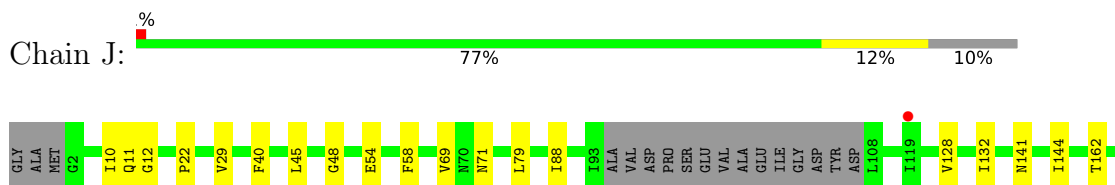
- Molecule 1: Circadian clock protein KaiC

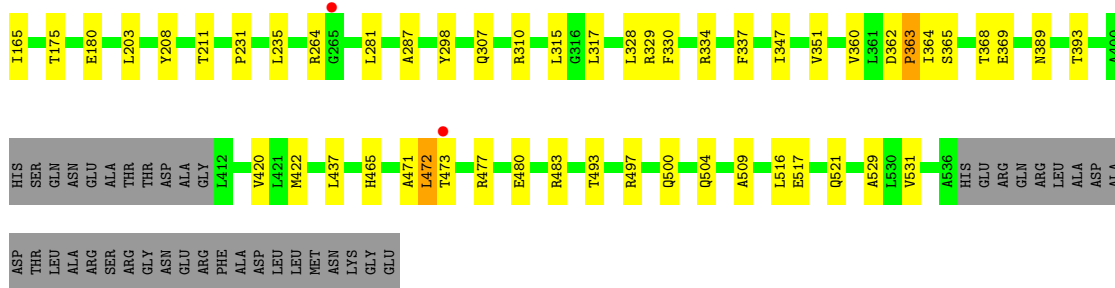


- Molecule 1: Circadian clock protein KaiC

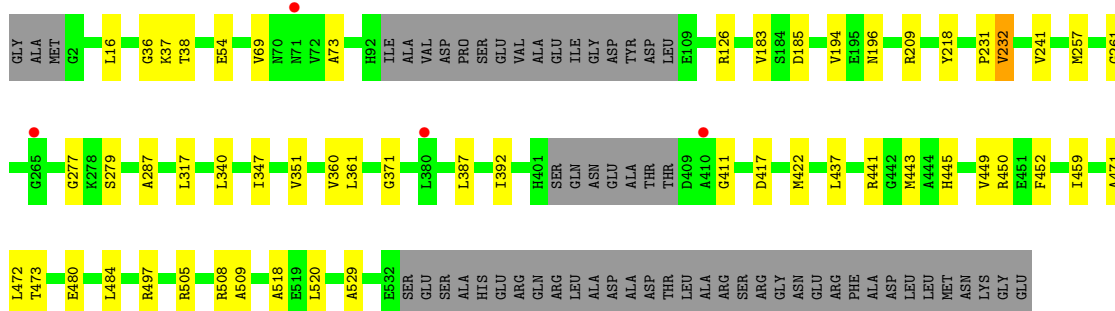
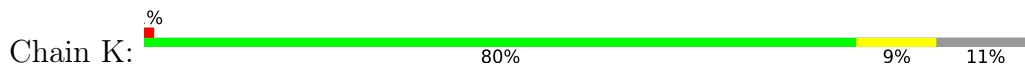


- Molecule 1: Circadian clock protein KaiC

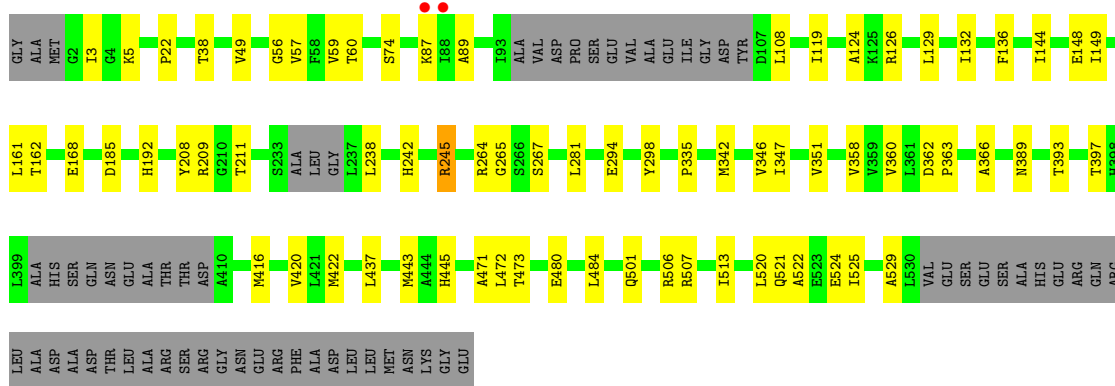




● Molecule 1: Circadian clock protein KaiC



● Molecule 1: Circadian clock protein KaiC



4 Data and refinement statistics

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) 97.6 (48.10-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.236 , 0.279 0.236 , 0.279	Depositor DCC
R_{free} test set	1988 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	90.8	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 90.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	93625	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/3938	0.28	0/5312
1	B	0.12	0/3930	0.28	0/5296
1	C	0.14	0/3941	0.29	0/5312
1	D	0.12	0/3975	0.31	0/5361
1	E	0.12	0/3976	0.28	0/5364
1	F	0.12	0/3910	0.28	0/5268
1	G	0.13	0/4057	0.30	0/5474
1	H	0.12	0/3969	0.29	0/5352
1	I	0.12	0/3875	0.29	0/5219
1	J	0.12	0/3961	0.29	0/5344
1	K	0.13	0/3944	0.29	0/5320
1	L	0.13	0/3946	0.30	0/5316
All	All	0.12	0/47422	0.29	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3879	3810	3876	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3875	3812	3871	50	0
1	C	3885	3821	3872	59	0
1	D	3916	3859	3929	65	2
1	E	3916	3862	3900	45	2
1	F	3852	3810	3851	57	0
1	G	3995	3913	4002	52	0
1	H	3910	3887	3917	44	3
1	I	3819	3695	3816	54	0
1	J	3902	3812	3900	48	0
1	K	3884	3822	3872	49	0
1	L	3888	3786	3899	58	1
2	A	54	23	24	1	0
2	B	54	24	24	2	0
2	C	54	23	24	5	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	549	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 6.

The worst 5 of 549 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:B:256:MET:HE1	1:B:435:LEU:HD22	1.58	0.84
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

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%)	30	62
1	B	495/568 (87%)	473 (96%)	21 (4%)	1 (0%)	43	74
1	C	498/568 (88%)	472 (95%)	25 (5%)	1 (0%)	43	74
1	D	502/568 (88%)	460 (92%)	36 (7%)	6 (1%)	10	41
1	E	505/568 (89%)	481 (95%)	23 (5%)	1 (0%)	43	74
1	F	492/568 (87%)	463 (94%)	28 (6%)	1 (0%)	43	74
1	G	514/568 (90%)	476 (93%)	34 (7%)	4 (1%)	16	49
1	H	503/568 (89%)	476 (95%)	27 (5%)	0	100	100
1	I	484/568 (85%)	455 (94%)	26 (5%)	3 (1%)	21	54
1	J	504/568 (89%)	472 (94%)	28 (6%)	4 (1%)	16	49
1	K	502/568 (88%)	479 (95%)	19 (4%)	4 (1%)	16	49
1	L	495/568 (87%)	462 (93%)	32 (6%)	1 (0%)	43	74
All	All	5993/6816 (88%)	5635 (94%)	330 (6%)	28 (0%)	24	57

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%)	398 (100%)	0	100	100
1	B	398/457 (87%)	398 (100%)	0	100	100
1	C	397/457 (87%)	397 (100%)	0	100	100
1	D	403/457 (88%)	403 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	403/457 (88%)	403 (100%)	0	100	100
1	F	397/457 (87%)	397 (100%)	0	100	100
1	G	415/457 (91%)	415 (100%)	0	100	100
1	H	404/457 (88%)	404 (100%)	0	100	100
1	I	394/457 (86%)	394 (100%)	0	100	100
1	J	401/457 (88%)	401 (100%)	0	100	100
1	K	397/457 (87%)	397 (100%)	0	100	100
1	L	402/457 (88%)	401 (100%)	1 (0%)	87	85
All	All	4809/5484 (88%)	4808 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	141	ASN
1	I	52	HIS
1	K	398	HIS
1	H	448	GLN
1	I	284	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	I	601	-	28,29,29	1.39	5 (17%)	43,45,45	1.88	11 (25%)
2	ADP	J	604	3	28,29,29	1.40	4 (14%)	43,45,45	1.91	11 (25%)
2	ADP	K	604	3	28,29,29	1.38	4 (14%)	43,45,45	1.90	12 (27%)
2	ADP	H	603	3	28,29,29	1.38	4 (14%)	43,45,45	1.91	12 (27%)
2	ADP	B	601	3	28,29,29	1.41	5 (17%)	43,45,45	1.92	12 (27%)
2	ADP	G	604	3	28,29,29	1.39	4 (14%)	43,45,45	1.89	12 (27%)
2	ADP	C	604	3	28,29,29	1.40	4 (14%)	43,45,45	1.92	12 (27%)
2	ADP	J	601	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	12 (27%)
2	ADP	G	601	3	28,29,29	1.40	5 (17%)	43,45,45	1.90	11 (25%)
2	ADP	F	603	3	28,29,29	1.39	4 (14%)	43,45,45	1.90	12 (27%)
2	ADP	F	601	-	28,29,29	1.39	4 (14%)	43,45,45	1.89	11 (25%)
2	ADP	C	601	3	28,29,29	1.38	5 (17%)	43,45,45	1.90	12 (27%)
2	ADP	H	601	3	28,29,29	1.41	4 (14%)	43,45,45	1.88	12 (27%)
2	ADP	A	604	3	28,29,29	1.39	4 (14%)	43,45,45	1.88	11 (25%)
2	ADP	K	601	-	28,29,29	1.38	5 (17%)	43,45,45	1.90	10 (23%)
2	ADP	D	604	3	28,29,29	1.39	4 (14%)	43,45,45	1.89	12 (27%)
2	ADP	E	604	3	28,29,29	1.39	4 (14%)	43,45,45	1.92	12 (27%)
2	ADP	B	604	3	28,29,29	1.39	4 (14%)	43,45,45	1.87	10 (23%)
2	ADP	A	601	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	12 (27%)
2	ADP	L	601	-	28,29,29	1.39	5 (17%)	43,45,45	1.90	12 (27%)
2	ADP	D	601	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	11 (25%)
2	ADP	I	604	3	28,29,29	1.38	4 (14%)	43,45,45	1.91	12 (27%)
2	ADP	E	601	-	28,29,29	1.41	5 (17%)	43,45,45	1.93	11 (25%)
2	ADP	L	602	3	28,29,29	1.40	4 (14%)	43,45,45	1.92	11 (25%)

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	I	601	-	-	6/16/32/32	0/3/3/3
2	ADP	J	604	3	-	3/16/32/32	0/3/3/3
2	ADP	K	604	3	-	1/16/32/32	0/3/3/3
2	ADP	H	603	3	-	4/16/32/32	0/3/3/3
2	ADP	B	601	3	-	4/16/32/32	0/3/3/3
2	ADP	G	604	3	-	4/16/32/32	0/3/3/3
2	ADP	C	604	3	-	5/16/32/32	0/3/3/3
2	ADP	J	601	-	-	5/16/32/32	0/3/3/3
2	ADP	G	601	3	-	4/16/32/32	0/3/3/3
2	ADP	F	603	3	-	5/16/32/32	0/3/3/3
2	ADP	F	601	-	-	1/16/32/32	0/3/3/3
2	ADP	C	601	3	-	4/16/32/32	0/3/3/3
2	ADP	H	601	3	-	7/16/32/32	0/3/3/3
2	ADP	A	604	3	-	4/16/32/32	0/3/3/3
2	ADP	K	601	-	-	6/16/32/32	0/3/3/3
2	ADP	D	604	3	-	5/16/32/32	0/3/3/3
2	ADP	E	604	3	-	1/16/32/32	0/3/3/3
2	ADP	B	604	3	-	5/16/32/32	0/3/3/3
2	ADP	A	601	-	-	7/16/32/32	0/3/3/3
2	ADP	L	601	-	-	0/16/32/32	0/3/3/3
2	ADP	D	601	-	-	4/16/32/32	0/3/3/3
2	ADP	I	604	3	-	5/16/32/32	0/3/3/3
2	ADP	E	601	-	-	2/16/32/32	0/3/3/3
2	ADP	L	602	3	-	4/16/32/32	0/3/3/3

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	ADP	C5-C4	4.63	1.47	1.39
2	D	601	ADP	C5-C4	4.61	1.47	1.39
2	A	601	ADP	C5-C4	4.60	1.47	1.39
2	B	601	ADP	C5-C4	4.59	1.47	1.39
2	J	604	ADP	C5-C4	4.58	1.47	1.39

The worst 5 of 276 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-5.79	118.75	126.72
2	A	601	ADP	C5-C4-N3	-5.76	118.79	126.72
2	K	601	ADP	C5-C4-N3	-5.75	118.80	126.72
2	I	601	ADP	C5-C4-N3	-5.75	118.80	126.72
2	D	601	ADP	C5-C4-N3	-5.73	118.83	126.72

There are no chirality outliers.

5 of 96 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	604	ADP	C5'-O5'-PA-O1A
2	A	604	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	O4'-C4'-C5'-O5'

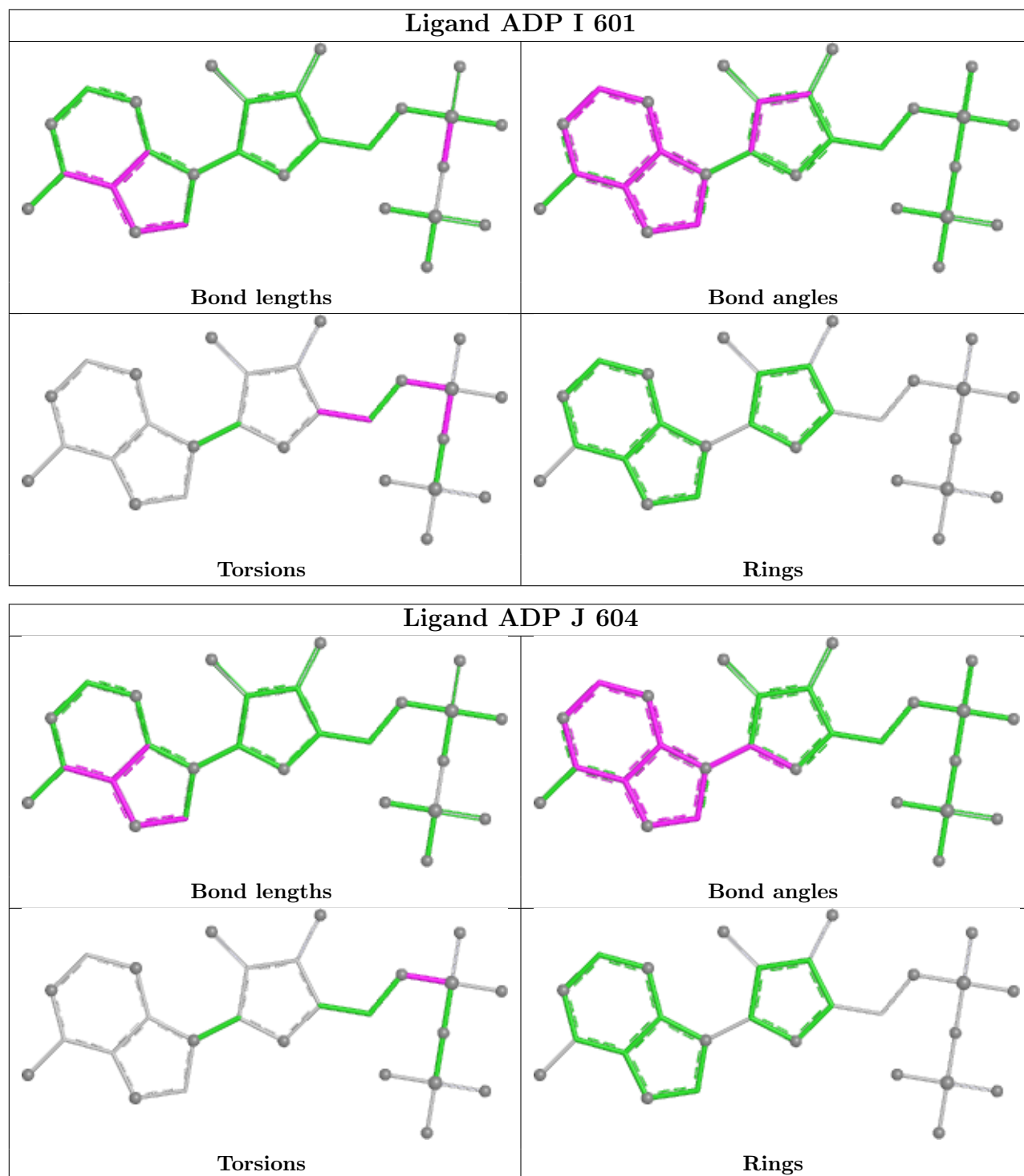
There are no ring outliers.

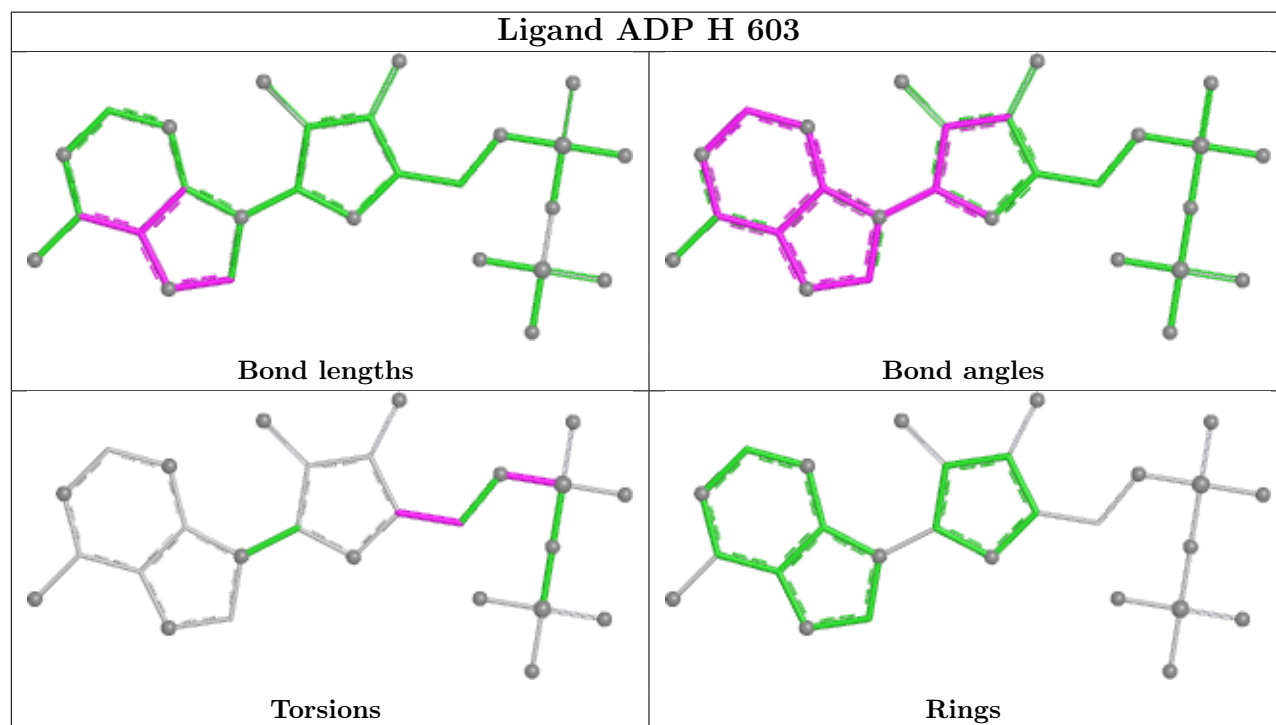
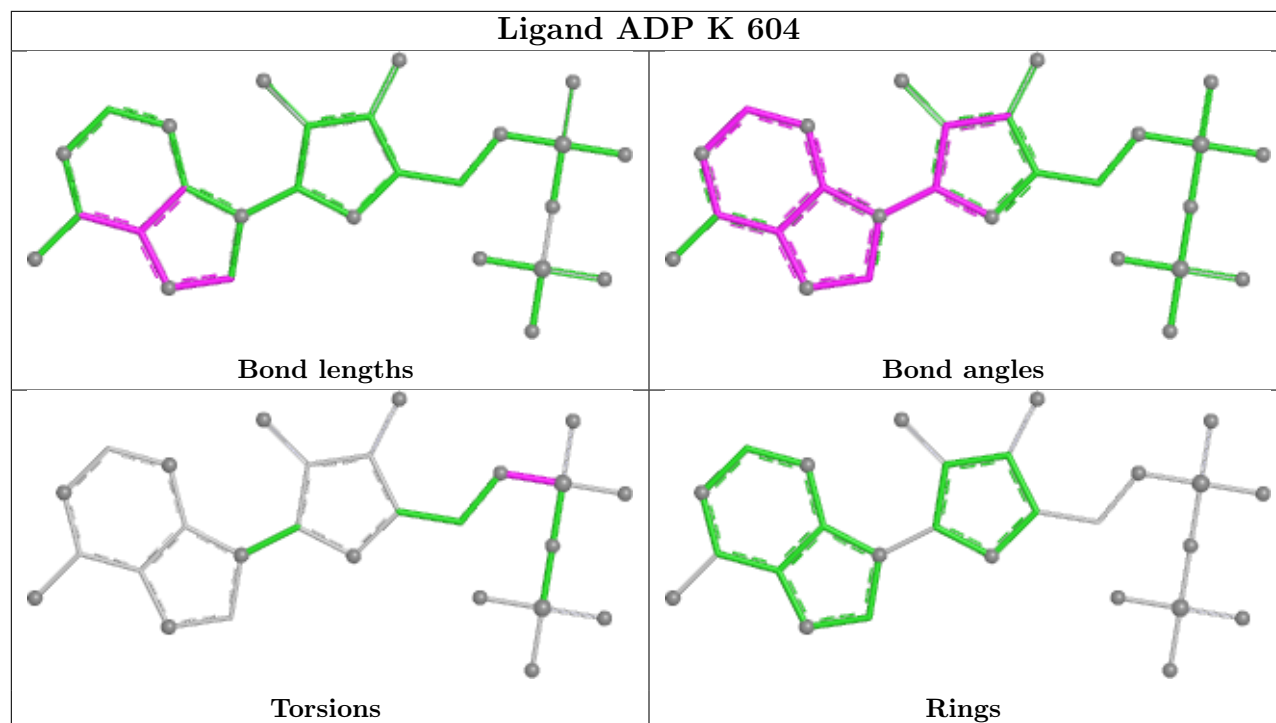
14 monomers are involved in 21 short contacts:

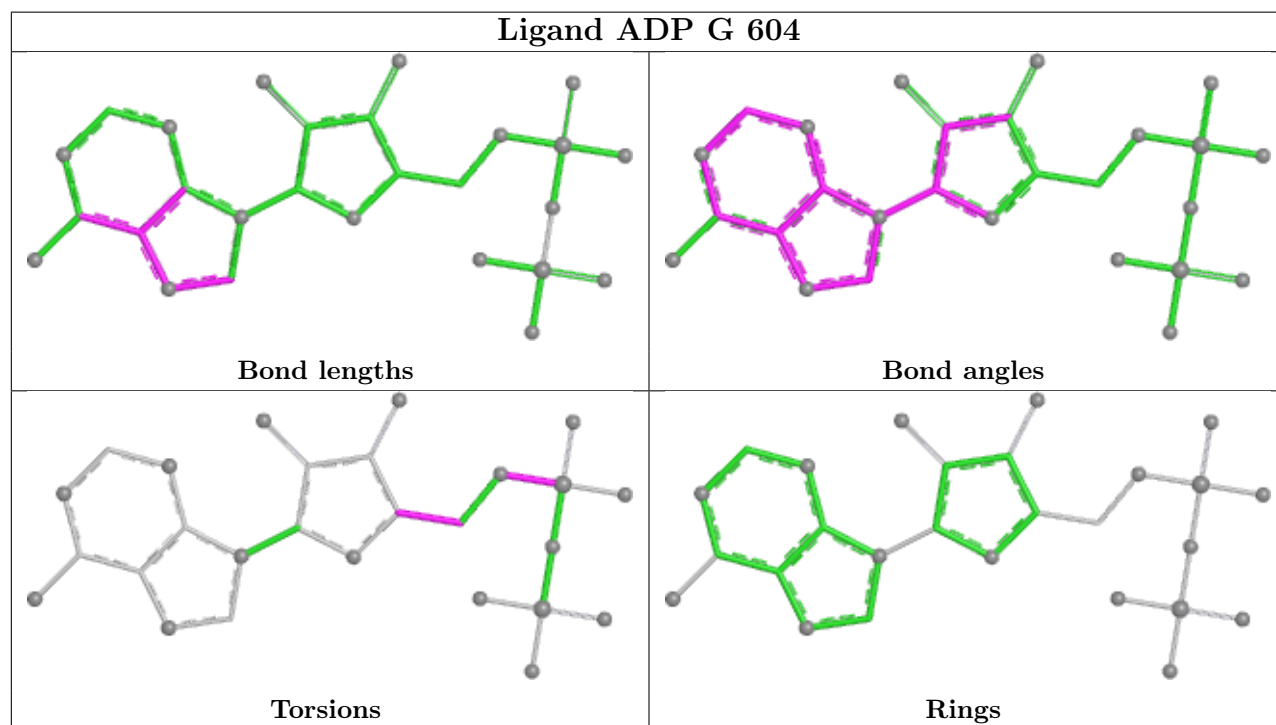
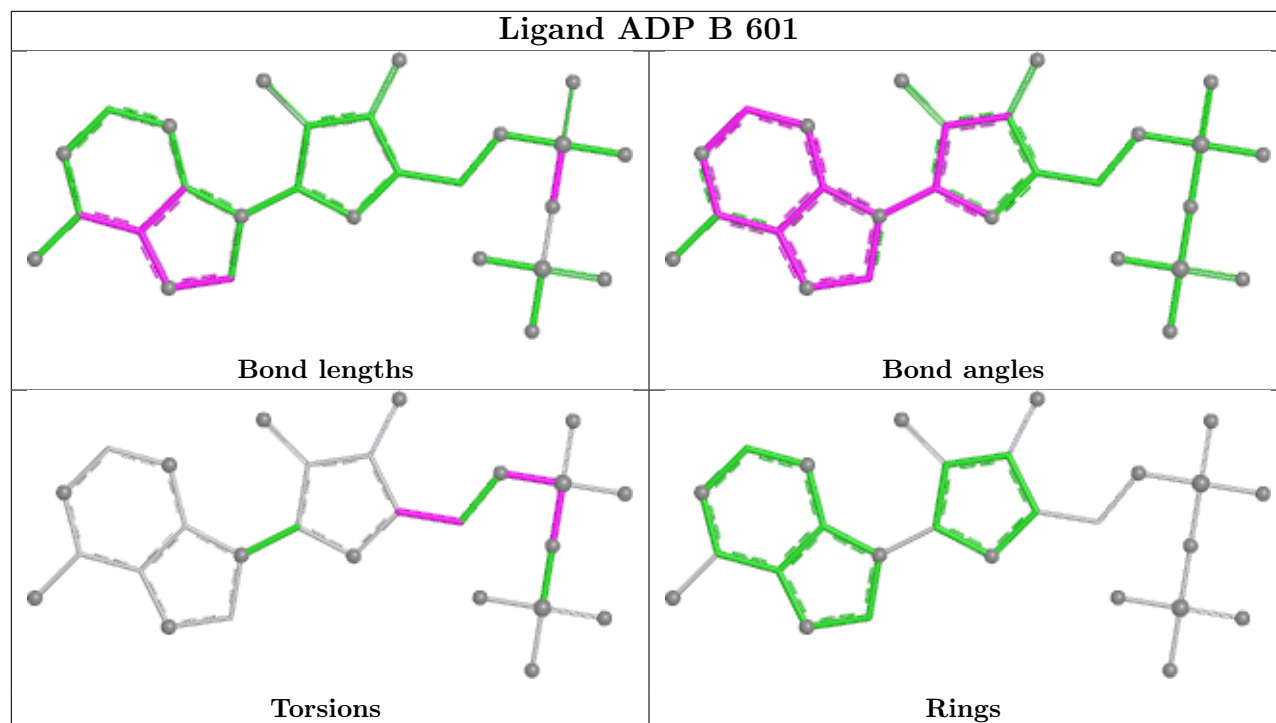
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	601	ADP	1	0
2	K	604	ADP	1	0
2	G	604	ADP	2	0
2	C	604	ADP	2	0
2	G	601	ADP	1	0
2	C	601	ADP	3	0
2	H	601	ADP	1	0
2	A	604	ADP	1	0
2	K	601	ADP	2	0
2	D	604	ADP	1	0
2	E	604	ADP	1	0
2	B	604	ADP	2	0
2	L	601	ADP	2	0
2	E	601	ADP	1	0

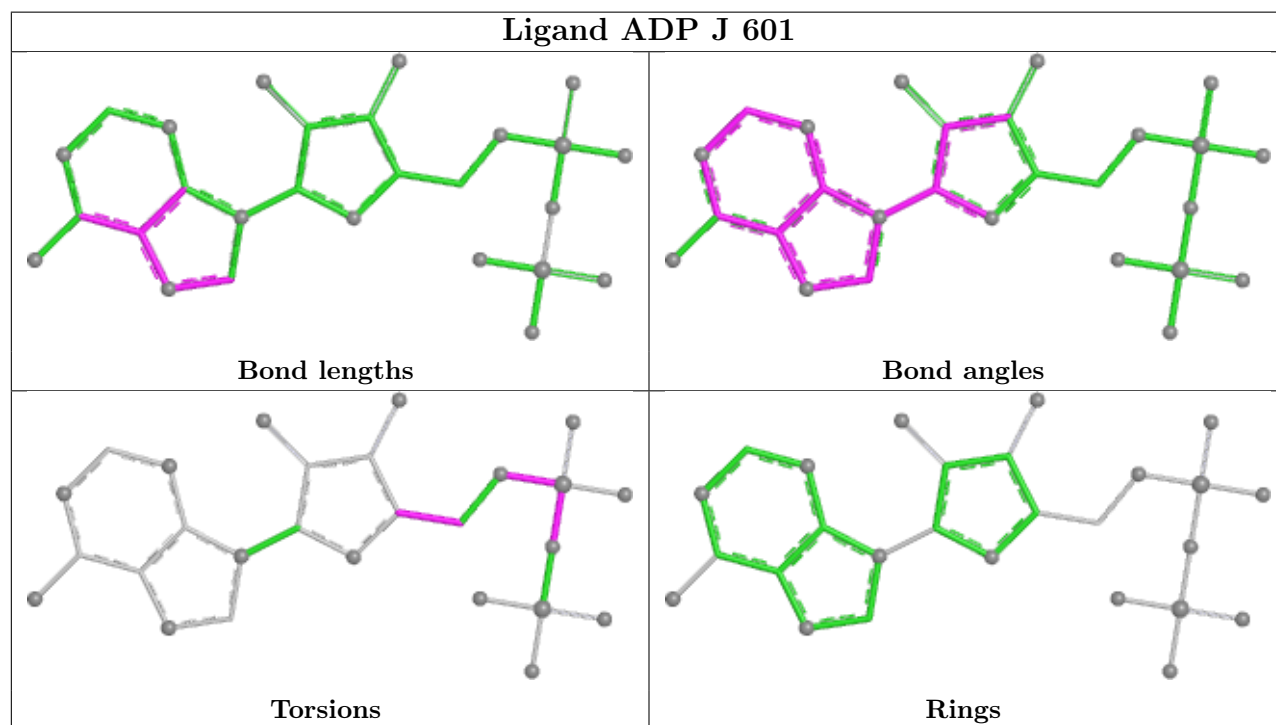
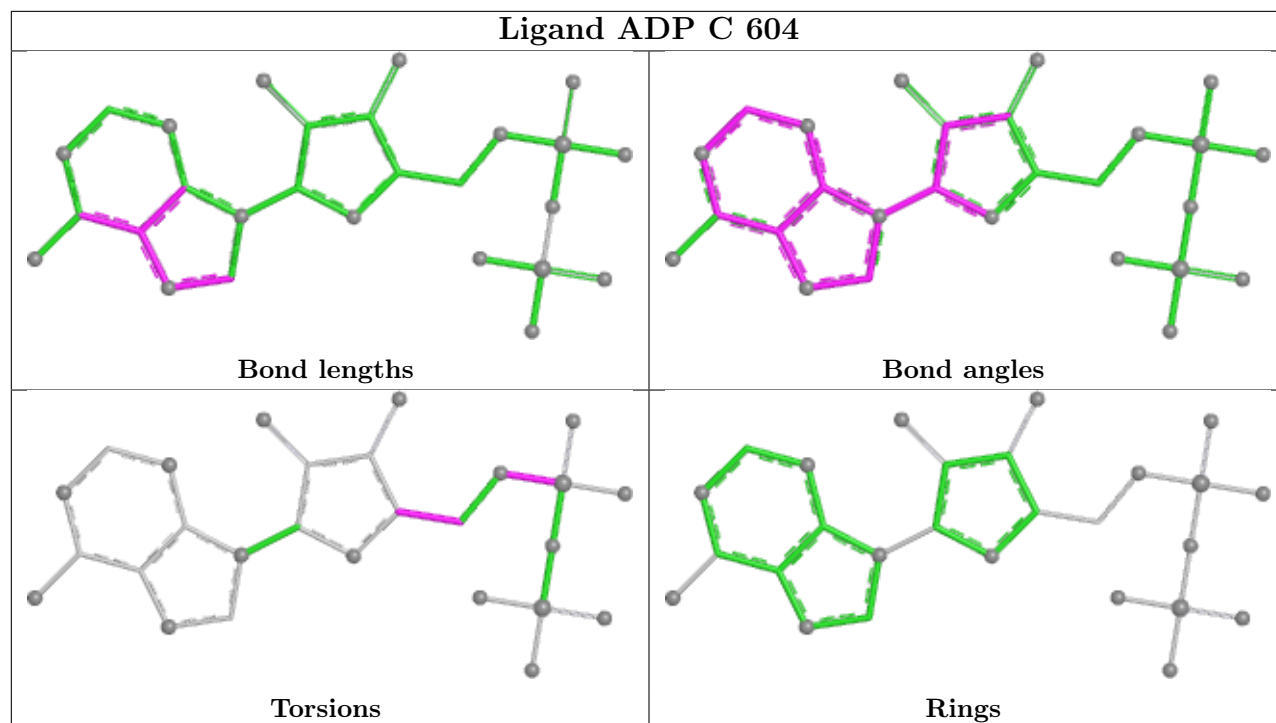
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

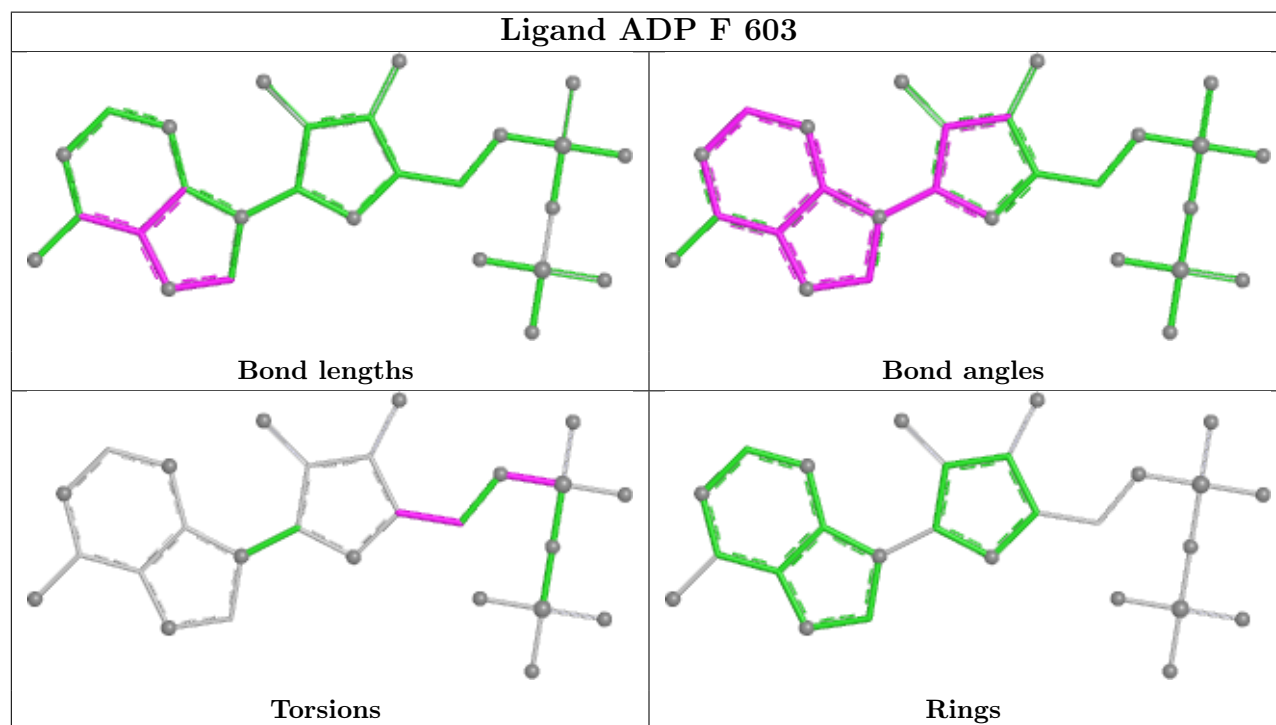
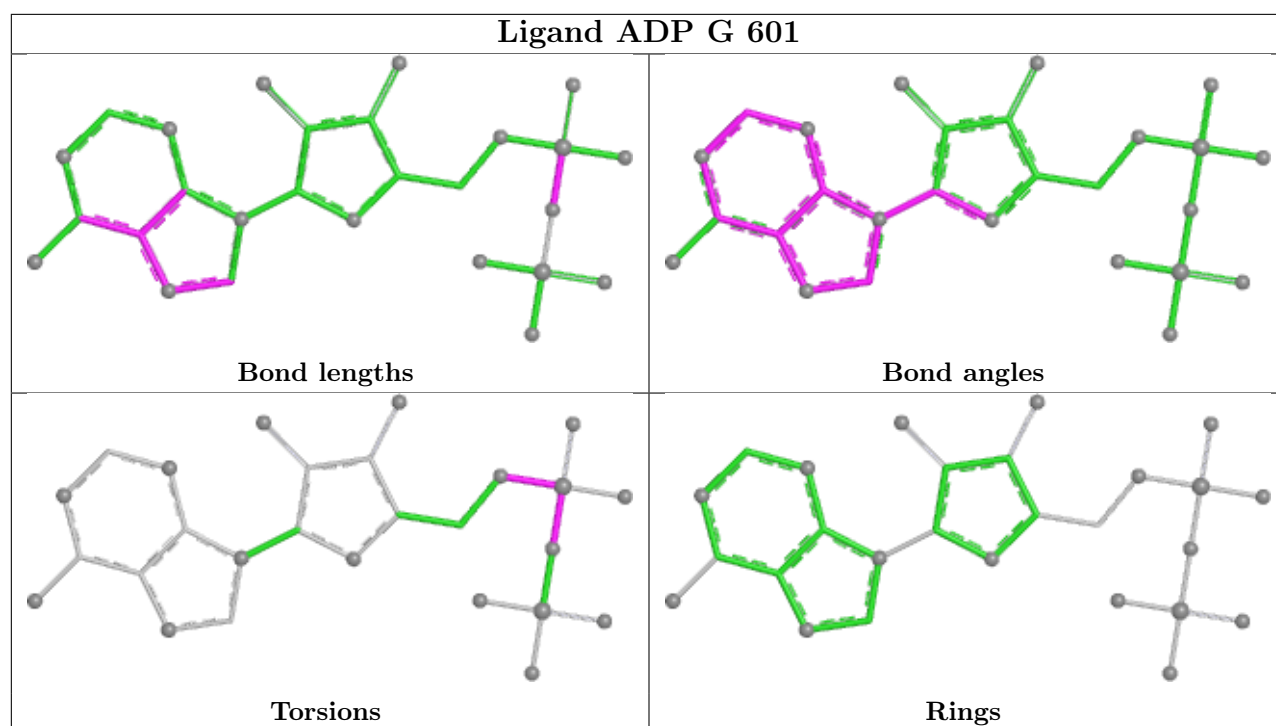
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

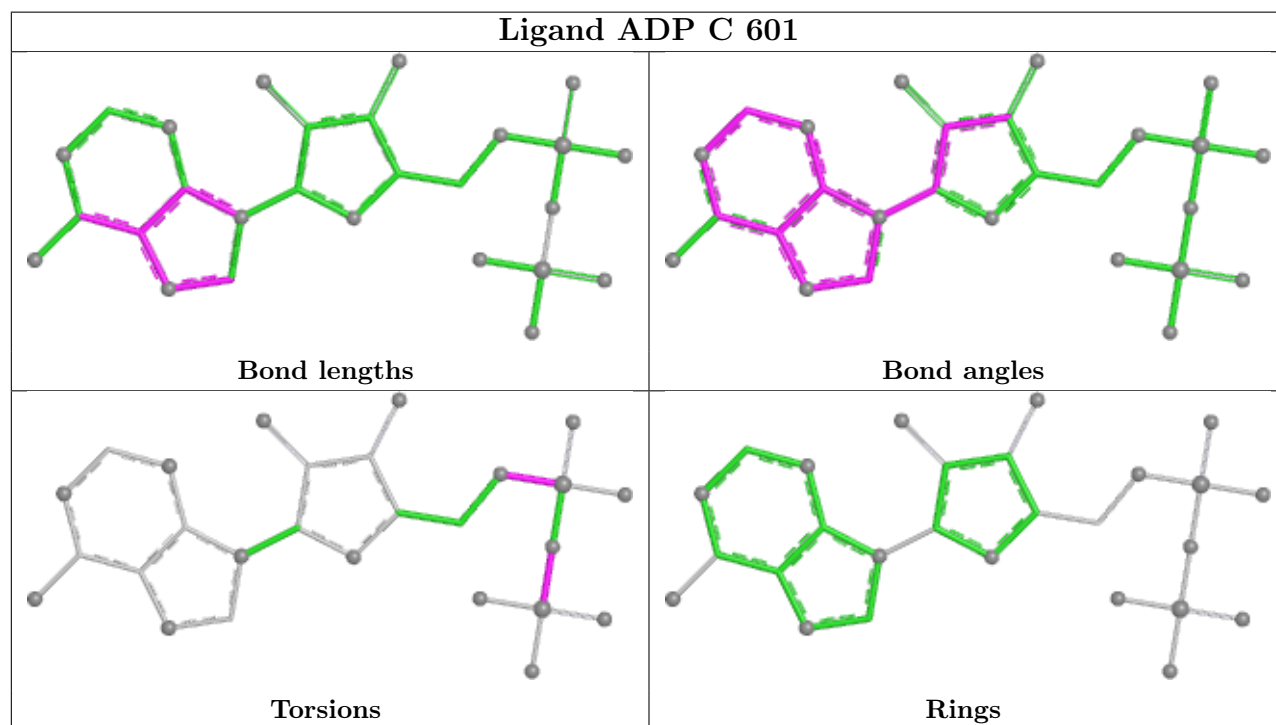
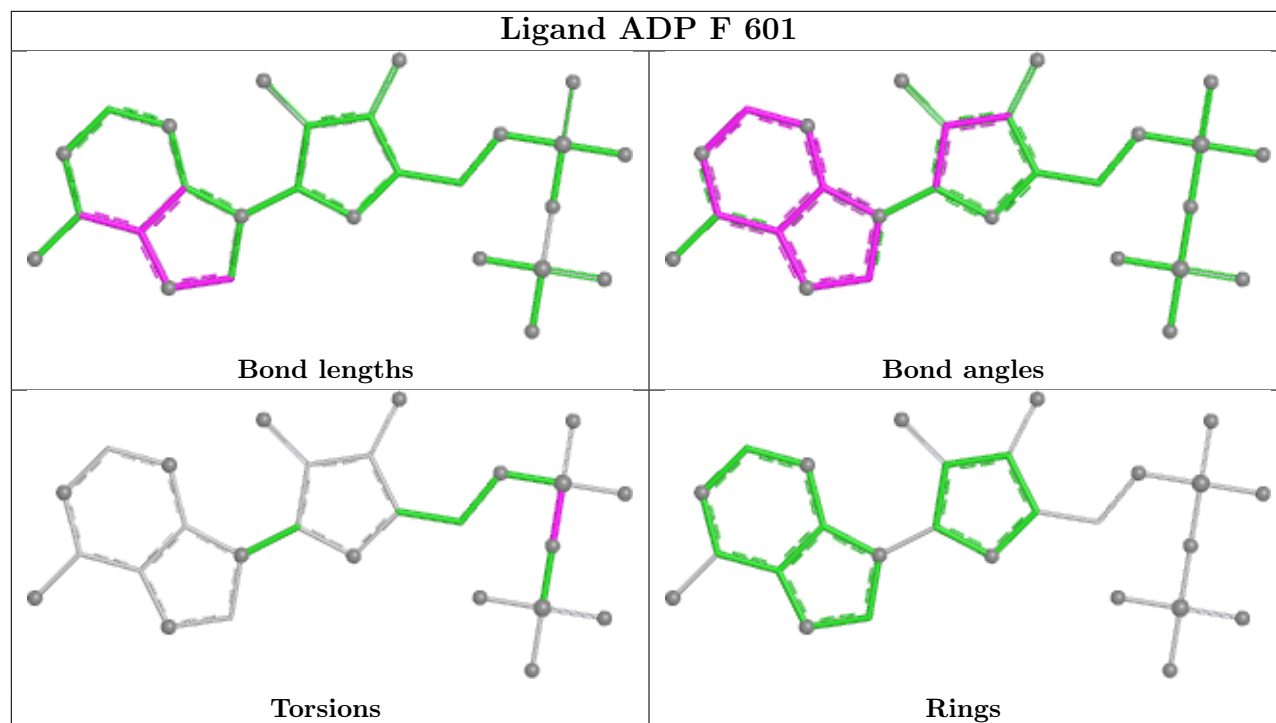


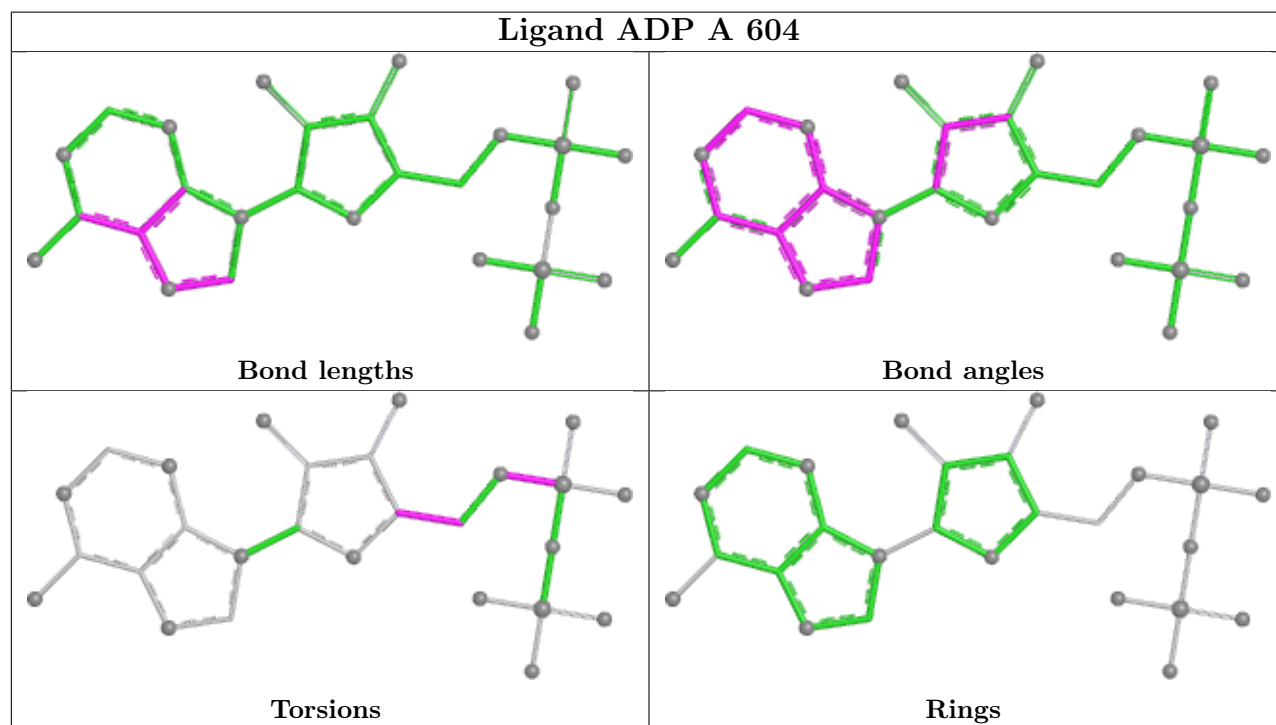
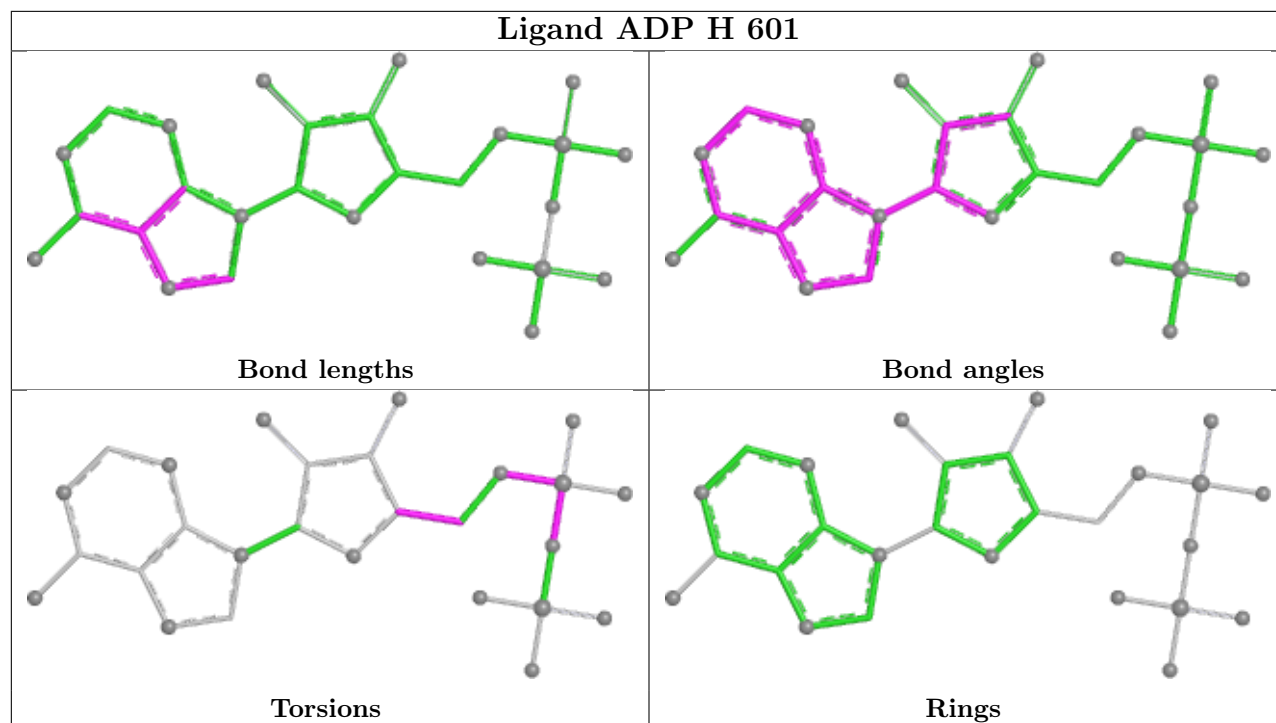


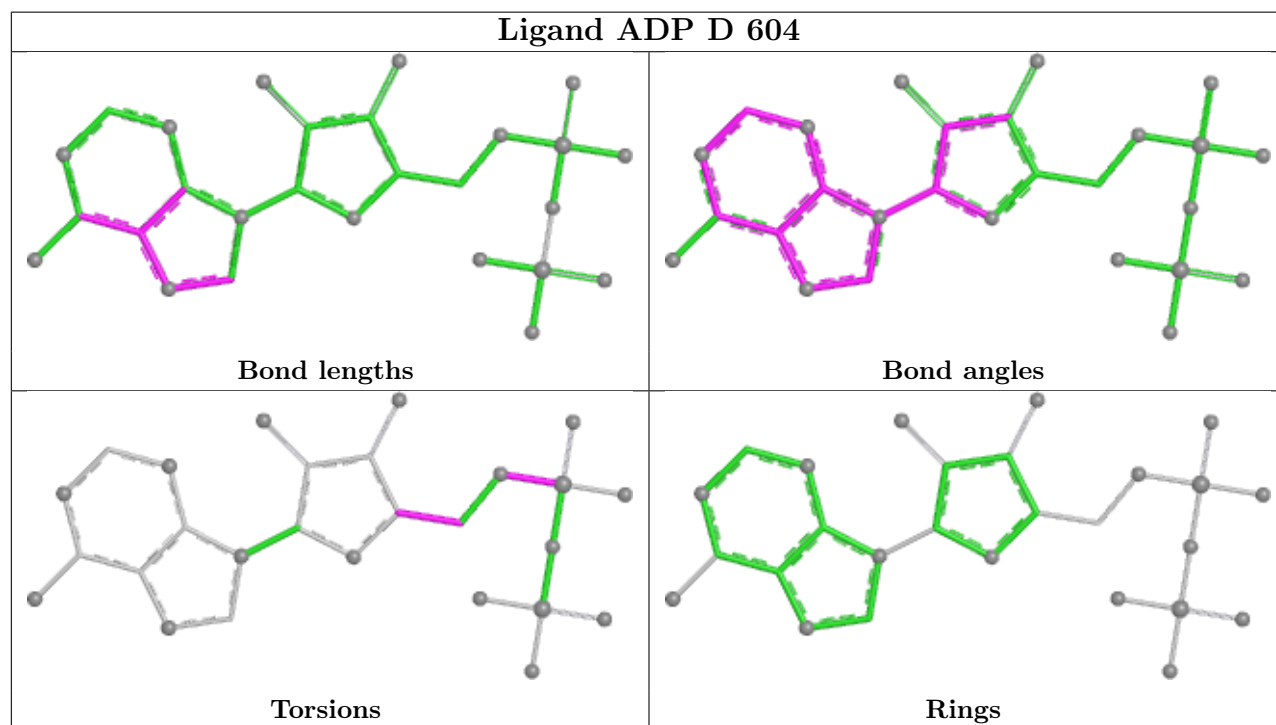
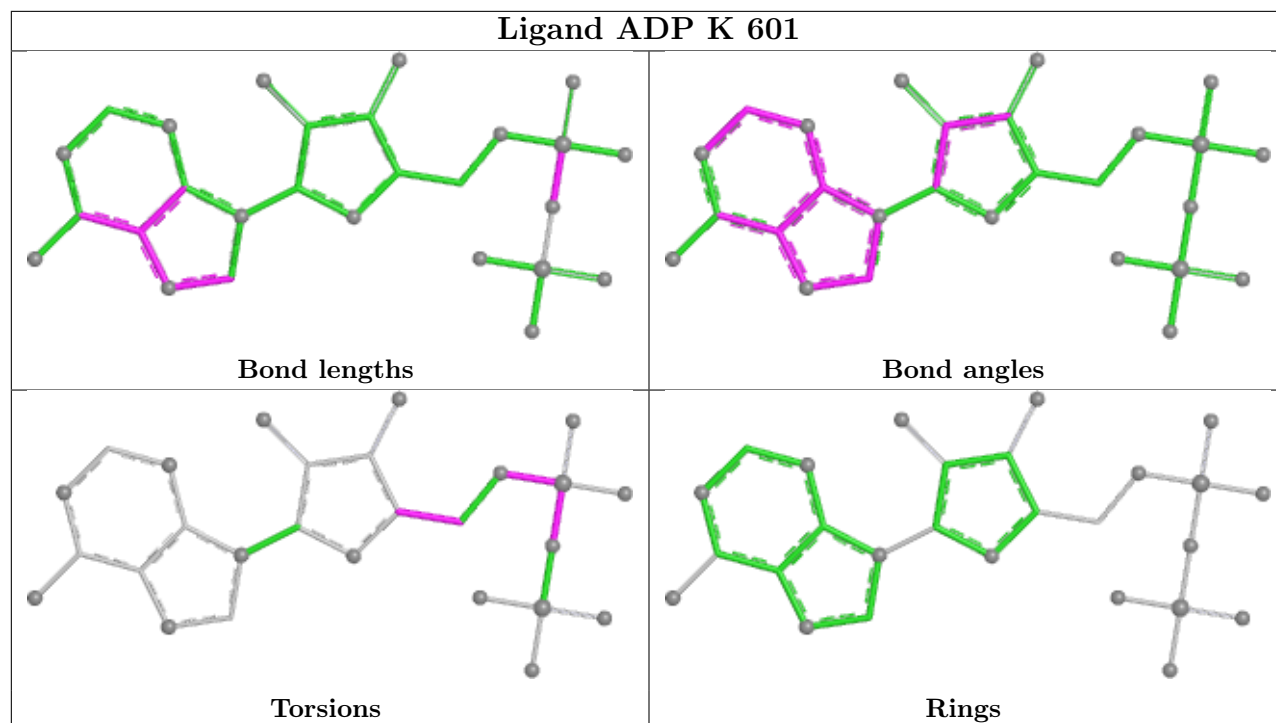


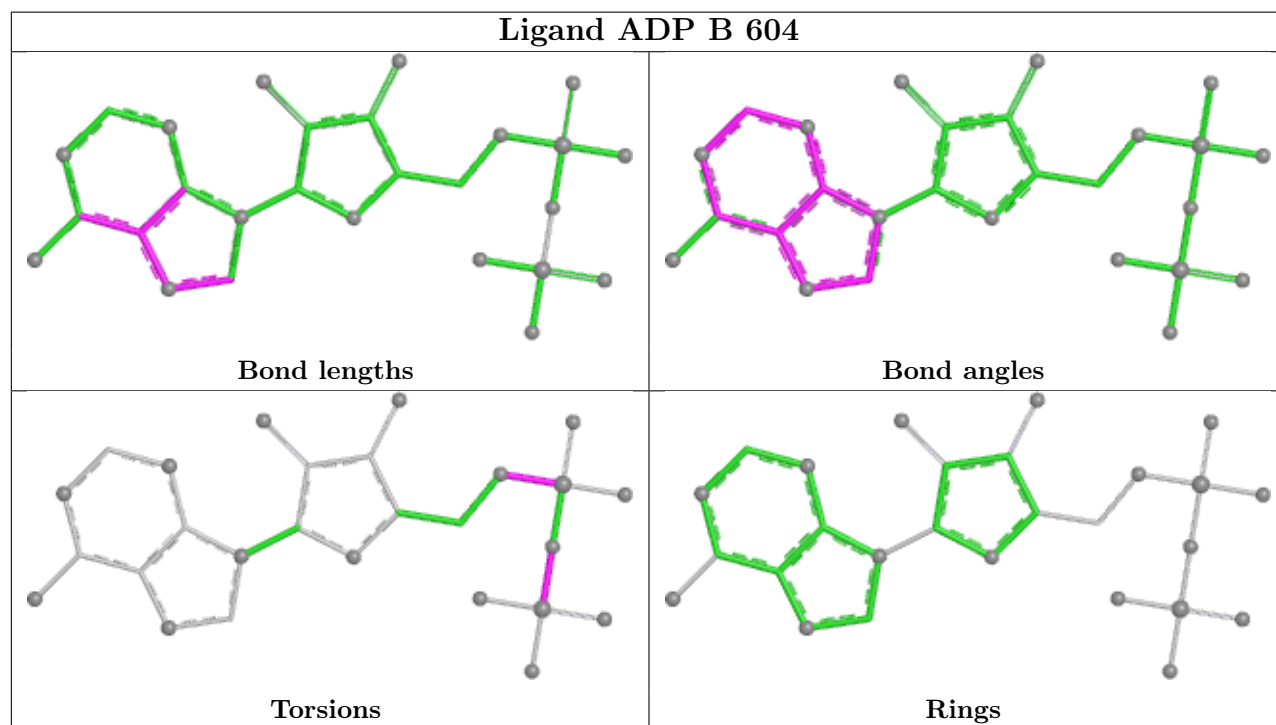
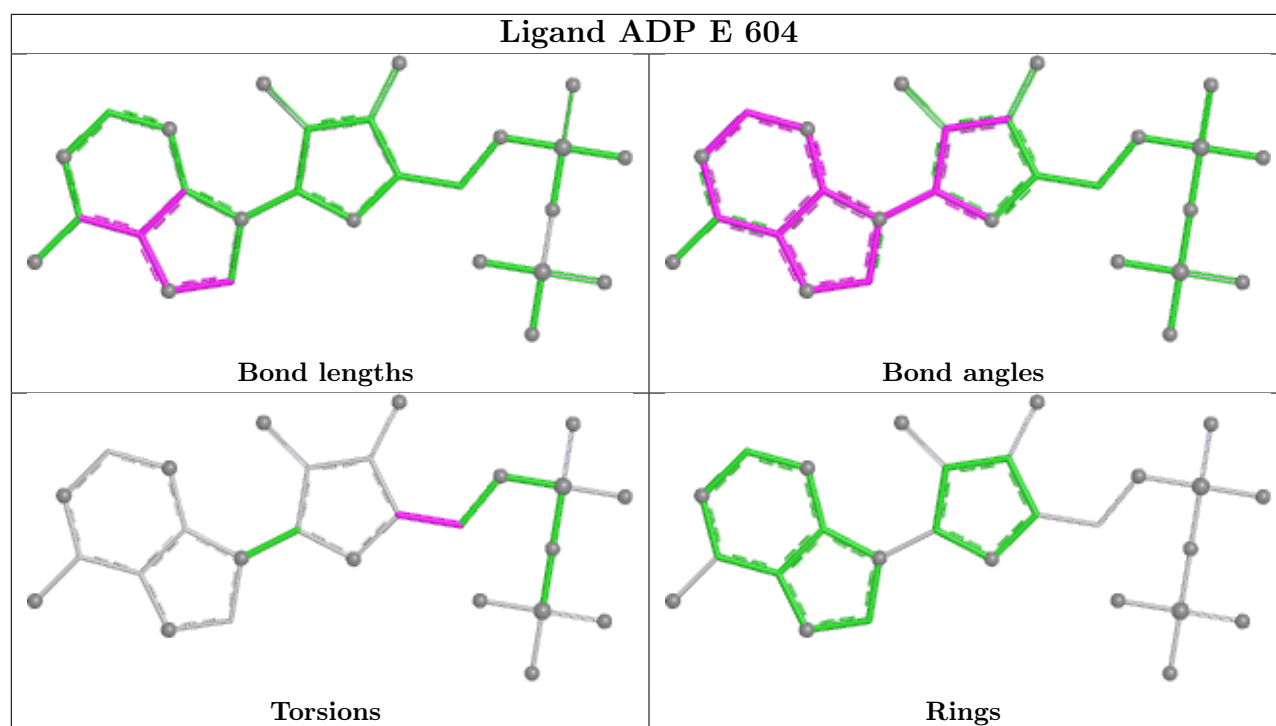


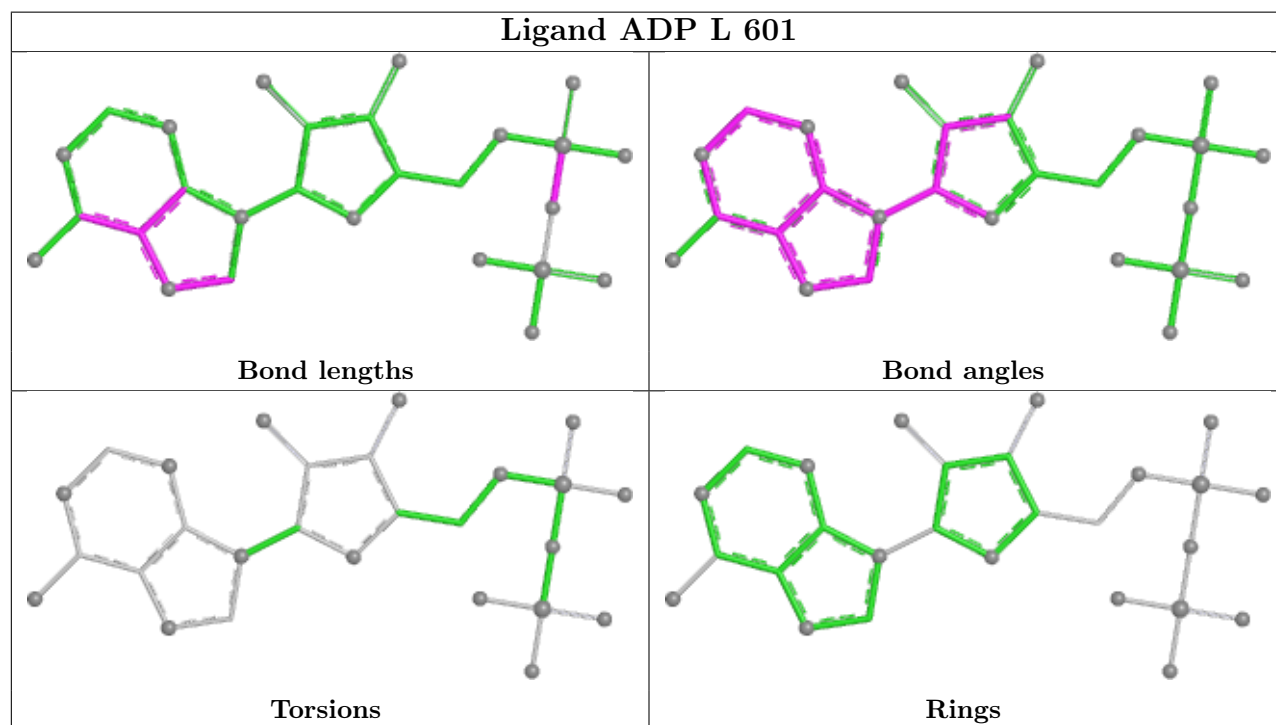
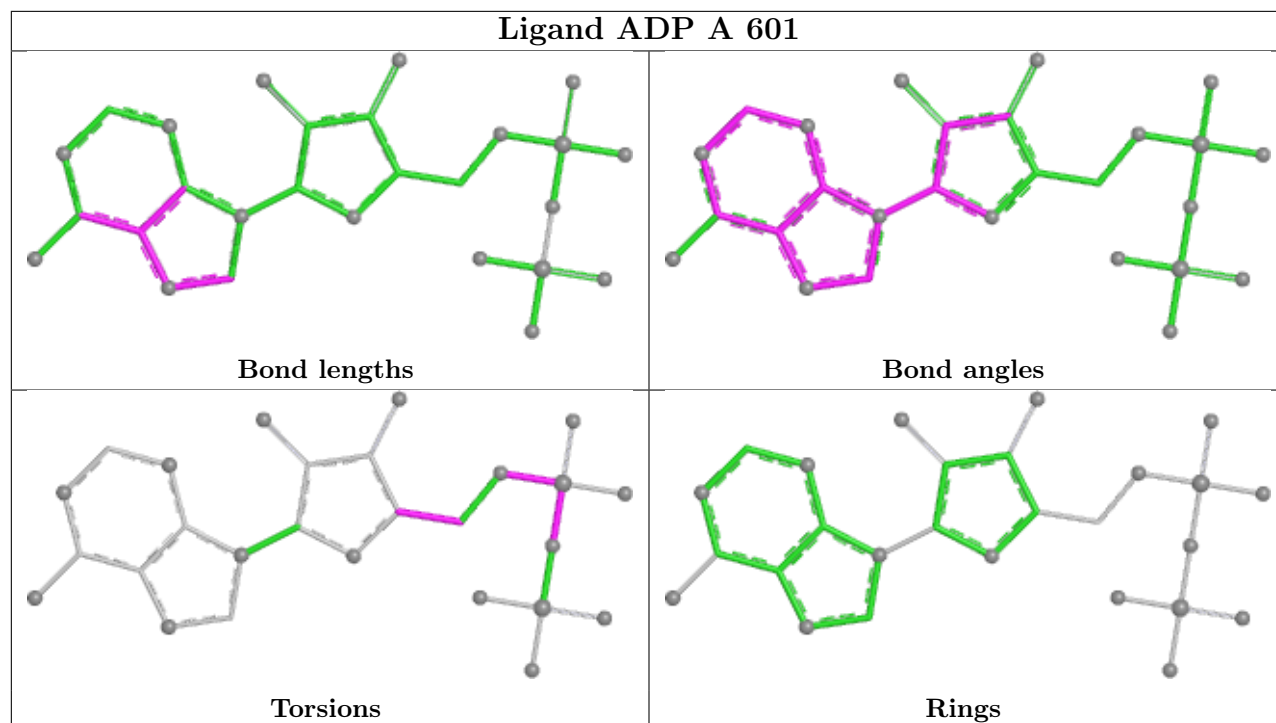


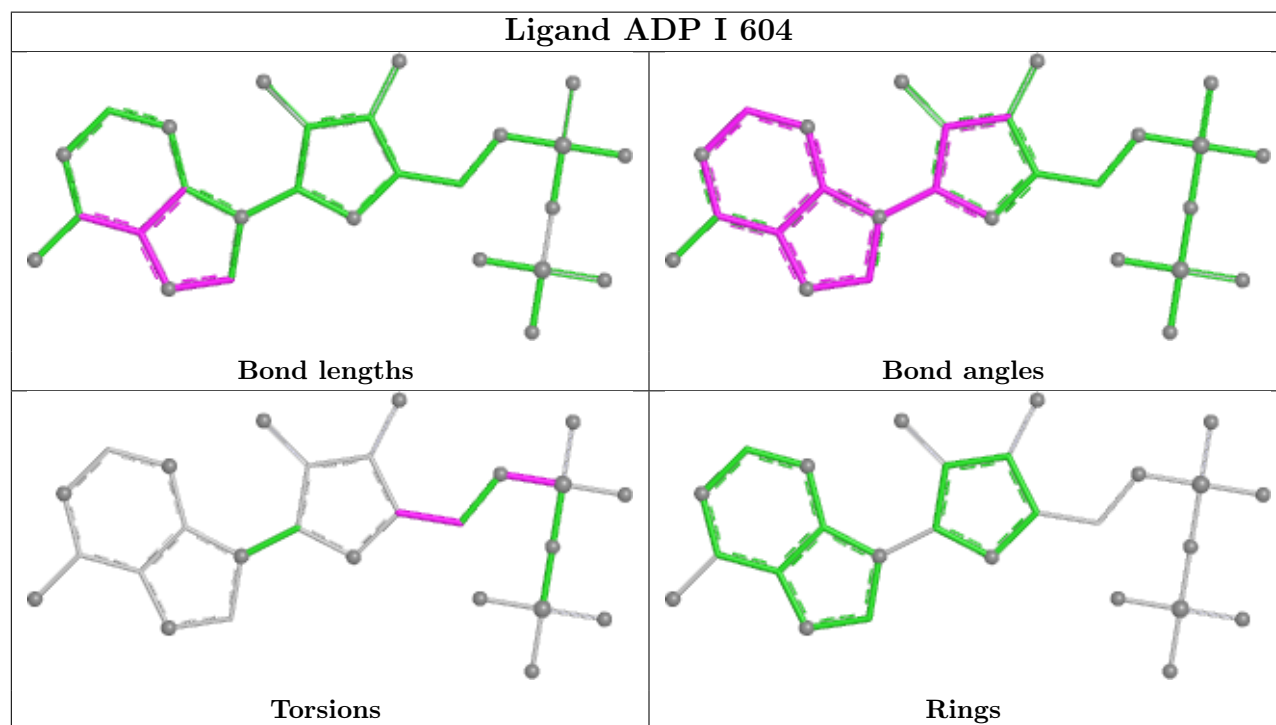
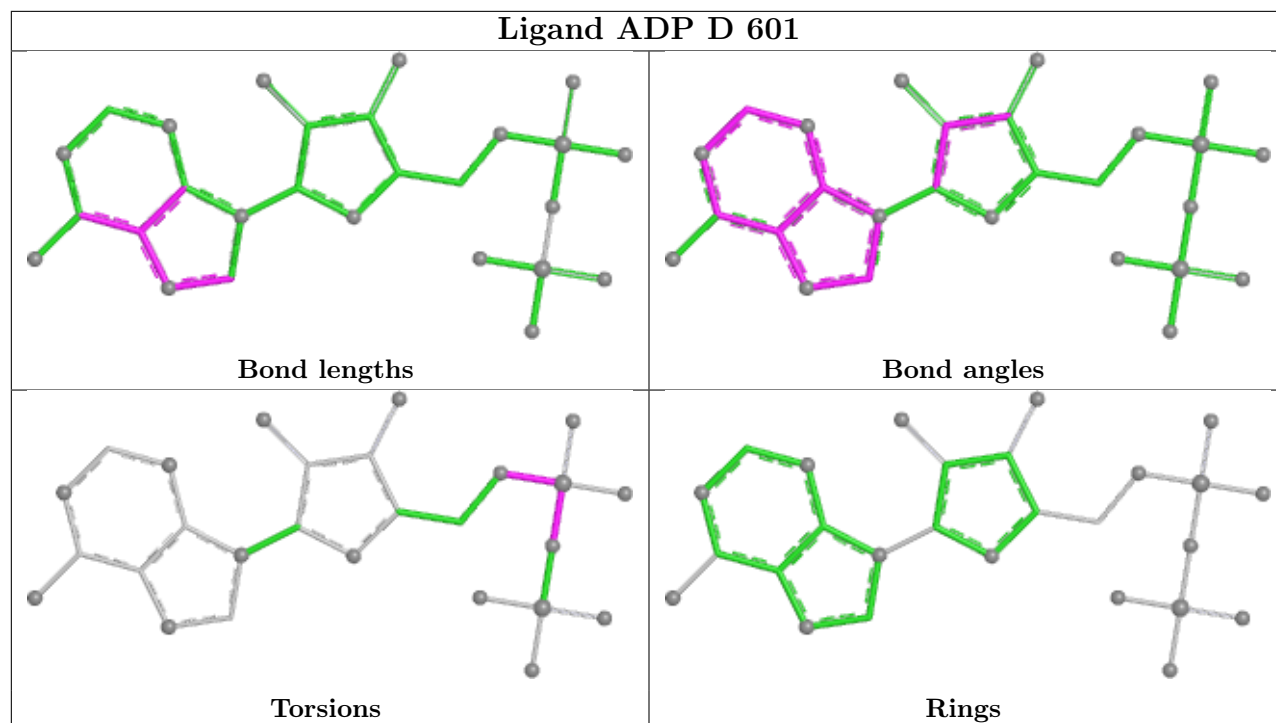


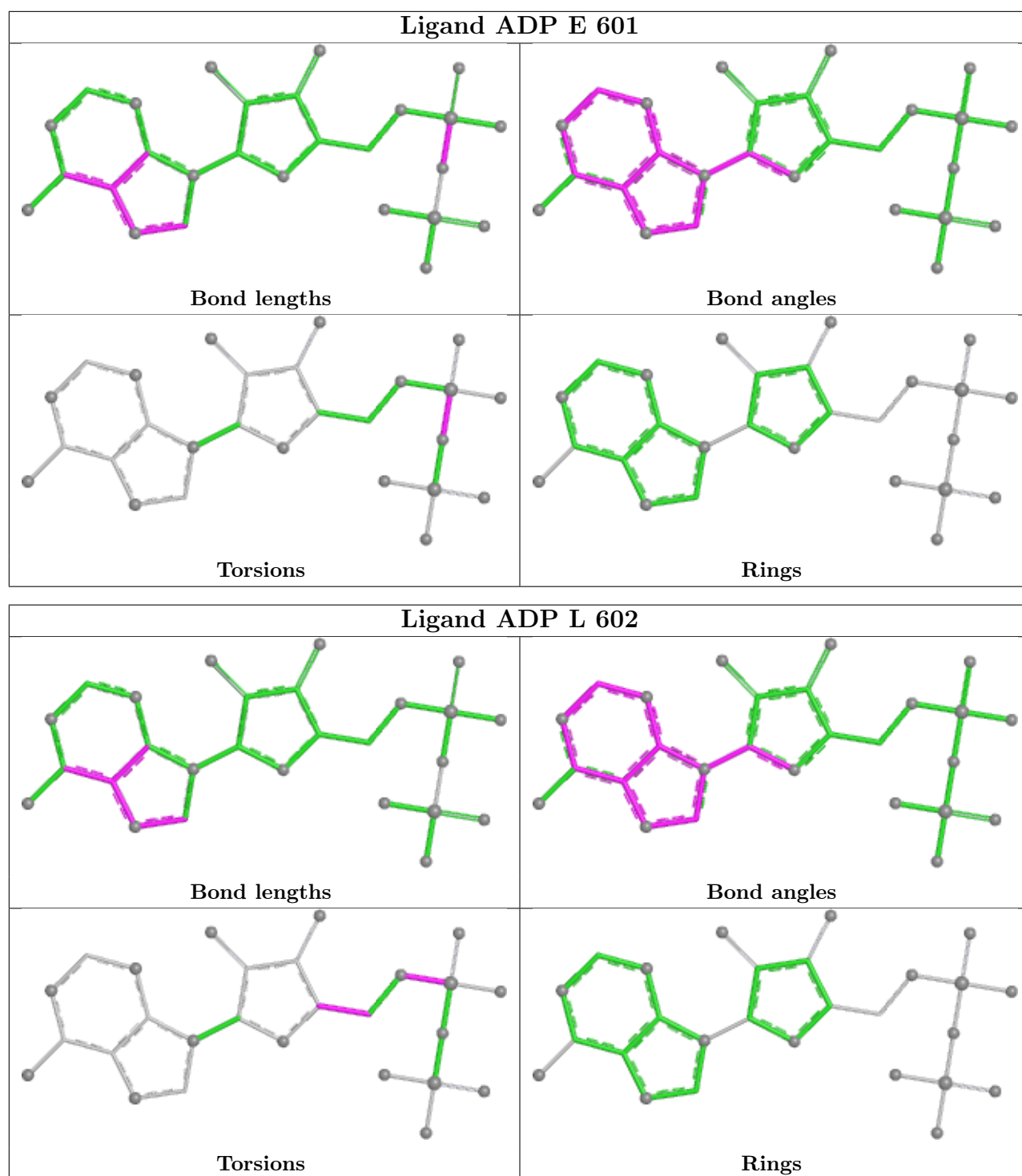












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	507/568 (89%)	-0.18	0 100 100	58, 106, 178, 225	0
1	B	505/568 (88%)	-0.16	0 100 100	54, 109, 158, 180	0
1	C	508/568 (89%)	-0.20	0 100 100	59, 108, 167, 206	0
1	D	510/568 (89%)	-0.15	0 100 100	63, 100, 158, 229	0
1	E	511/568 (89%)	-0.18	2 (0%) 88 72	57, 97, 150, 191	0
1	F	500/568 (88%)	-0.19	2 (0%) 88 72	43, 104, 153, 217	0
1	G	518/568 (91%)	-0.17	2 (0%) 88 72	57, 109, 176, 238	0
1	H	509/568 (89%)	-0.20	0 100 100	47, 101, 162, 230	0
1	I	494/568 (86%)	-0.14	0 100 100	62, 110, 163, 190	0
1	J	510/568 (89%)	-0.09	3 (0%) 85 65	71, 133, 188, 224	0
1	K	508/568 (89%)	-0.07	4 (0%) 82 60	69, 126, 180, 217	0
1	L	503/568 (88%)	-0.12	2 (0%) 88 72	50, 117, 181, 199	0
All	All	6083/6816 (89%)	-0.15	15 (0%) 91 82	43, 109, 172, 238	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	368	THR	3.6
1	J	265	GLY	2.9
1	E	254	ASP	2.8
1	F	266	SER	2.6
1	F	265	GLY	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	605	1/1	0.80	0.20	84,84,84,84	0
3	MG	I	603	1/1	0.82	0.15	79,79,79,79	0
3	MG	F	602	1/1	0.85	0.19	82,82,82,82	0
2	ADP	L	601	27/27	0.86	0.12	94,126,152,158	0
2	ADP	B	601	27/27	0.86	0.12	87,114,141,141	0
3	MG	D	602	1/1	0.87	0.14	85,85,85,85	0
2	ADP	A	604	27/27	0.87	0.13	69,88,114,127	0
2	ADP	J	601	27/27	0.87	0.12	105,136,162,167	0
2	ADP	K	601	27/27	0.88	0.08	108,131,158,171	0
2	ADP	A	601	27/27	0.88	0.10	95,112,137,158	0
3	MG	J	603	1/1	0.88	0.07	104,104,104,104	0
2	ADP	C	601	27/27	0.89	0.11	73,95,115,117	0
2	ADP	F	601	27/27	0.89	0.12	72,117,146,151	0
2	ADP	B	604	27/27	0.90	0.10	58,75,91,106	0
3	MG	K	603	1/1	0.90	0.07	85,85,85,85	0
2	ADP	I	604	27/27	0.91	0.09	69,104,130,139	0
2	ADP	K	604	27/27	0.91	0.10	77,106,129,131	0
2	ADP	H	601	27/27	0.91	0.11	68,95,134,137	0
2	ADP	G	604	27/27	0.92	0.10	47,77,119,137	0
3	MG	A	602	1/1	0.92	0.09	76,76,76,76	0
3	MG	B	603	1/1	0.92	0.10	65,65,65,65	0
3	MG	J	602	1/1	0.92	0.14	62,62,62,62	0
2	ADP	C	604	27/27	0.92	0.11	72,87,114,123	0
3	MG	C	602	1/1	0.92	0.23	63,63,63,63	0
2	ADP	G	601	27/27	0.93	0.09	89,114,139,143	0
2	ADP	E	604	27/27	0.93	0.12	51,78,112,113	0
3	MG	G	602	1/1	0.93	0.19	46,46,46,46	0
3	MG	H	602	1/1	0.93	0.14	77,77,77,77	0
2	ADP	J	604	27/27	0.93	0.09	64,84,108,124	0
2	ADP	D	601	27/27	0.93	0.12	72,97,132,137	0
2	ADP	H	603	27/27	0.93	0.11	65,93,117,137	0
3	MG	C	603	1/1	0.93	0.05	98,98,98,98	0

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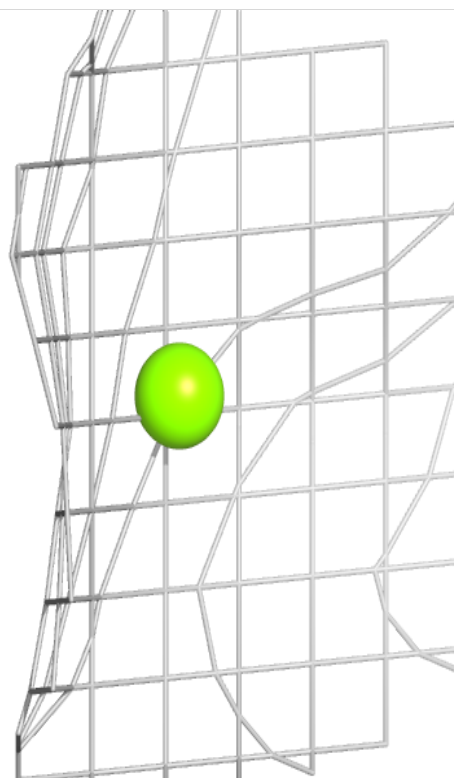
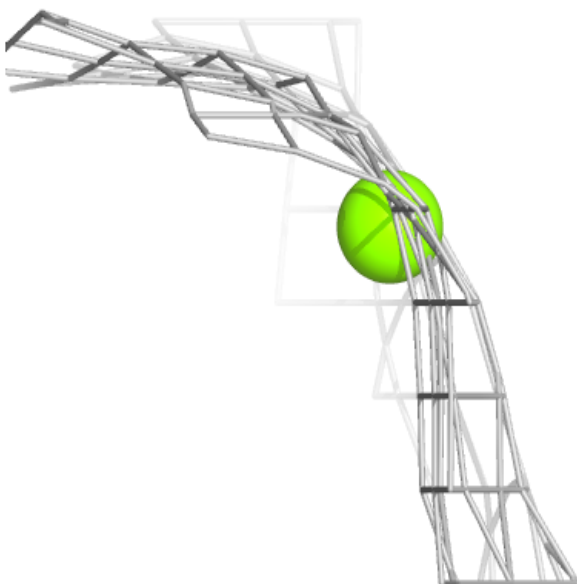
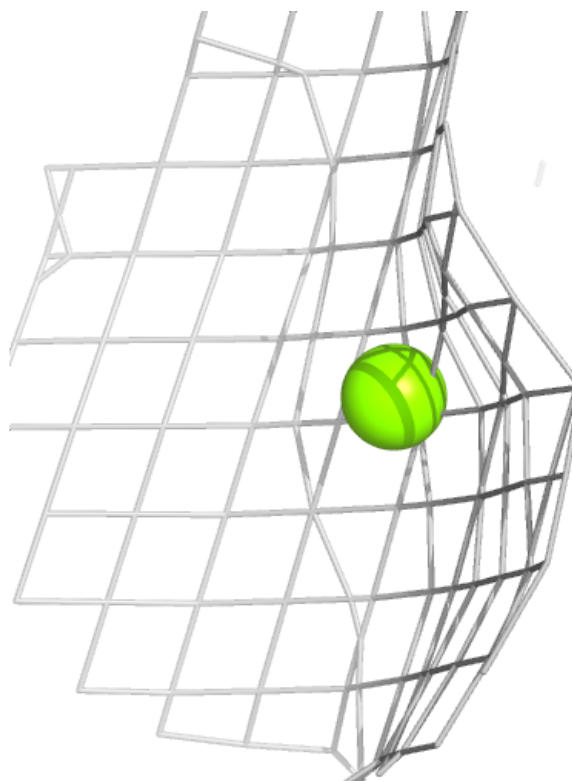
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	603	1/1	0.94	0.06	98,98,98,98	0
2	ADP	E	601	27/27	0.94	0.09	60,91,112,122	0
3	MG	D	603	1/1	0.94	0.14	68,68,68,68	0
2	ADP	I	601	27/27	0.94	0.09	100,123,156,158	0
3	MG	K	602	1/1	0.94	0.09	70,70,70,70	0
2	ADP	D	604	27/27	0.94	0.10	57,77,98,106	0
3	MG	H	604	1/1	0.95	0.07	77,77,77,77	0
3	MG	B	602	1/1	0.95	0.09	36,36,36,36	0
2	ADP	F	603	27/27	0.95	0.09	58,94,119,126	0
3	MG	G	605	1/1	0.96	0.15	58,58,58,58	0
2	ADP	L	602	27/27	0.96	0.07	41,78,99,103	0
3	MG	I	602	1/1	0.97	0.06	53,53,53,53	0
3	MG	E	602	1/1	0.97	0.15	46,46,46,46	0
3	MG	G	603	1/1	0.98	0.07	98,98,98,98	0
3	MG	E	603	1/1	0.99	0.05	66,66,66,66	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.

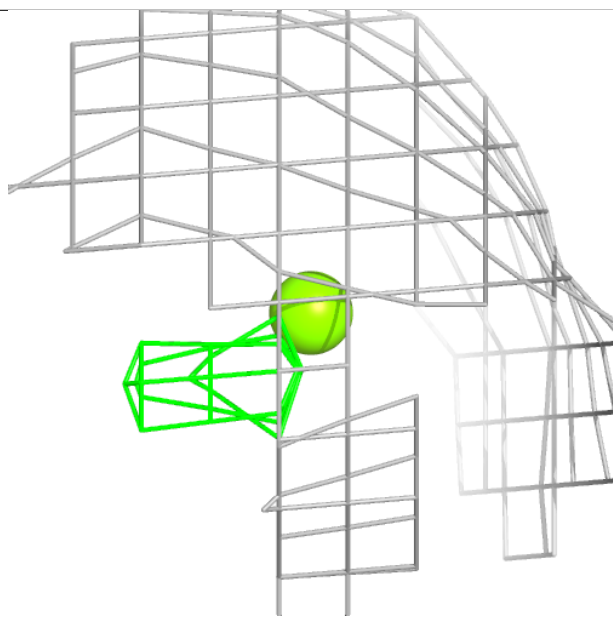
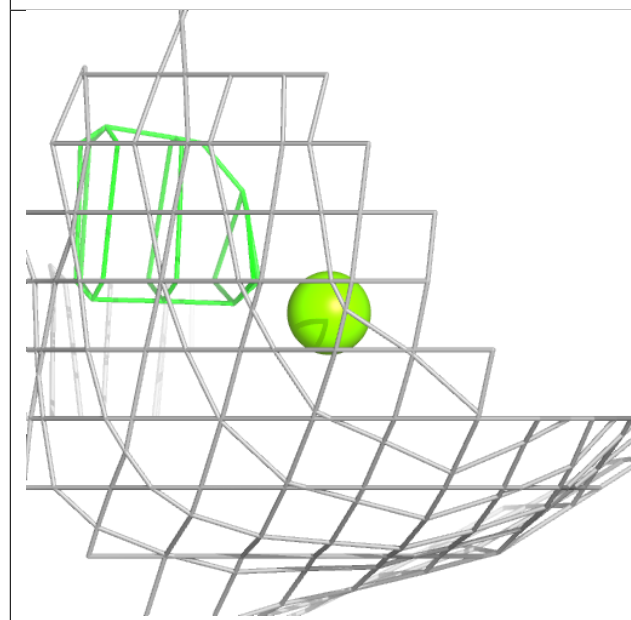
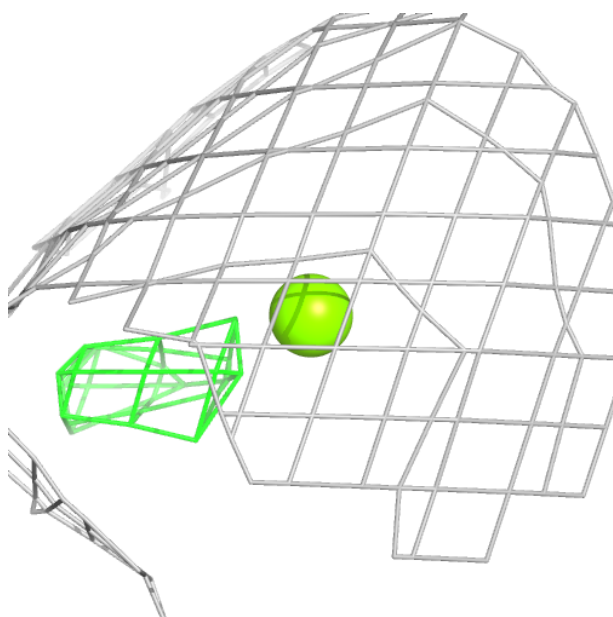
Electron density around MG B 605:

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



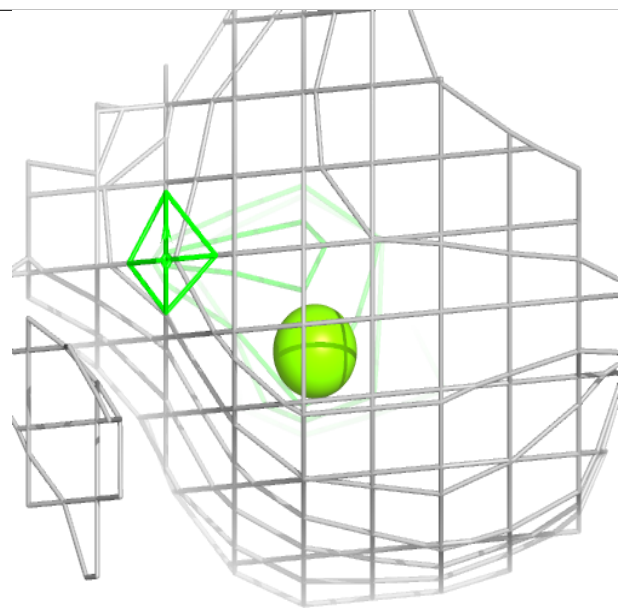
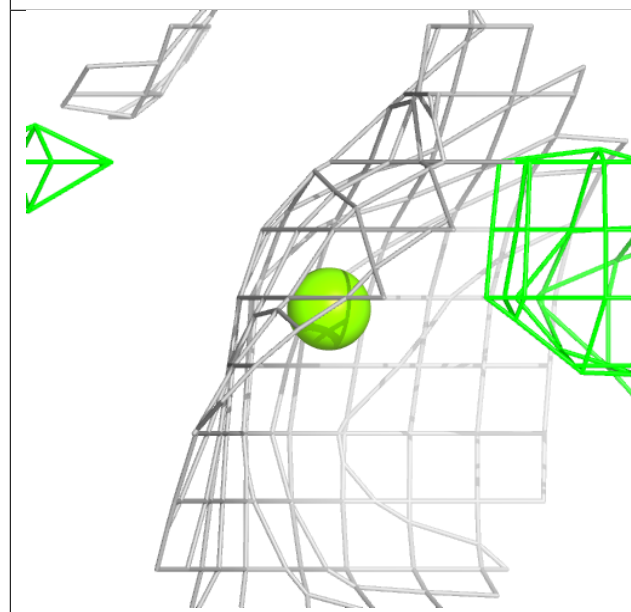
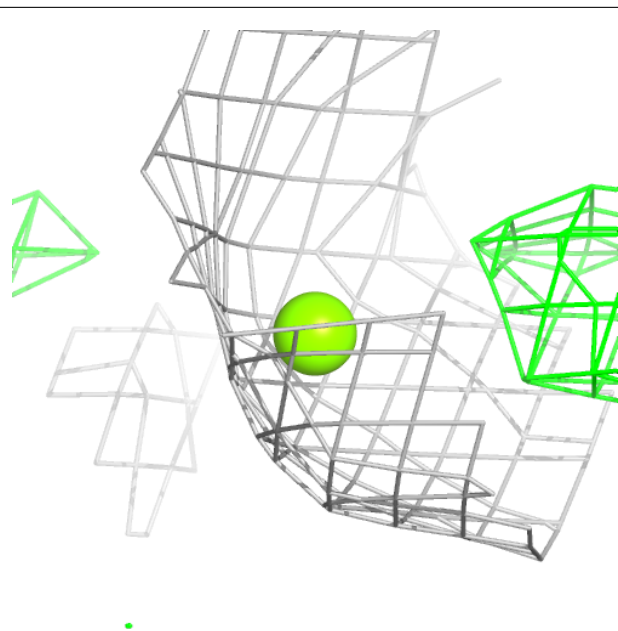
Electron density around MG I 603:

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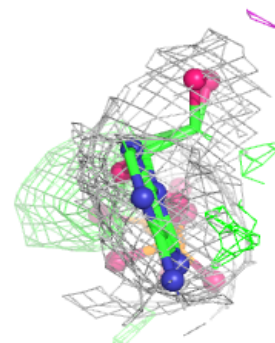
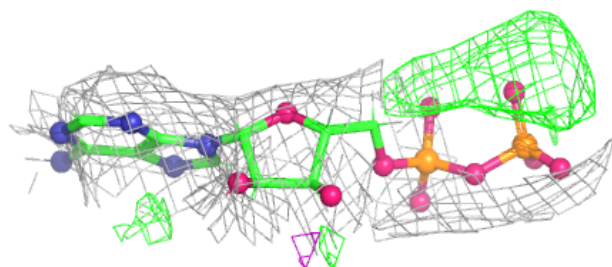
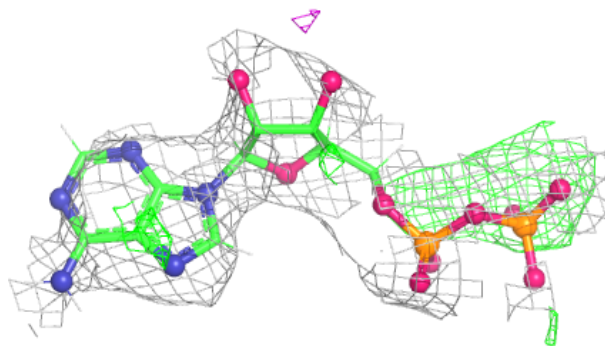
Electron density around MG F 602:

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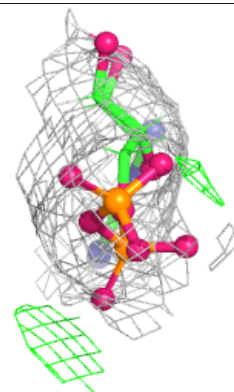
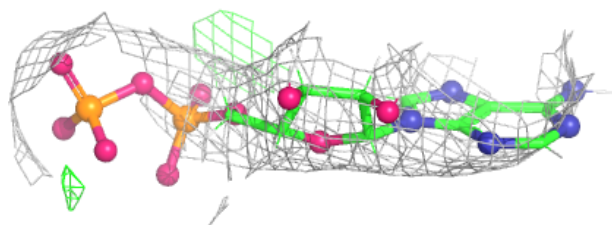
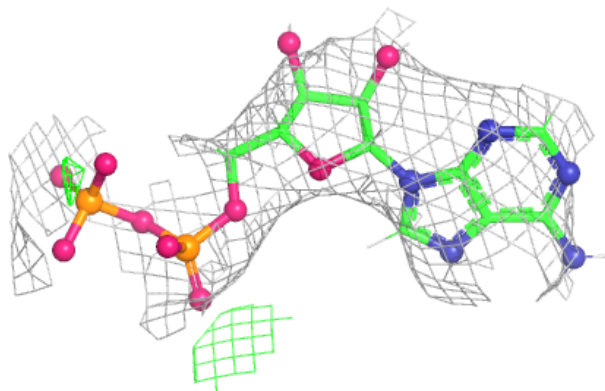


Electron density around ADP L 601:

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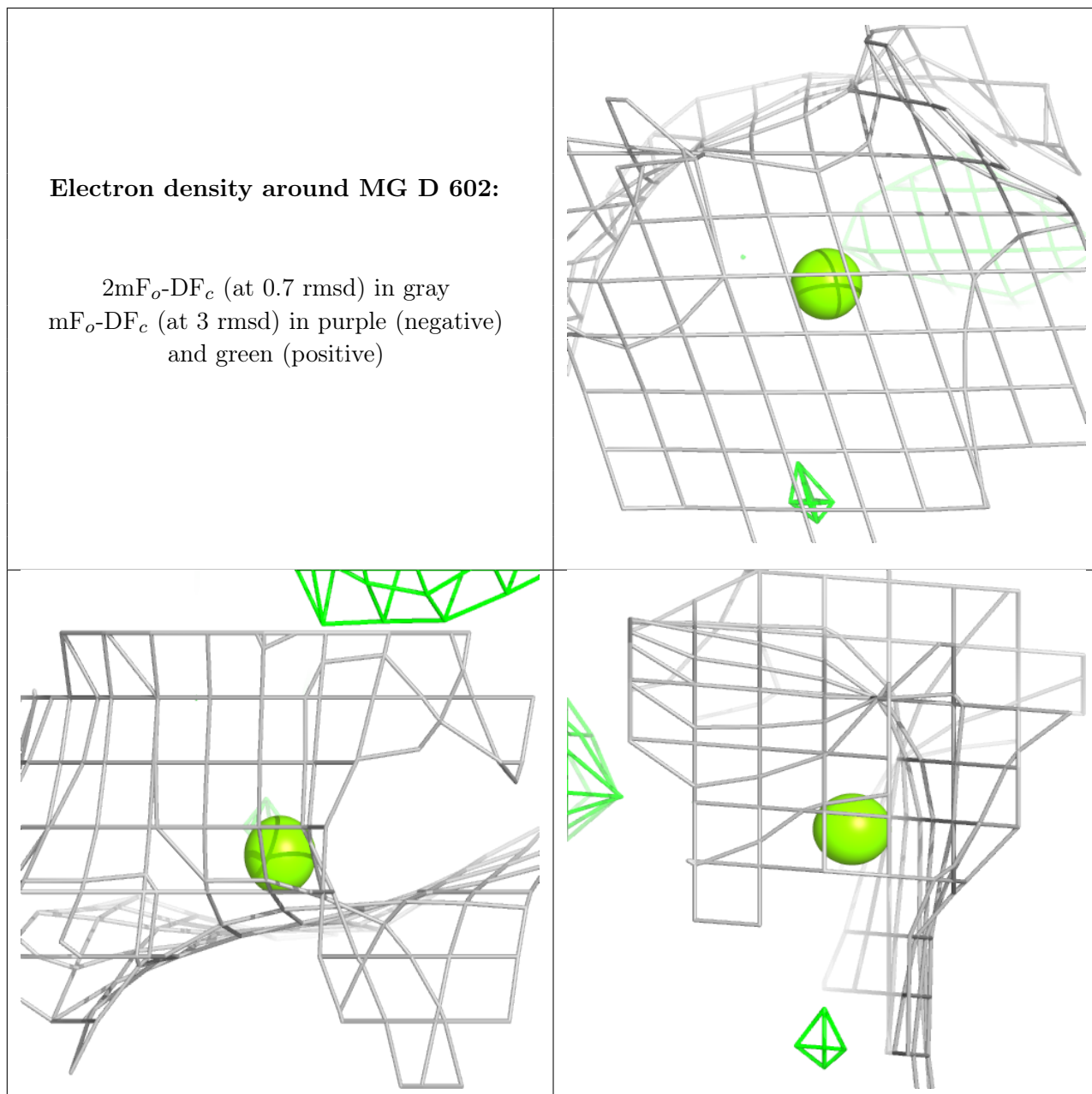
**Electron density around ADP B 601:**

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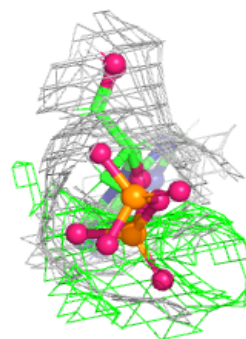
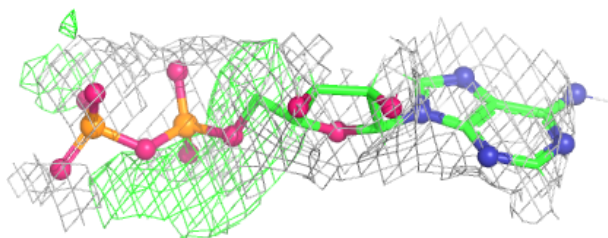
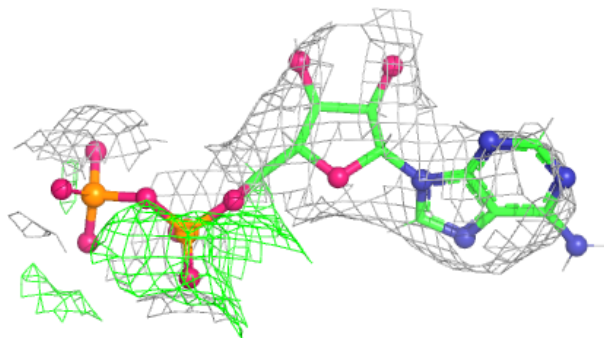
Electron density around MG D 602:

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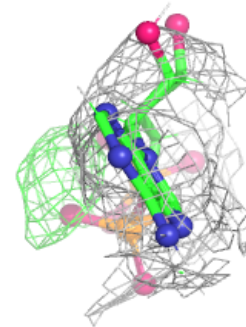
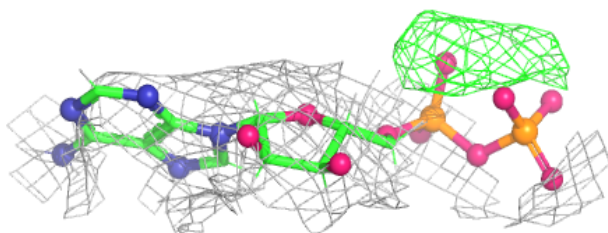
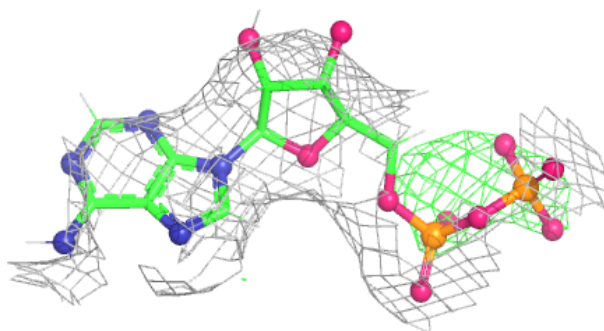


Electron density around ADP A 604:

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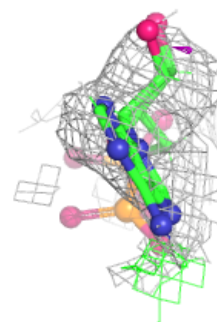
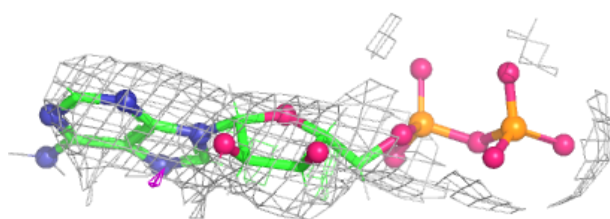
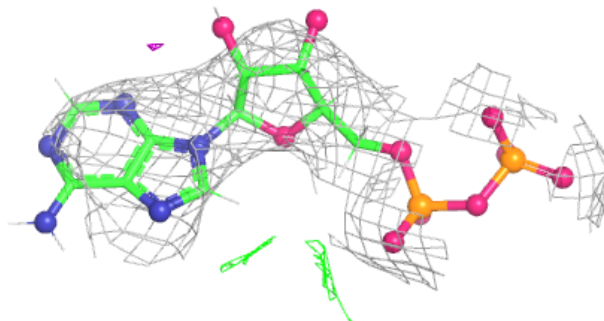
**Electron density around ADP J 601:**

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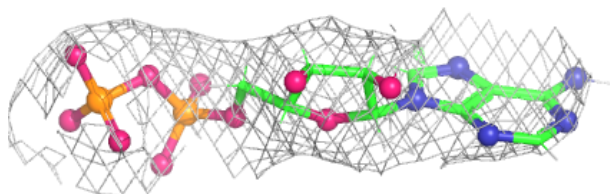
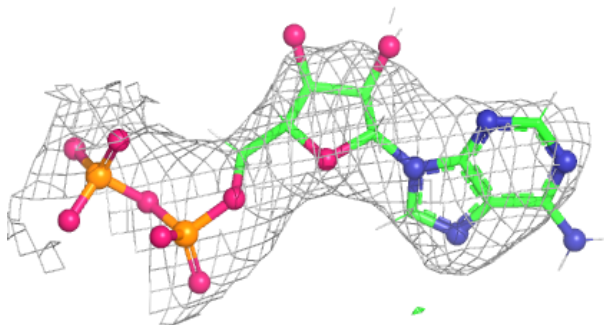


Electron density around ADP K 601:

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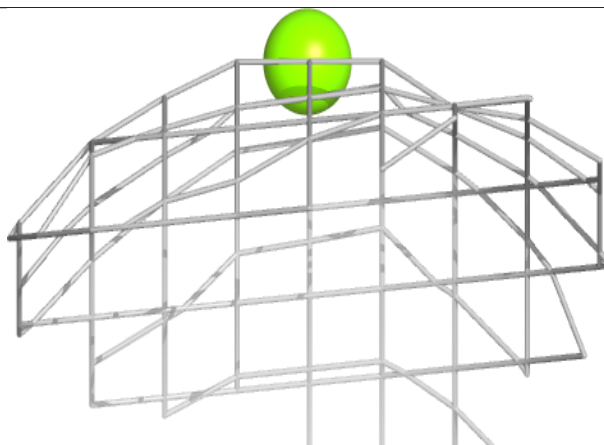
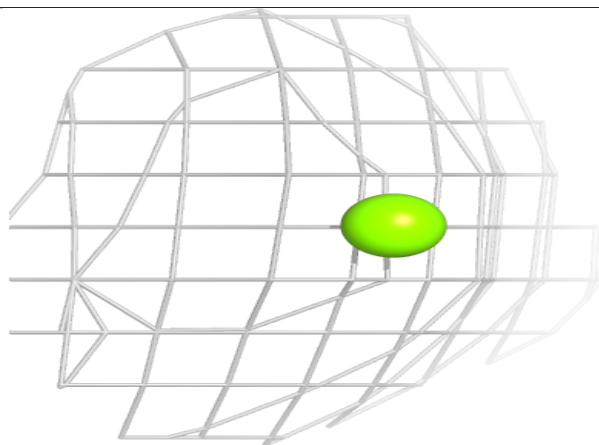
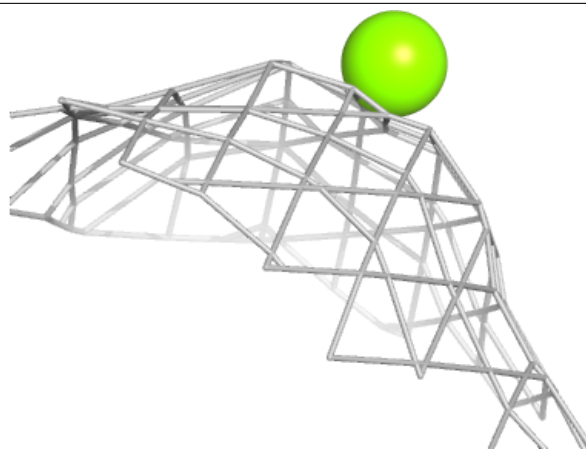
**Electron density around ADP A 601:**

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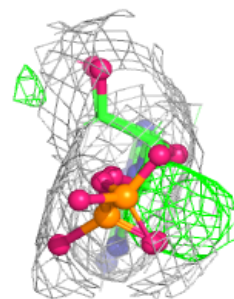
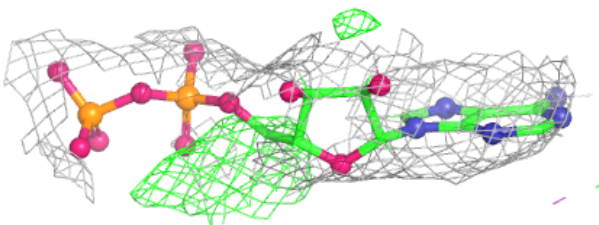
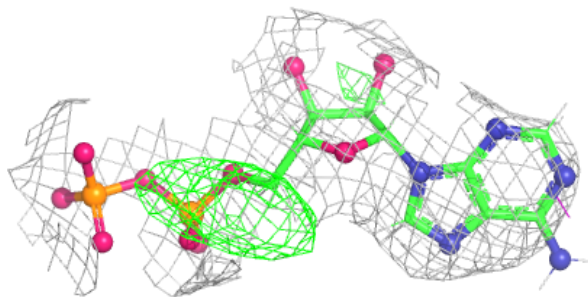


Electron density around MG J 603:

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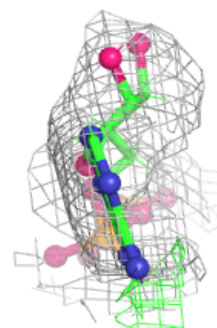
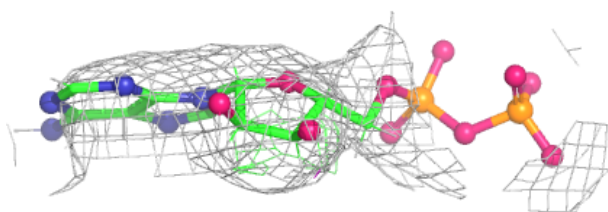
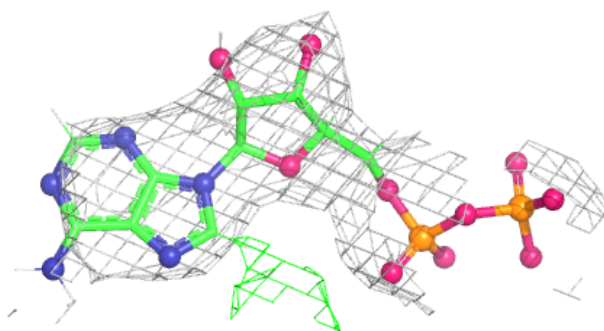
**Electron density around ADP C 601:**

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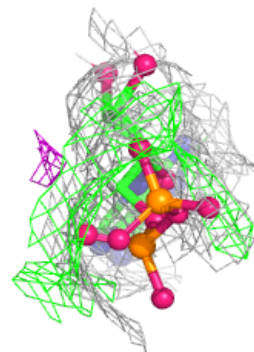
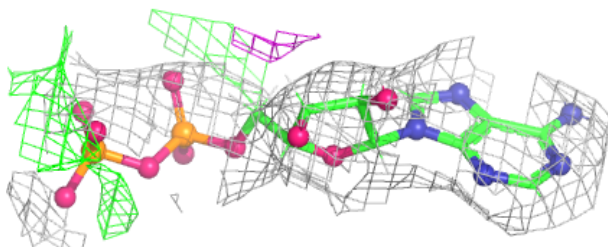
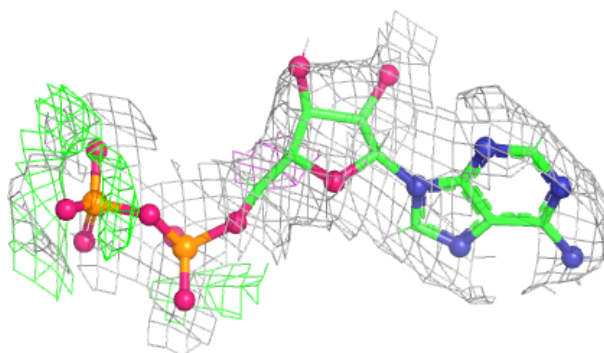


Electron density around ADP F 601:

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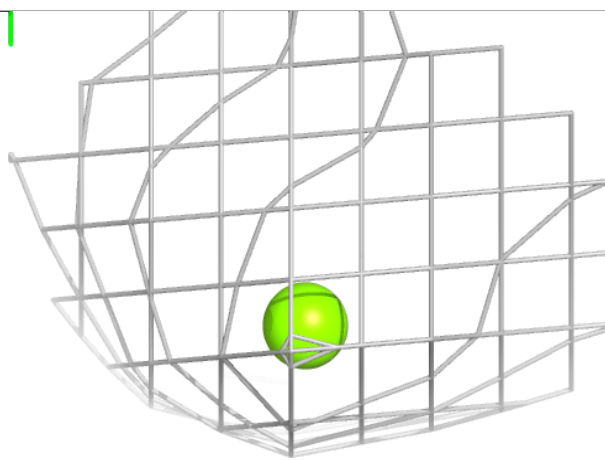
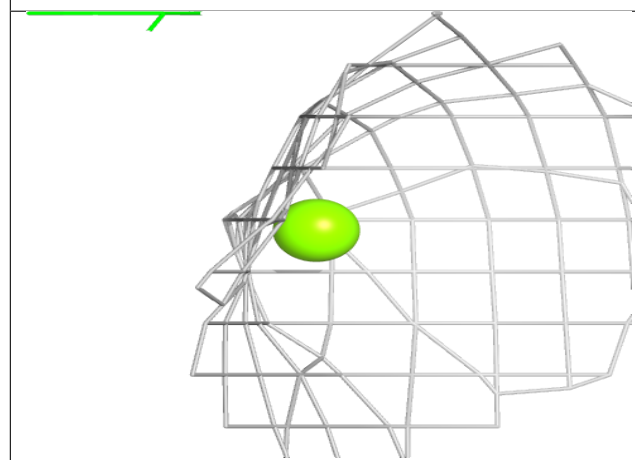
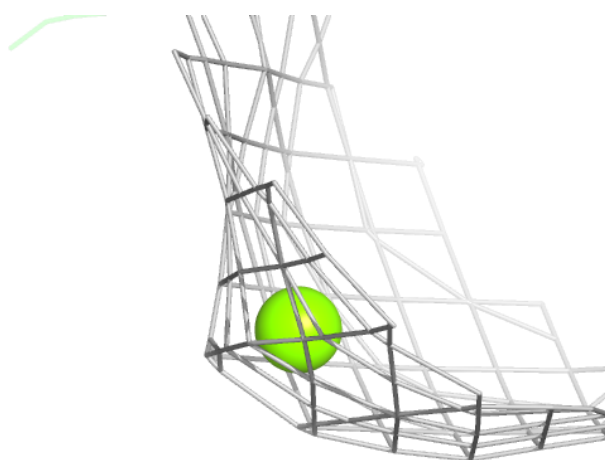
**Electron density around ADP B 604:**

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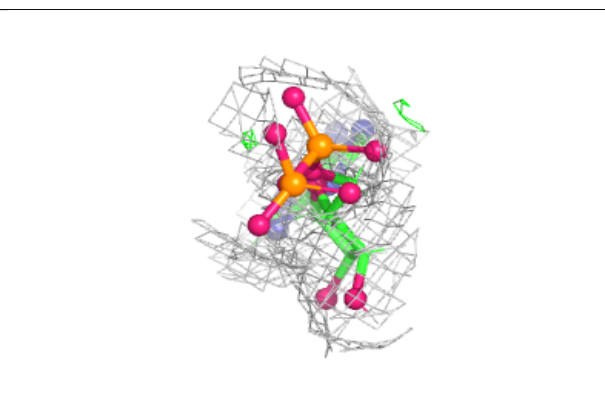
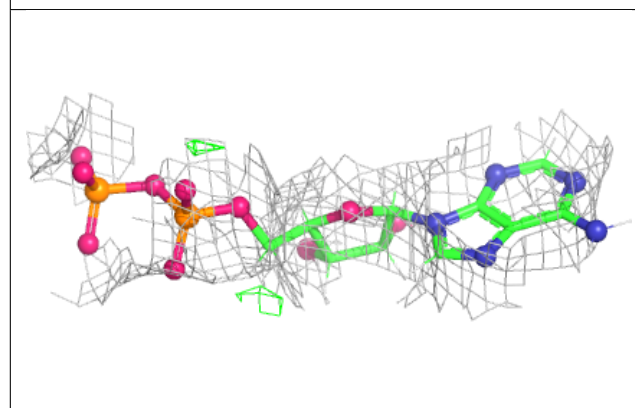
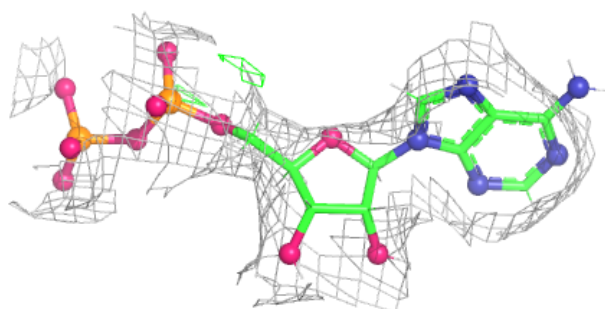


Electron density around MG K 603:

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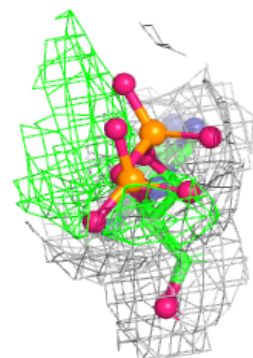
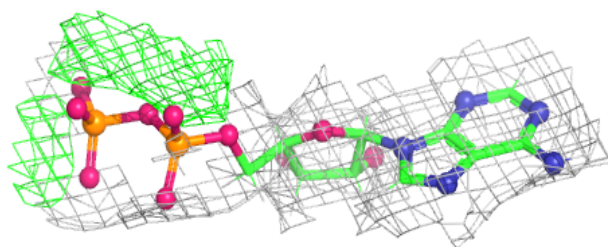
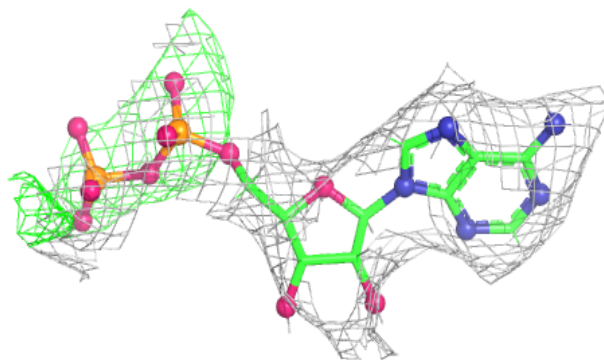
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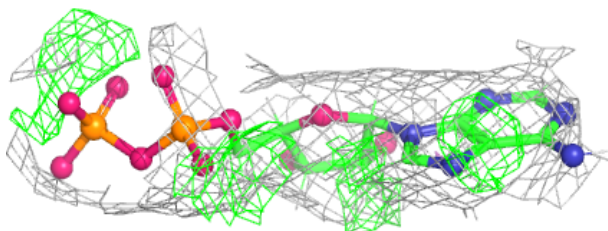
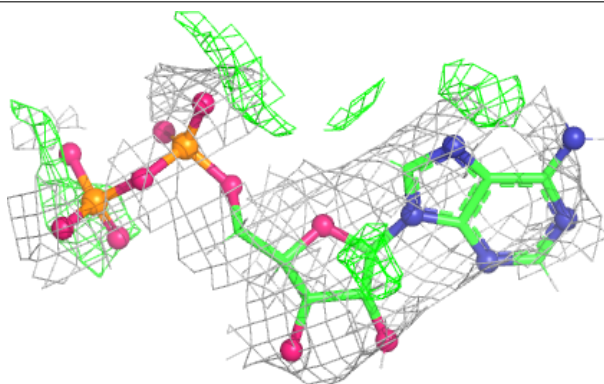


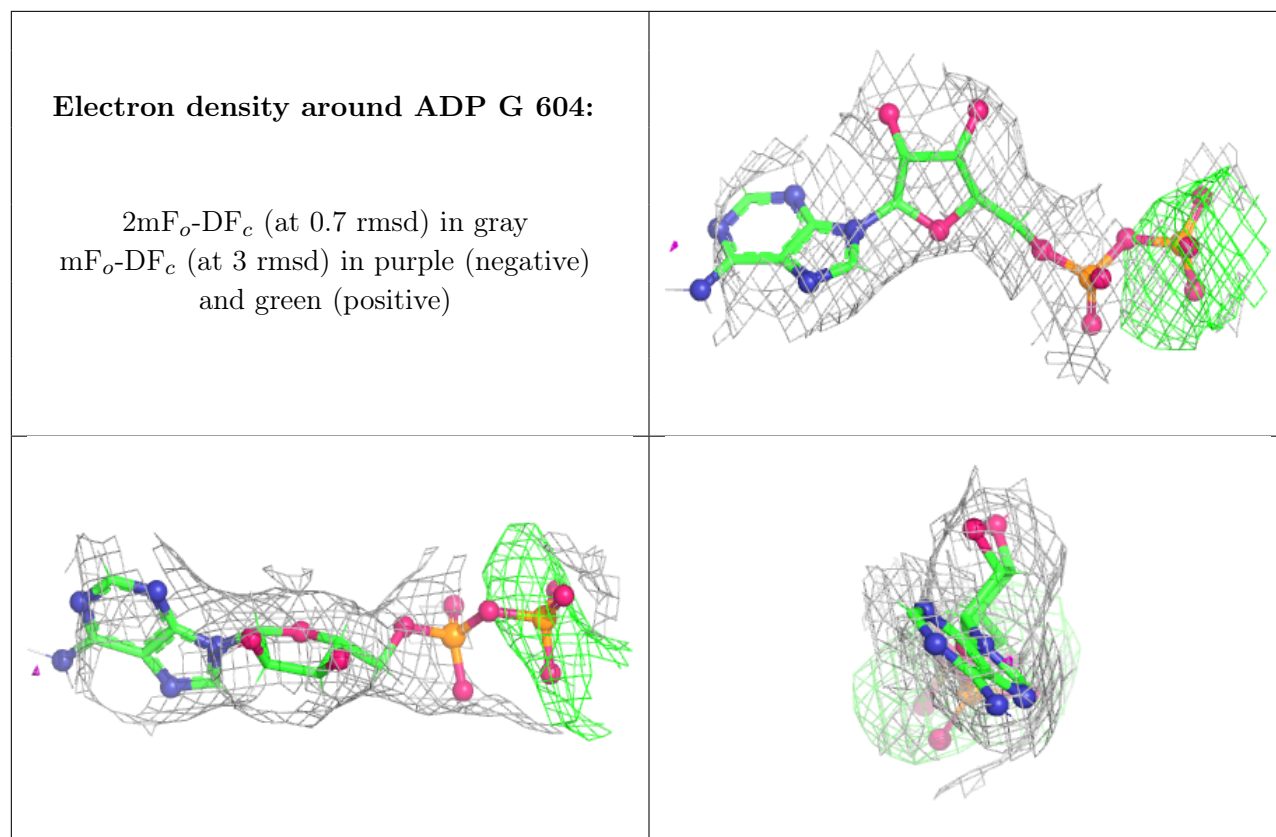
Electron density around ADP K 604:

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**Electron density around ADP H 601:**

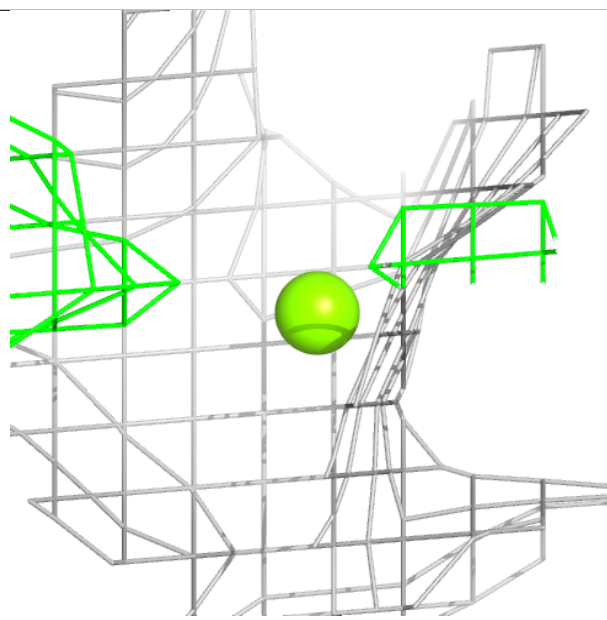
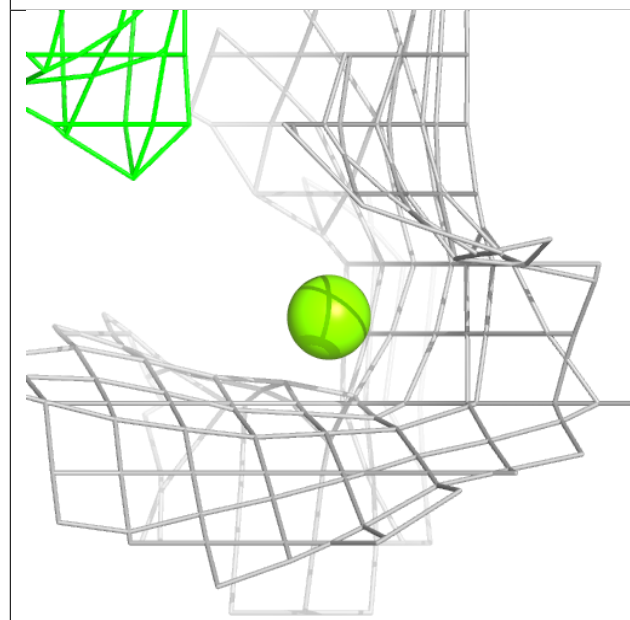
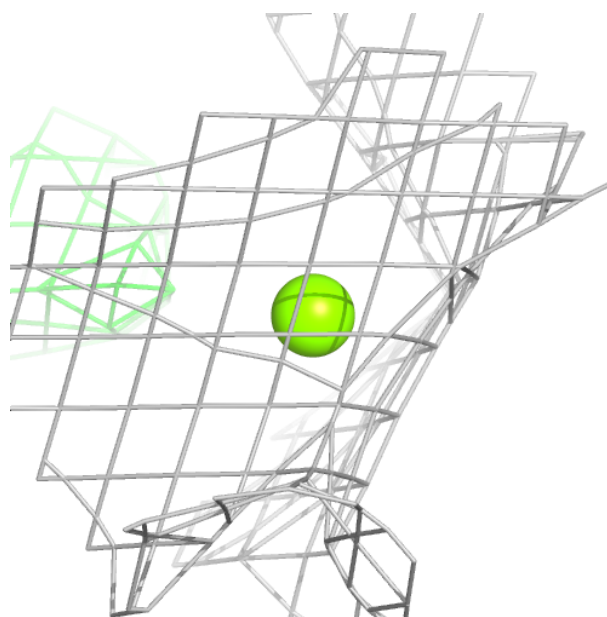
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and green (positive)





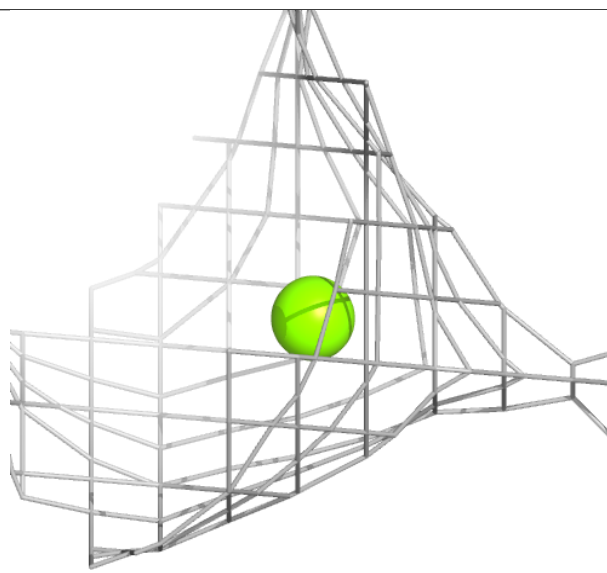
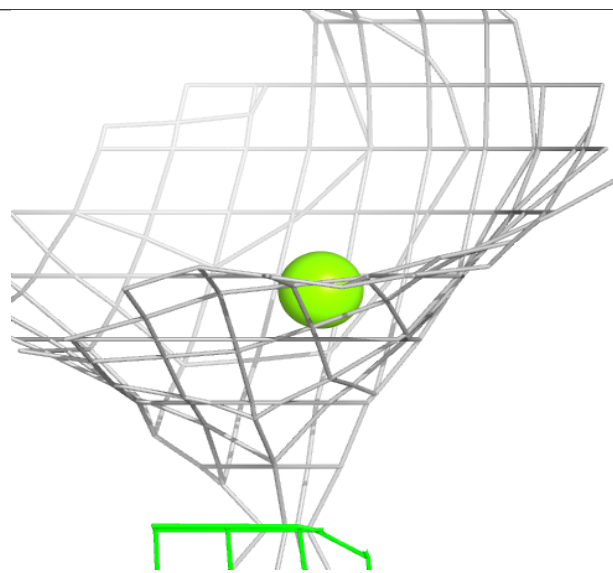
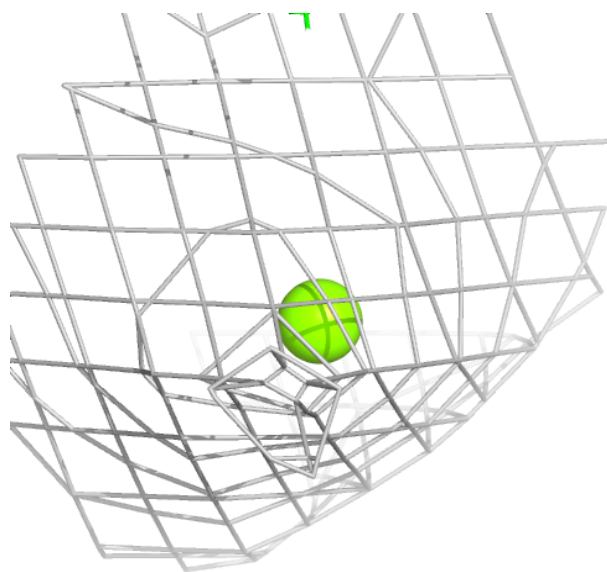
Electron density around MG A 602:

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and green (positive)



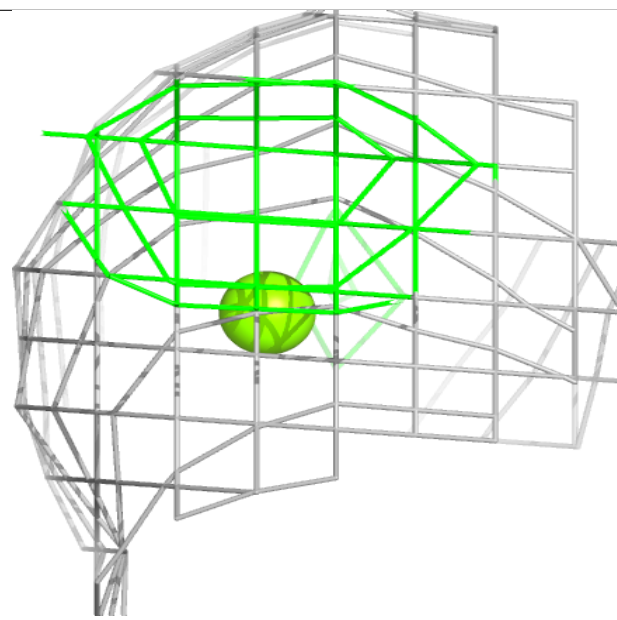
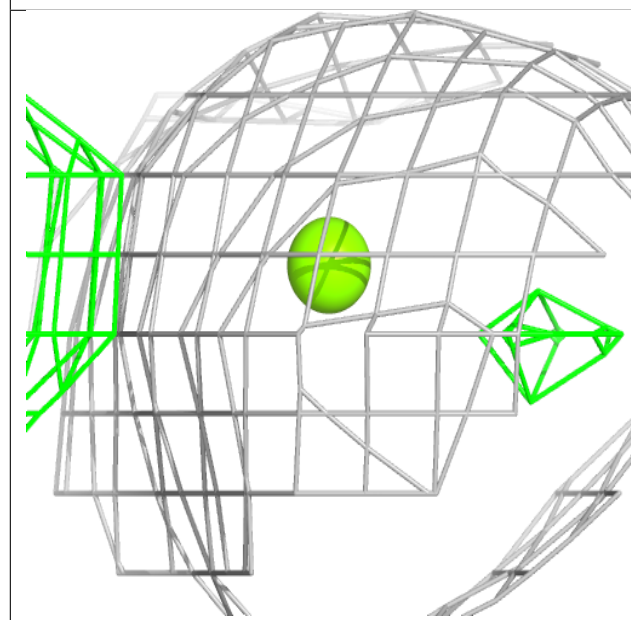
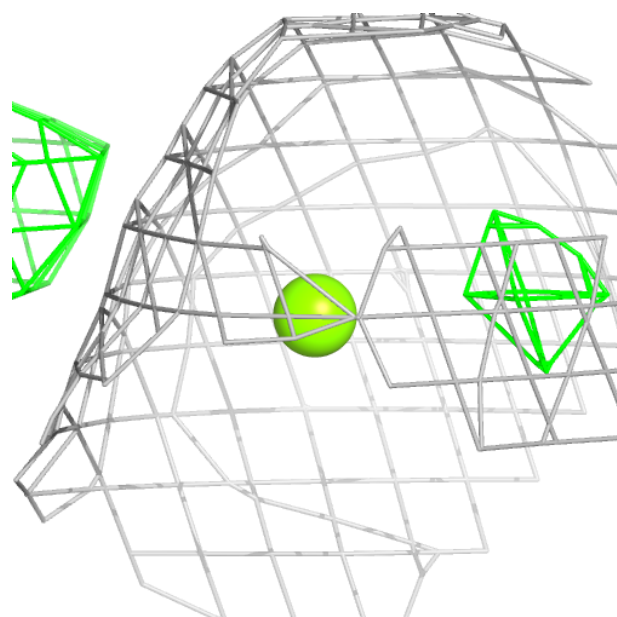
Electron density around MG B 603:

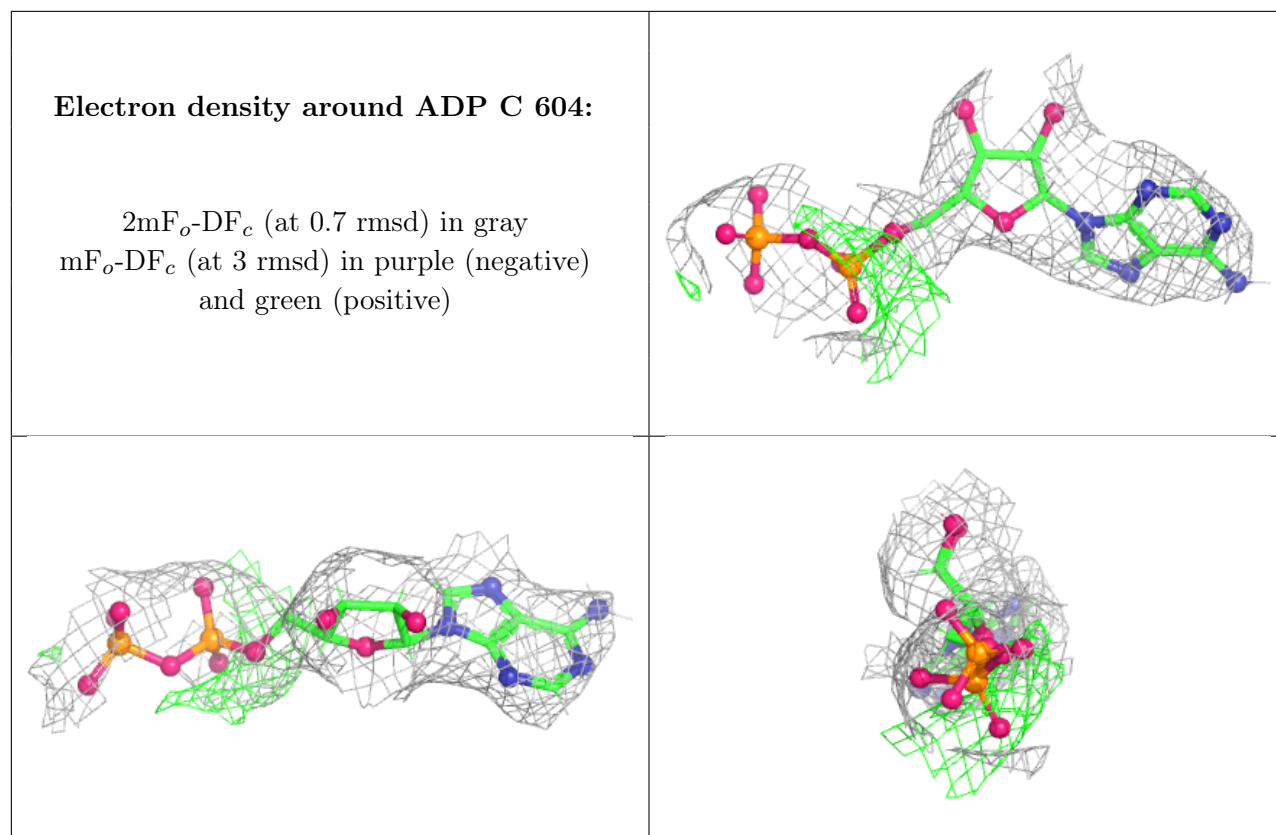
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Electron density around MG J 602:

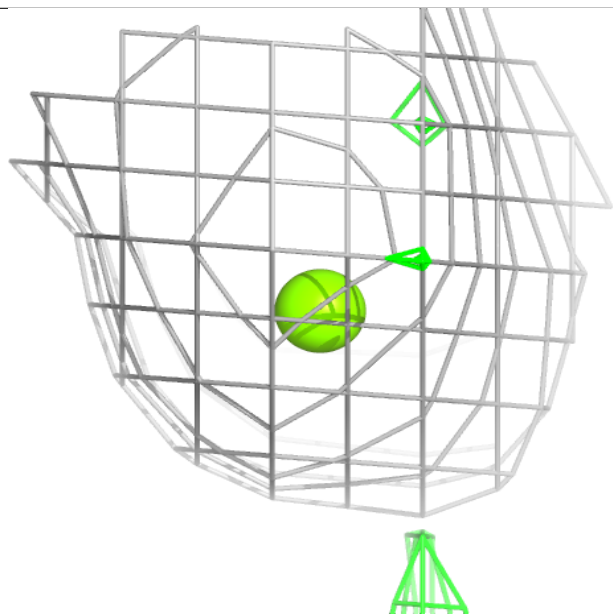
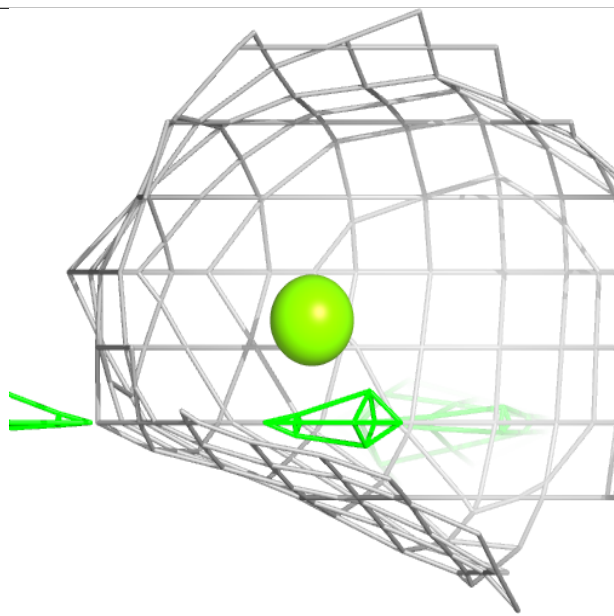
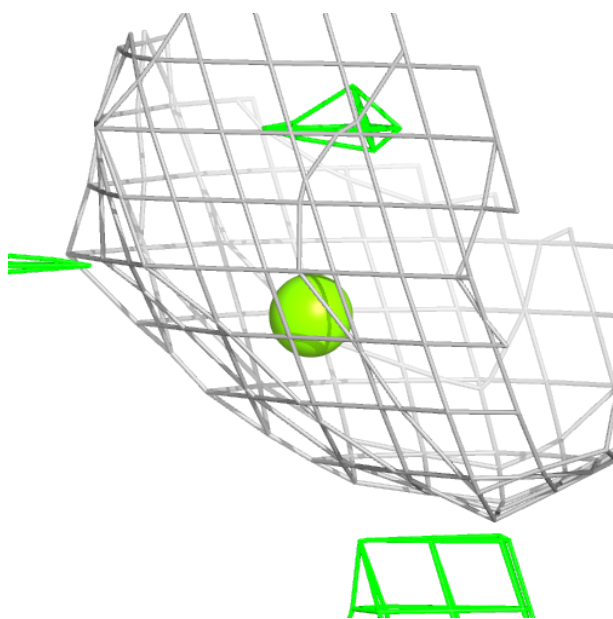
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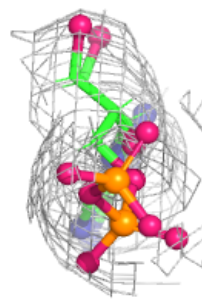
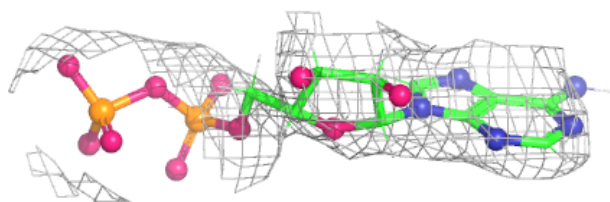
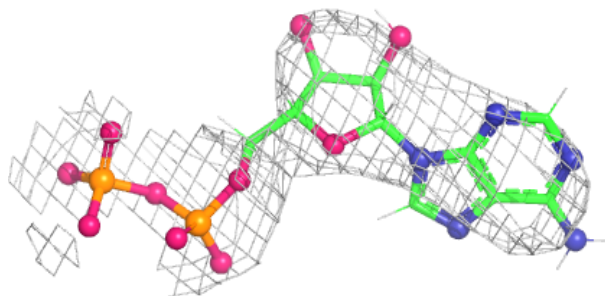
Electron density around MG C 602:

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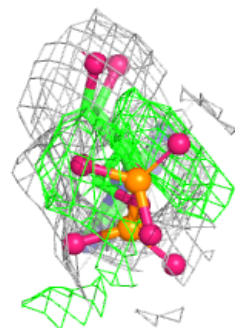
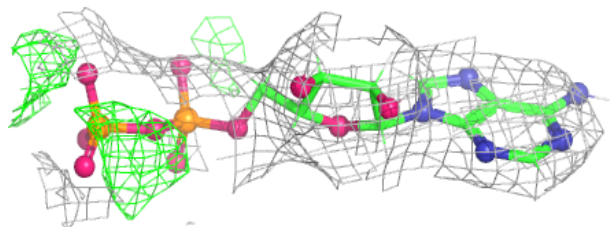
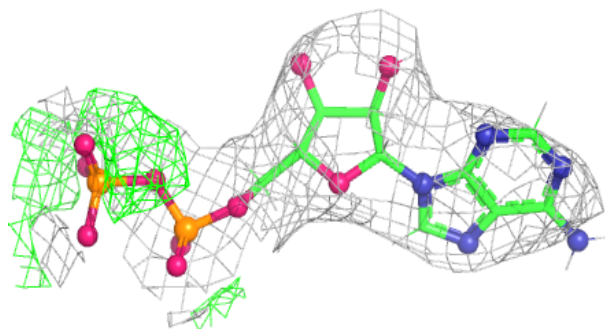


Electron density around ADP G 601:

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

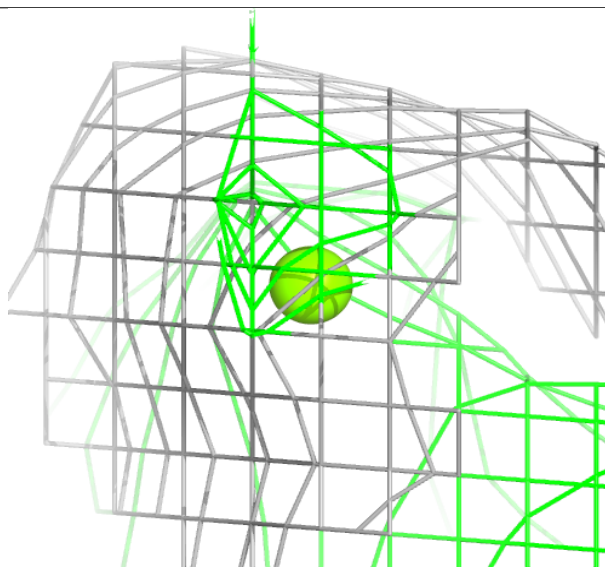
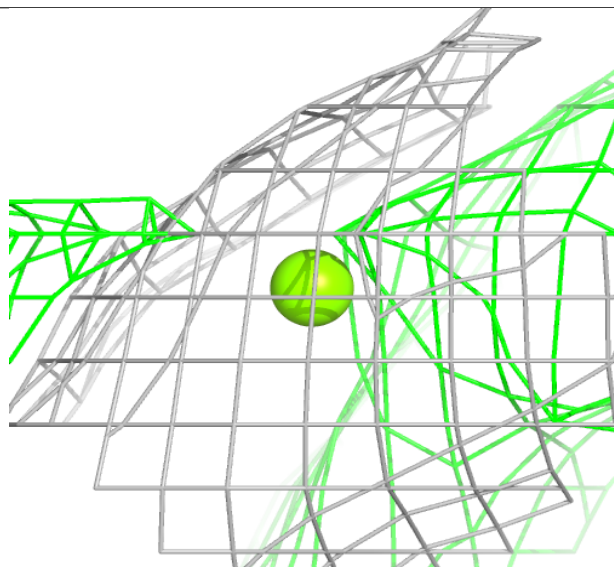
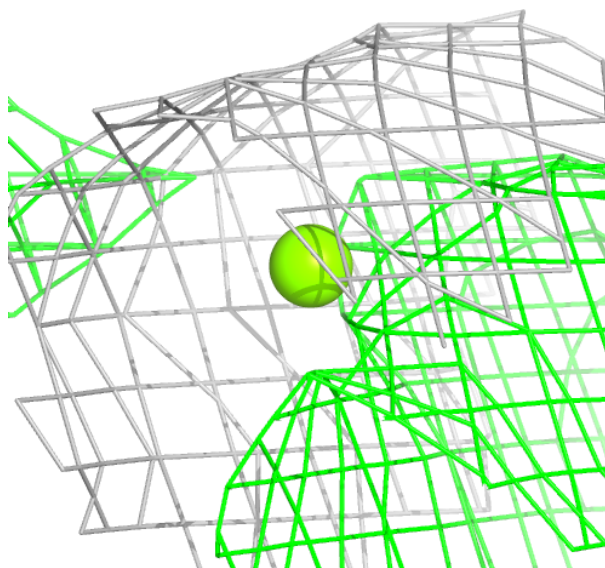
**Electron density around ADP E 604:**

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



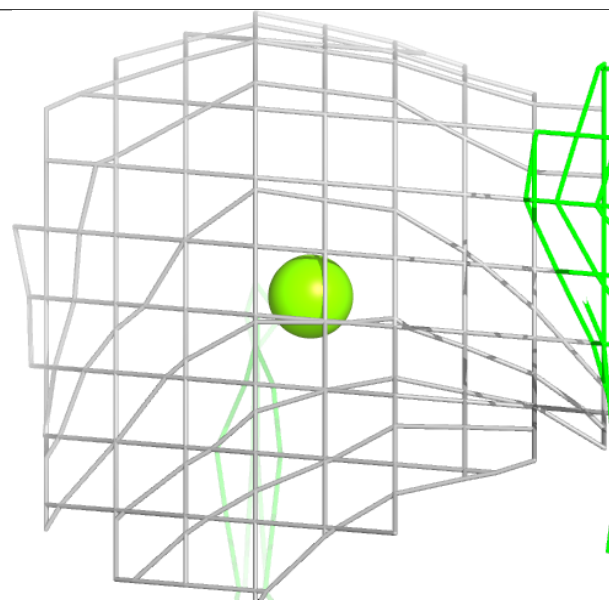
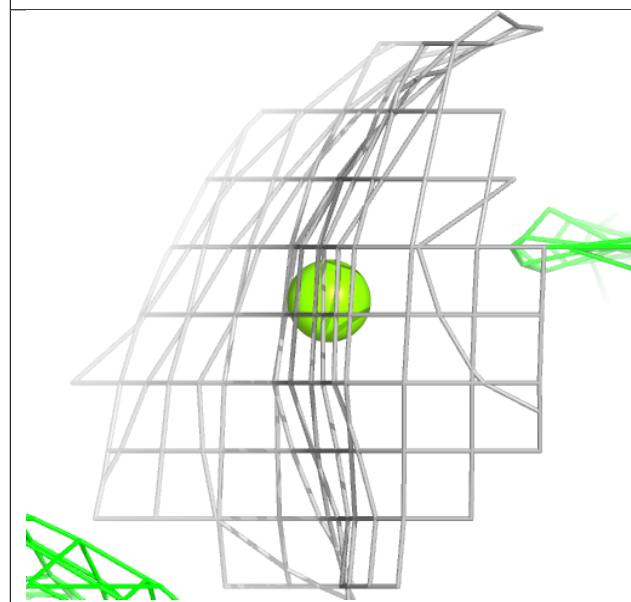
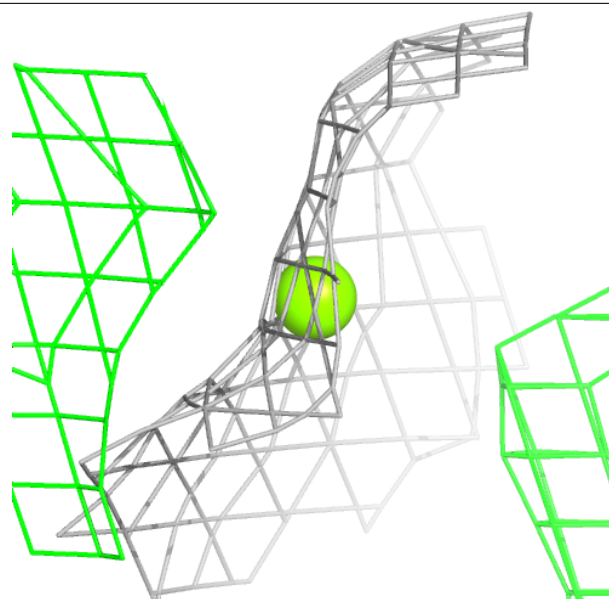
Electron density around MG G 602:

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



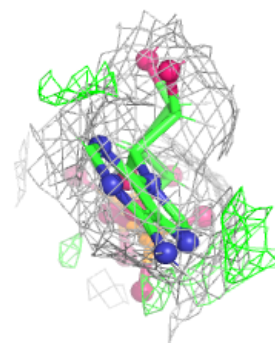
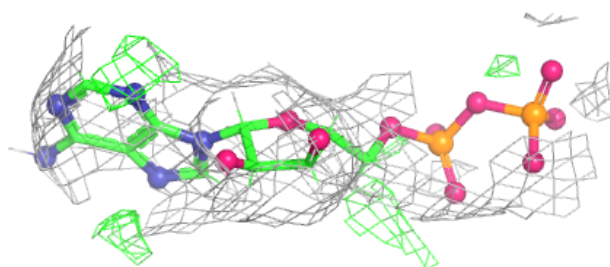
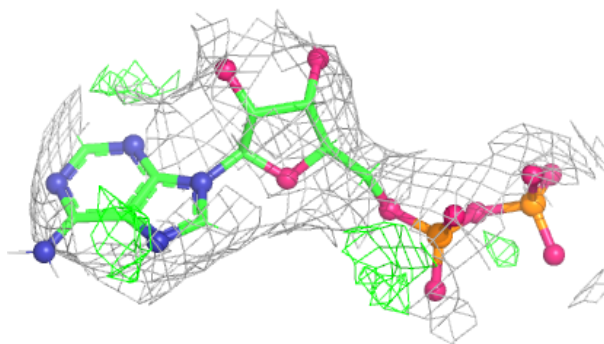
Electron density around MG H 602:

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

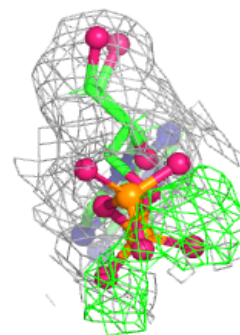
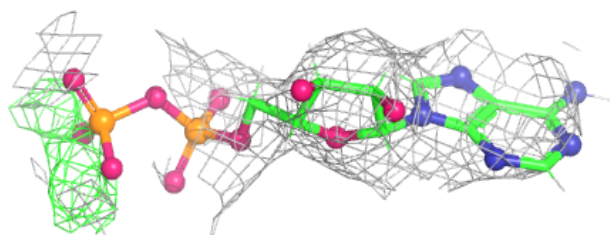
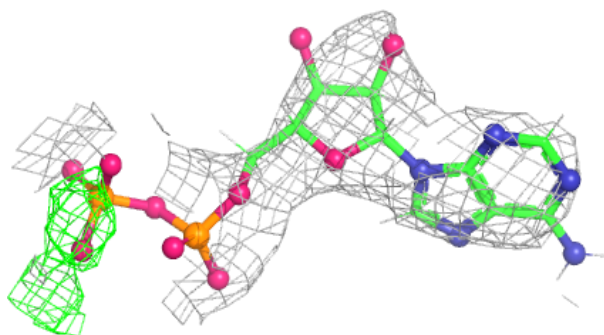


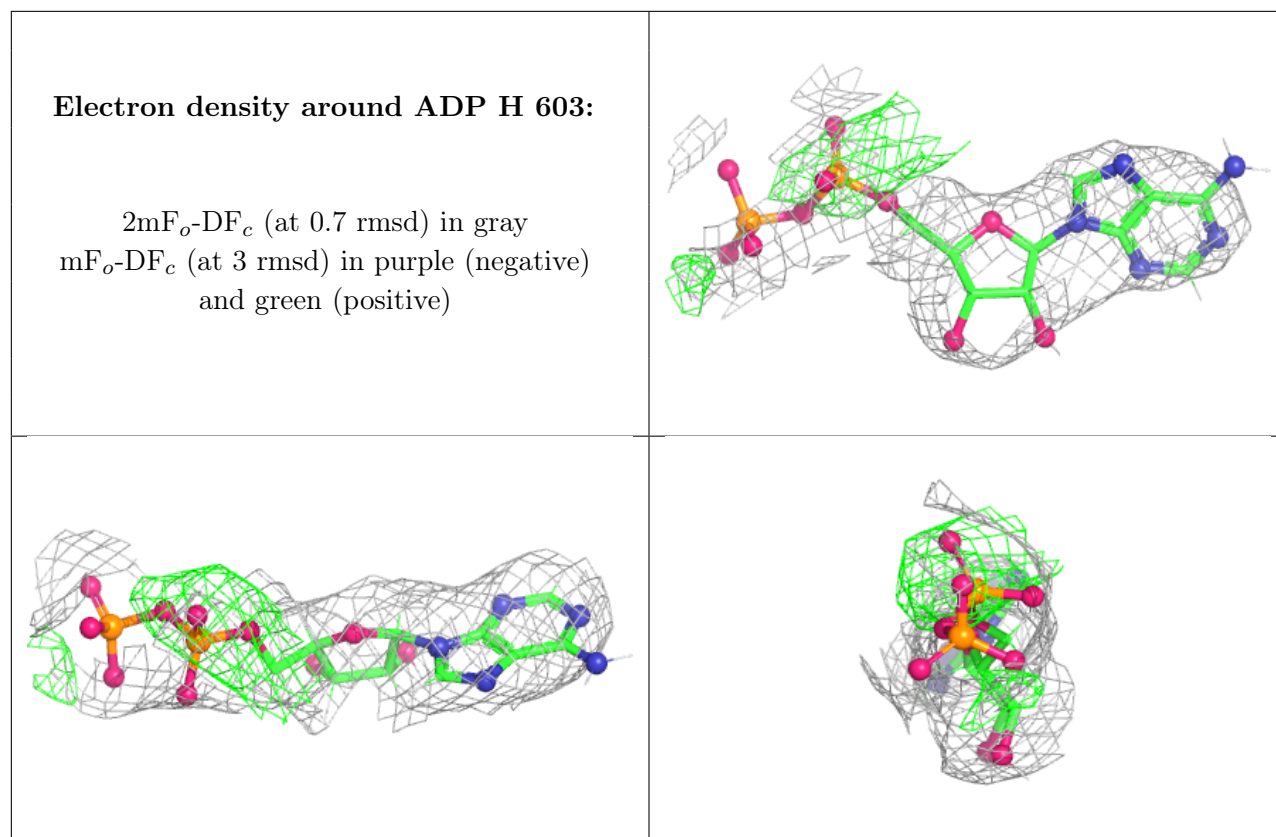
Electron density around ADP J 604:

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

**Electron density around ADP D 601:**

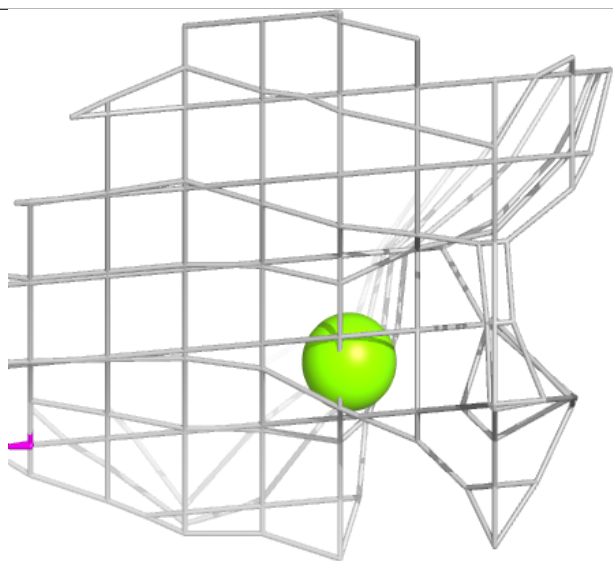
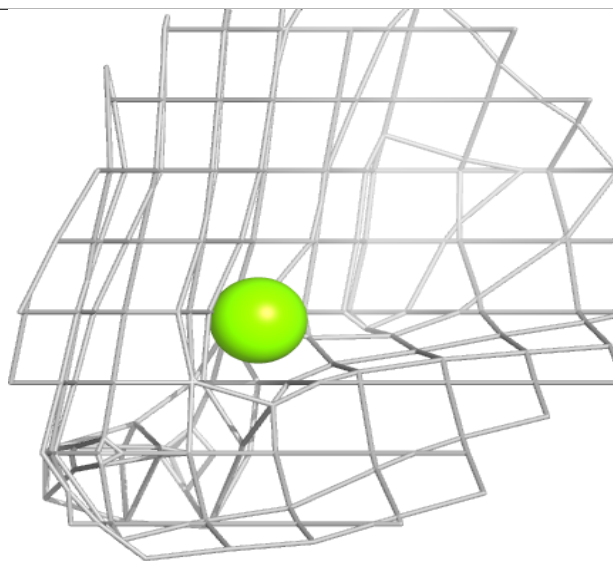
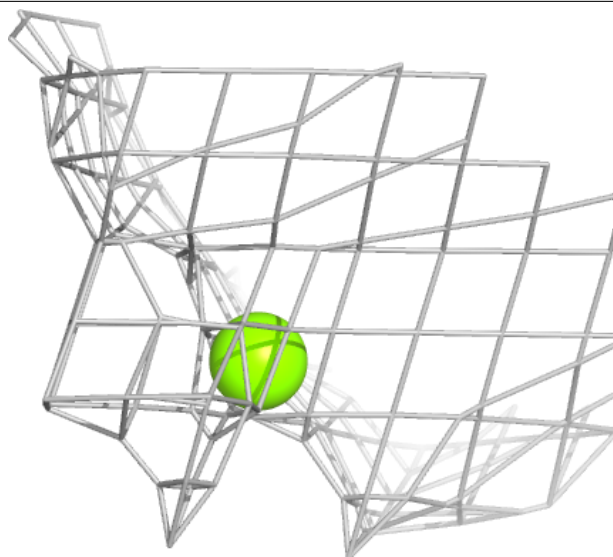
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





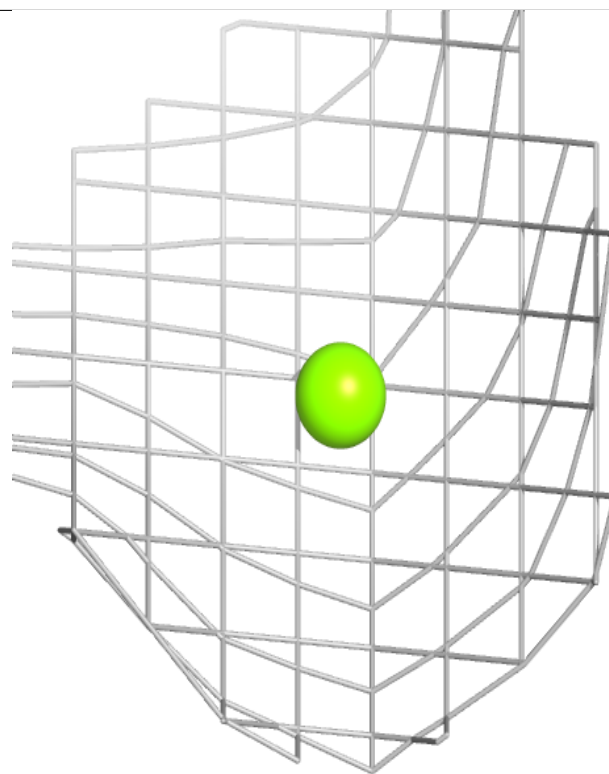
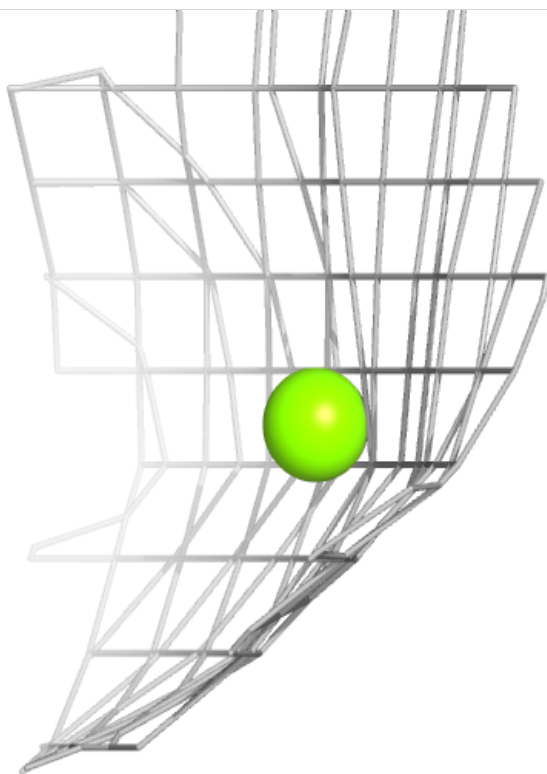
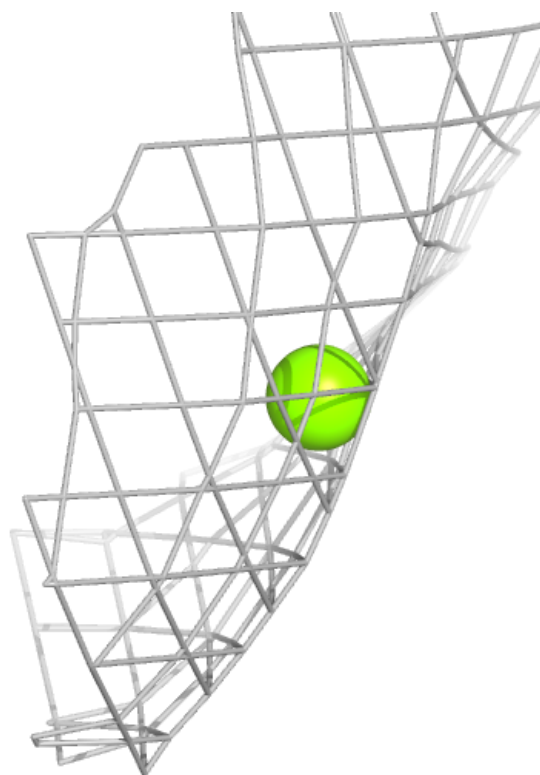
Electron density around MG C 603:

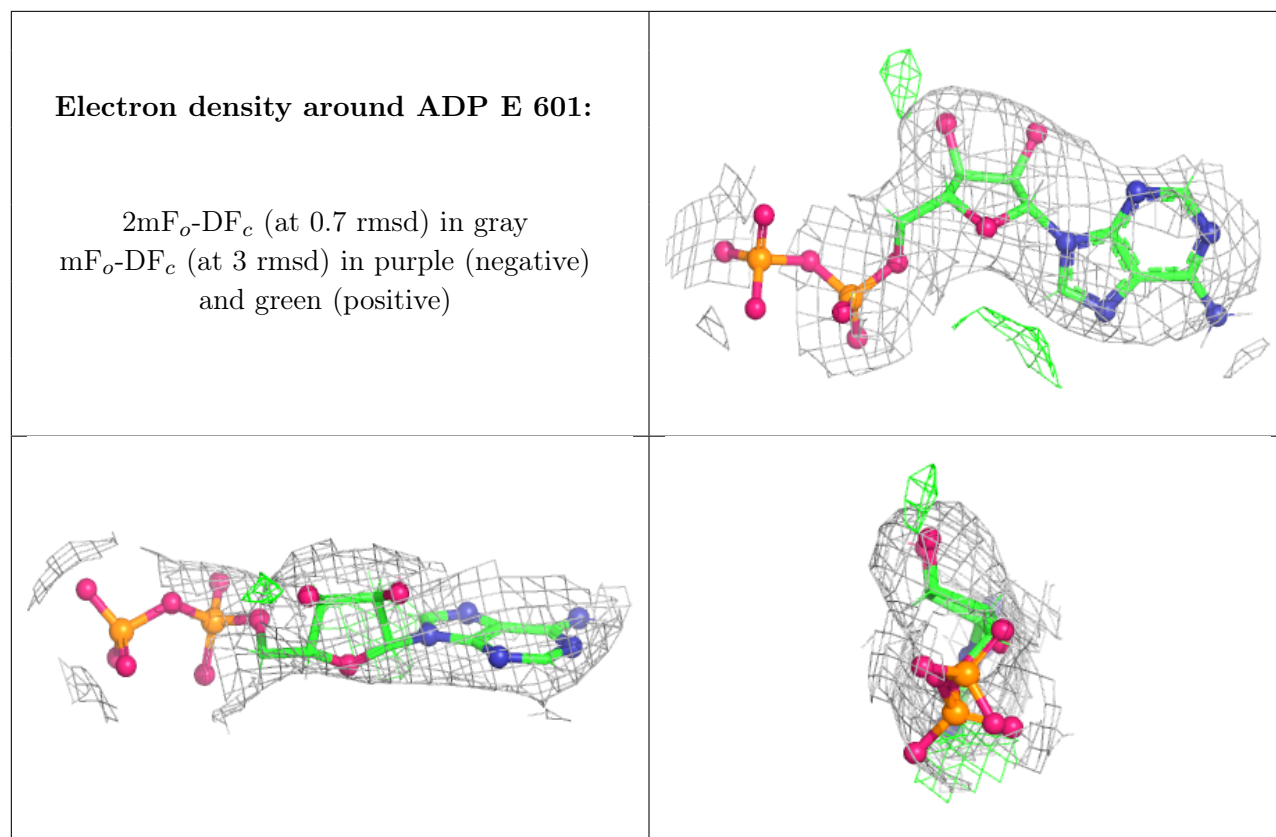
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 603:

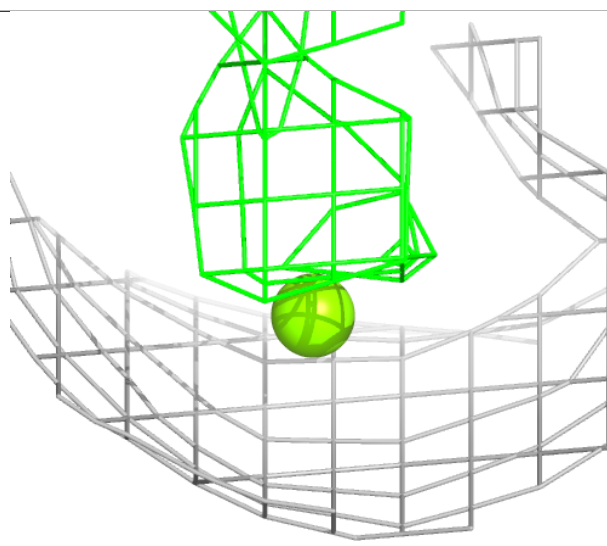
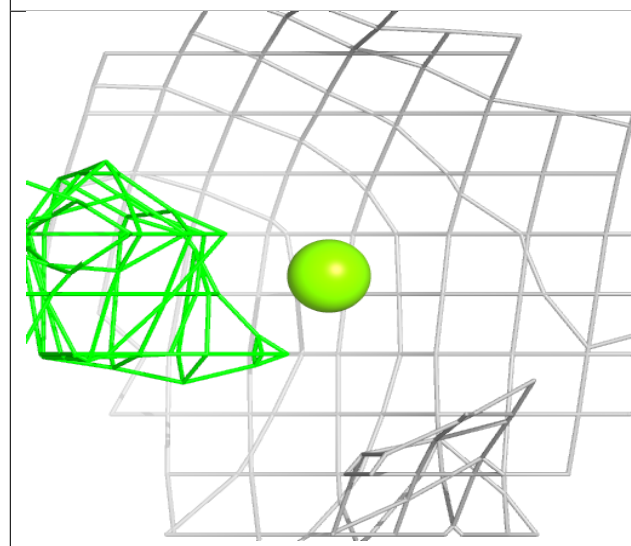
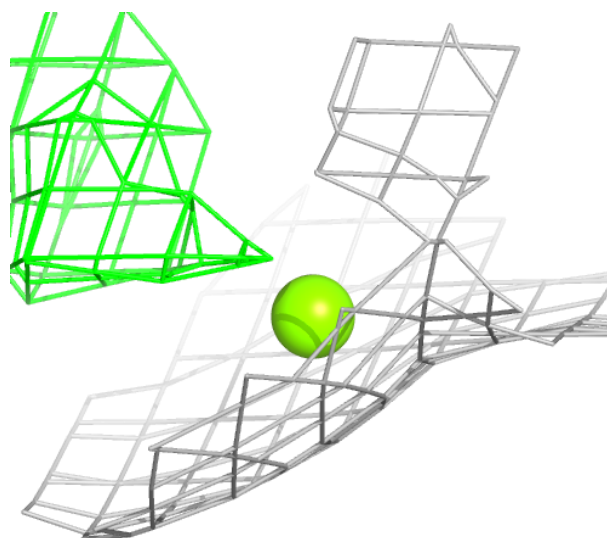
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





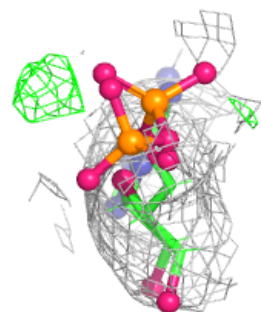
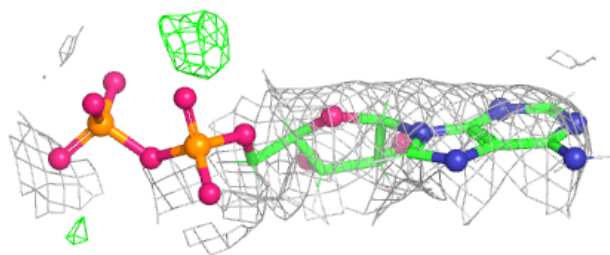
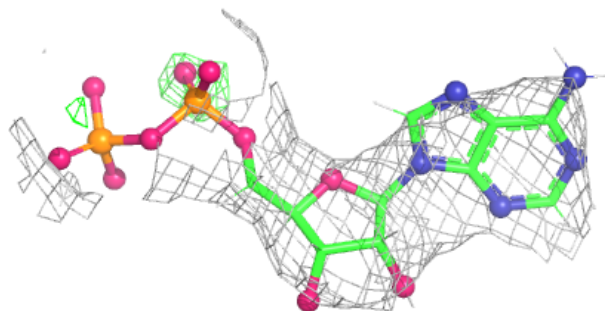
Electron density around MG D 603:

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



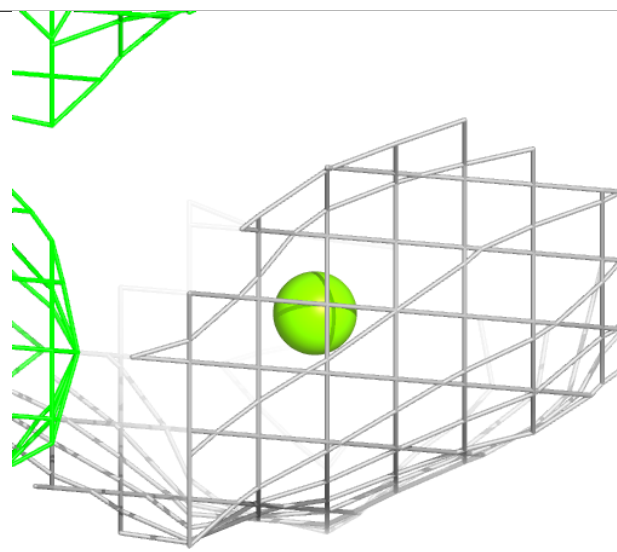
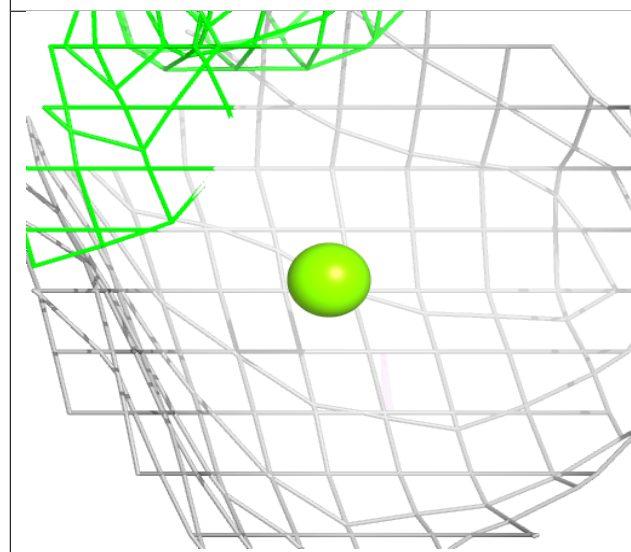
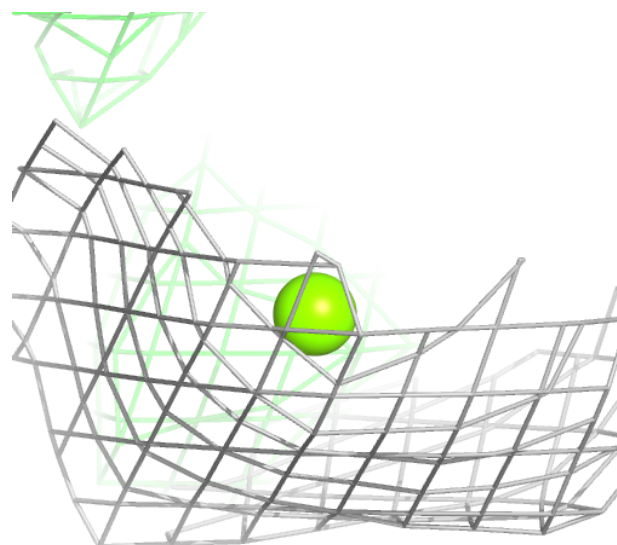
Electron density around ADP I 601:

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



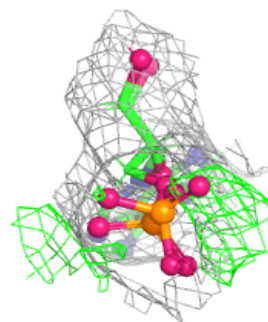
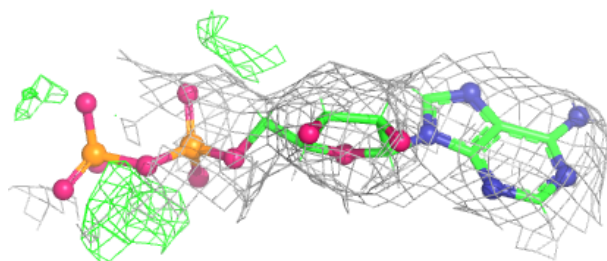
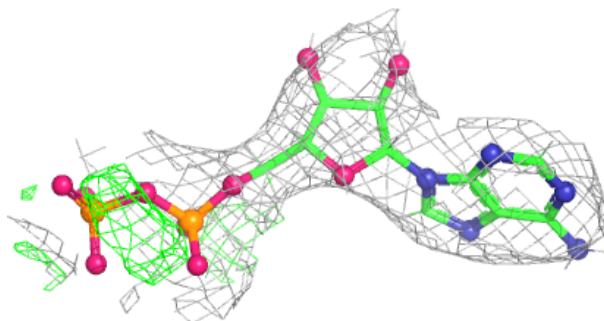
Electron density around MG K 602:

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



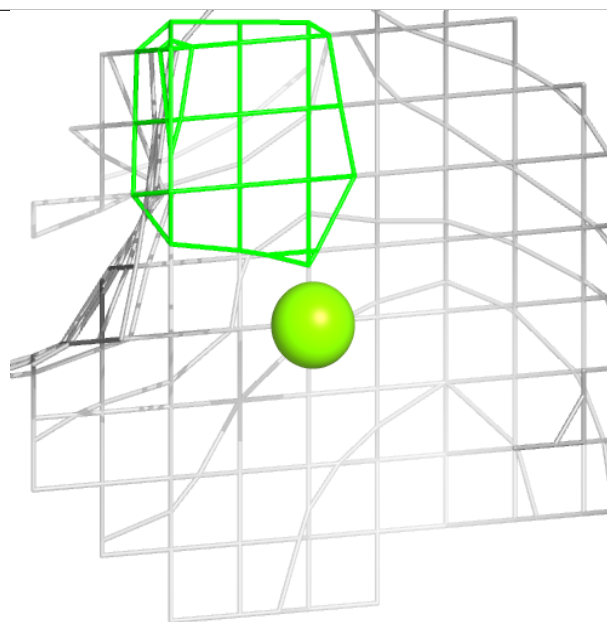
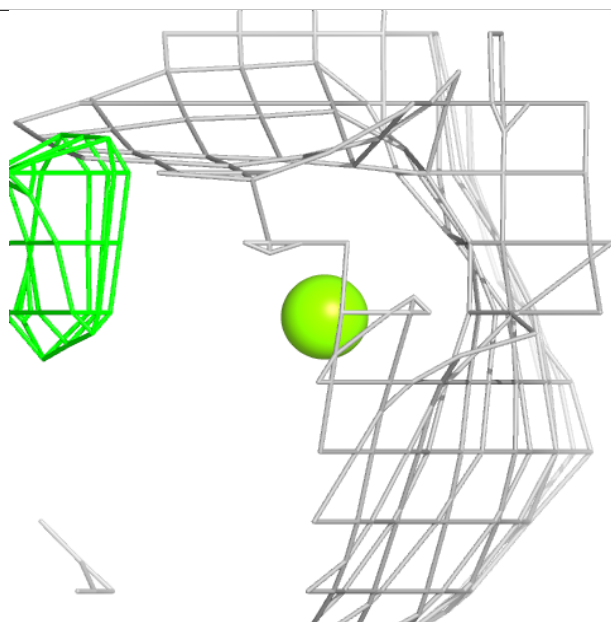
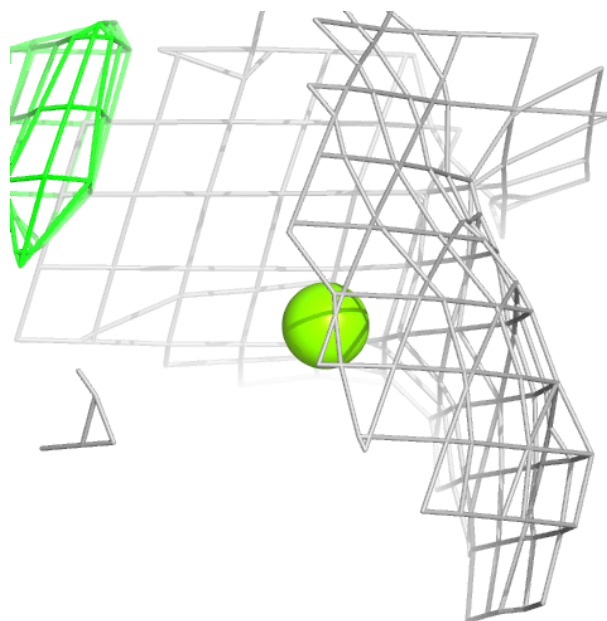
Electron density around ADP D 604:

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



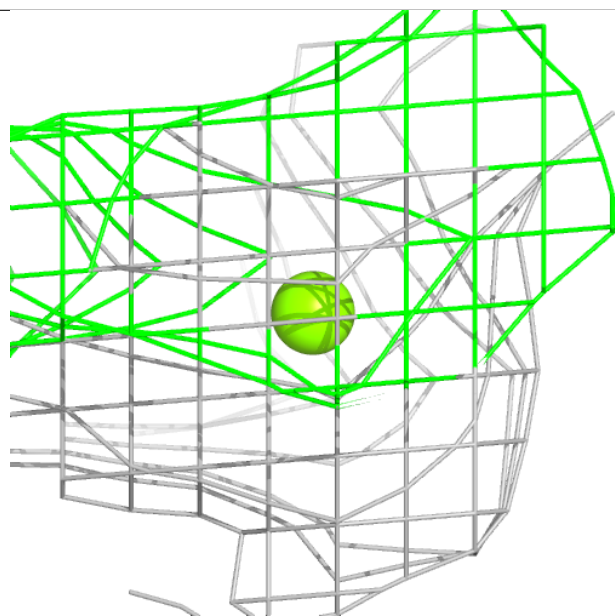
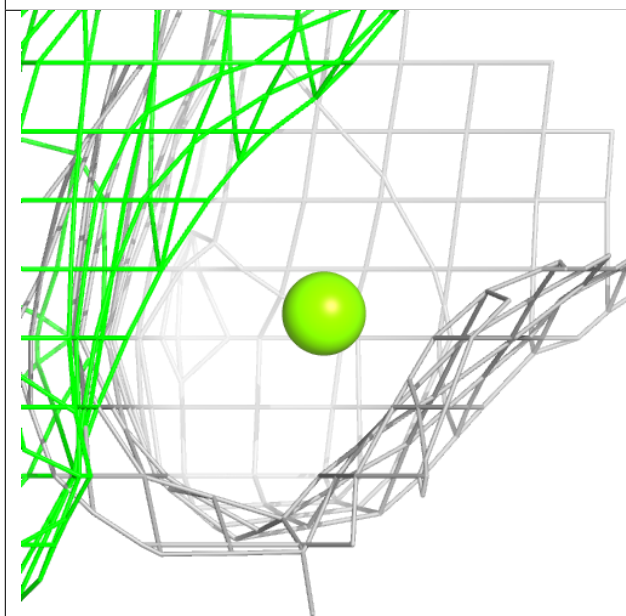
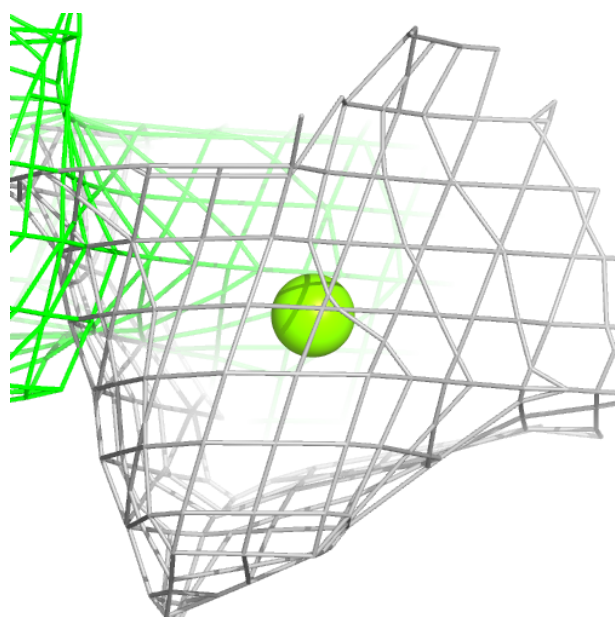
Electron density around MG H 604:

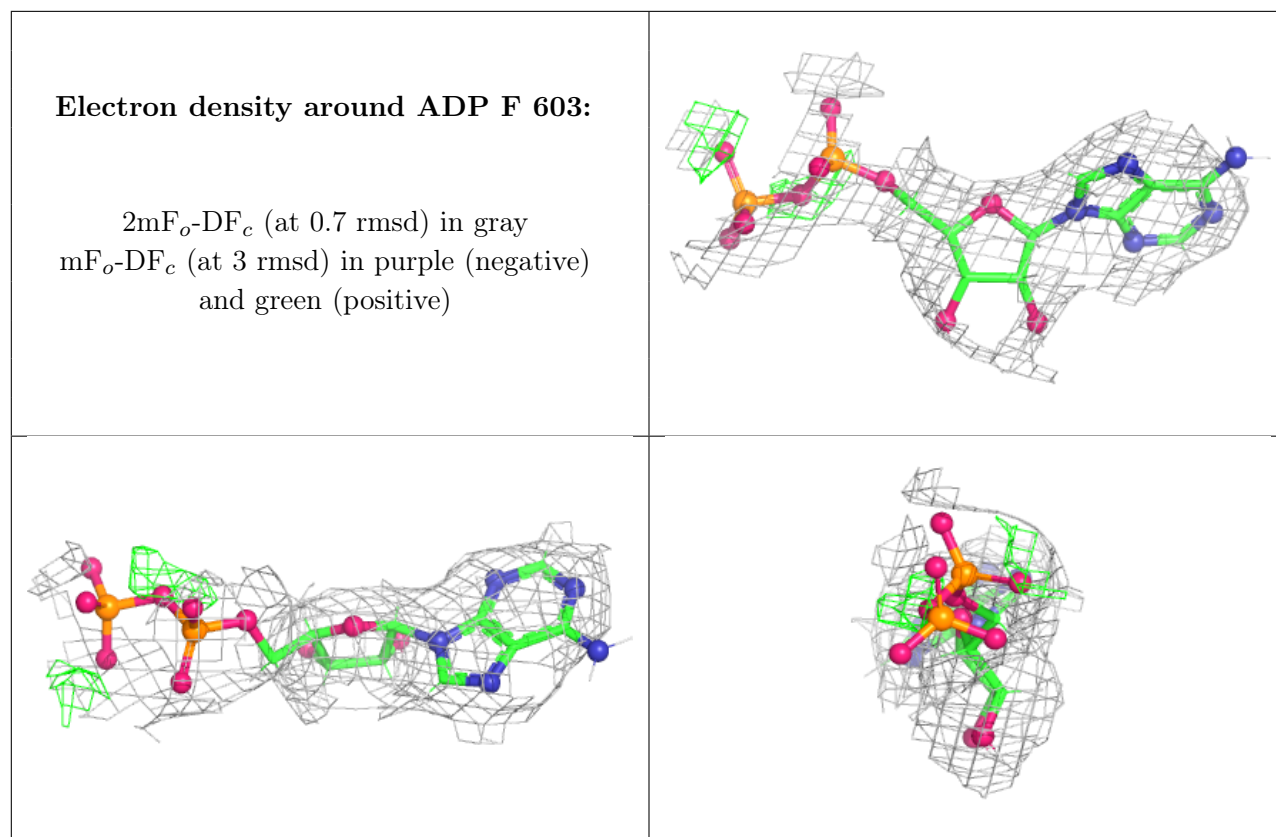
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 602:

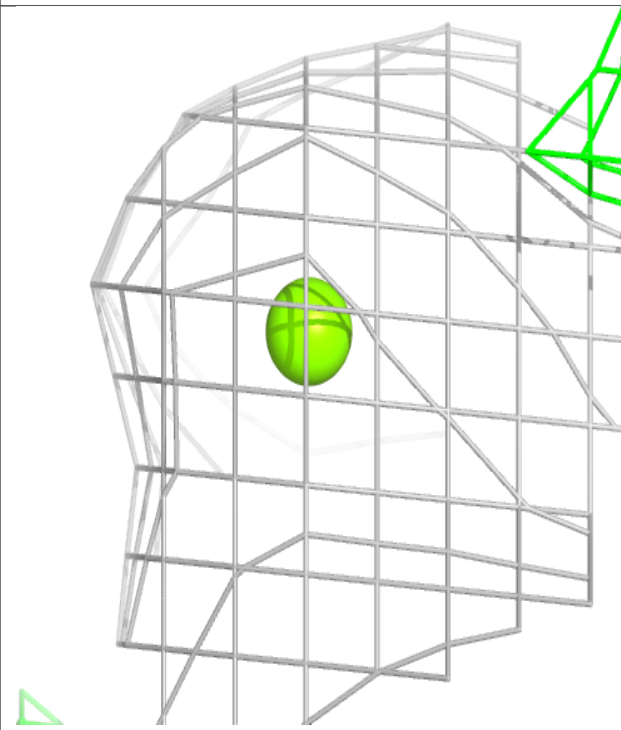
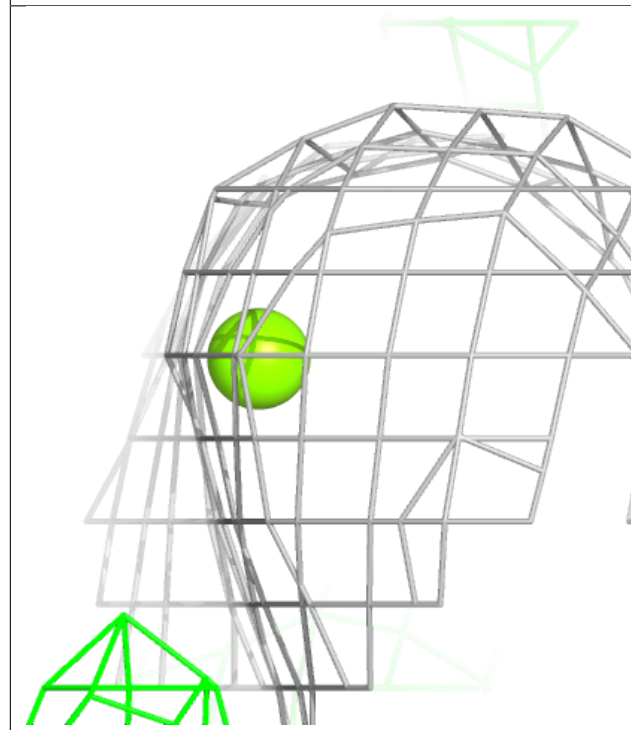
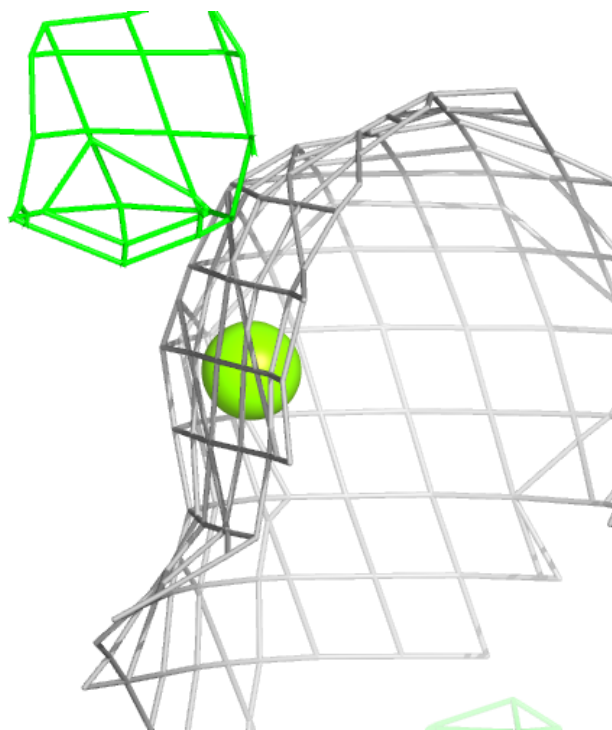
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





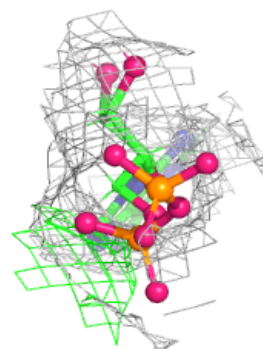
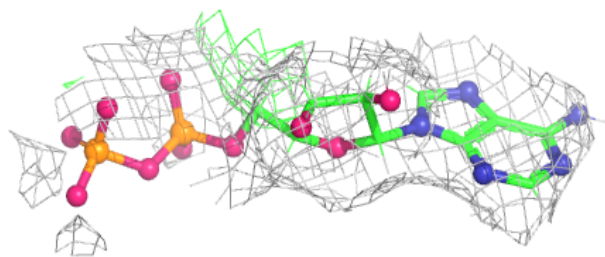
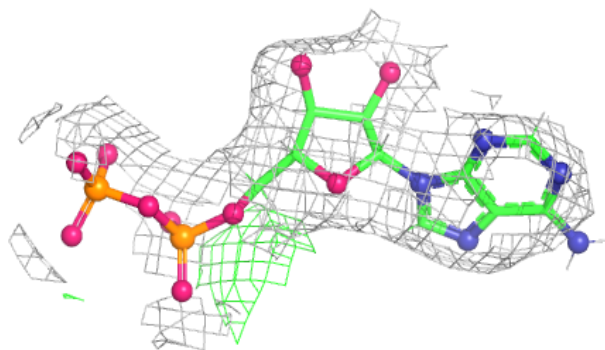
Electron density around MG G 605:

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



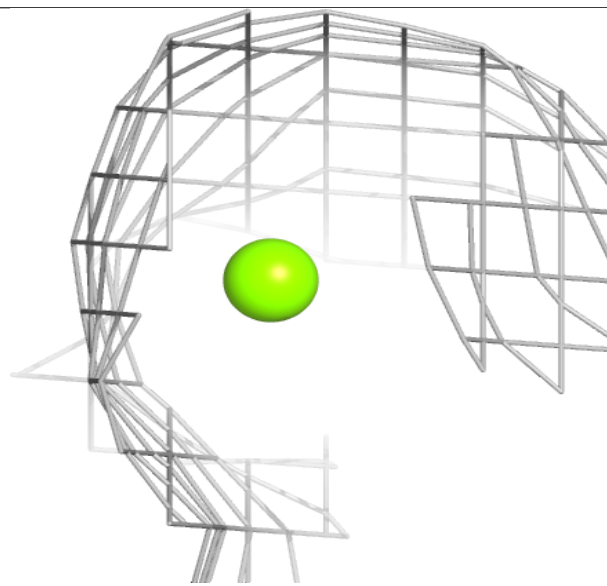
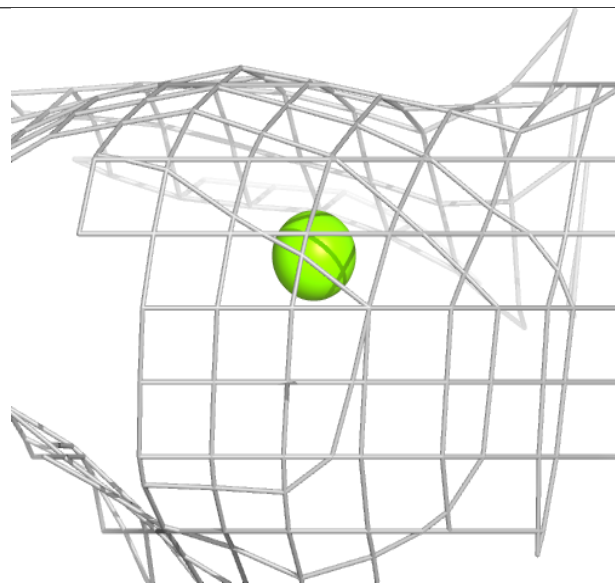
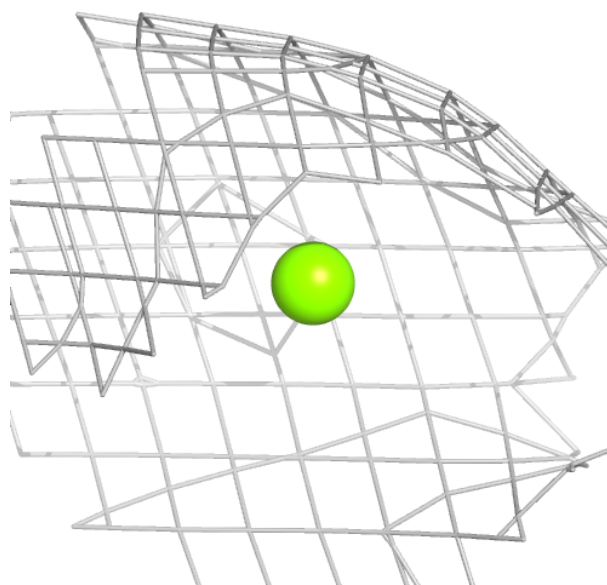
Electron density around ADP L 602:

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



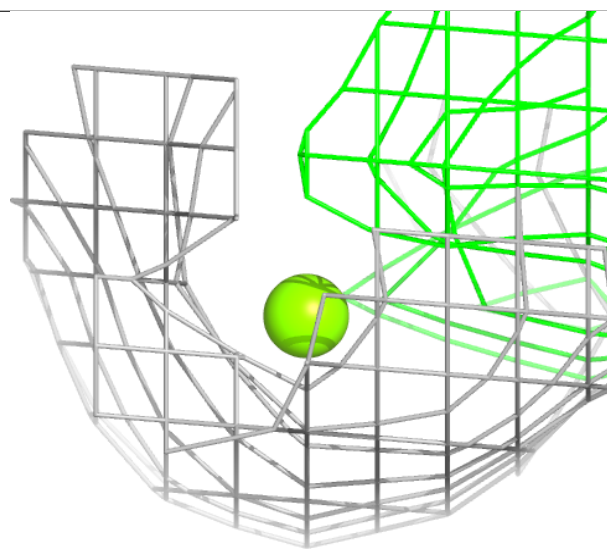
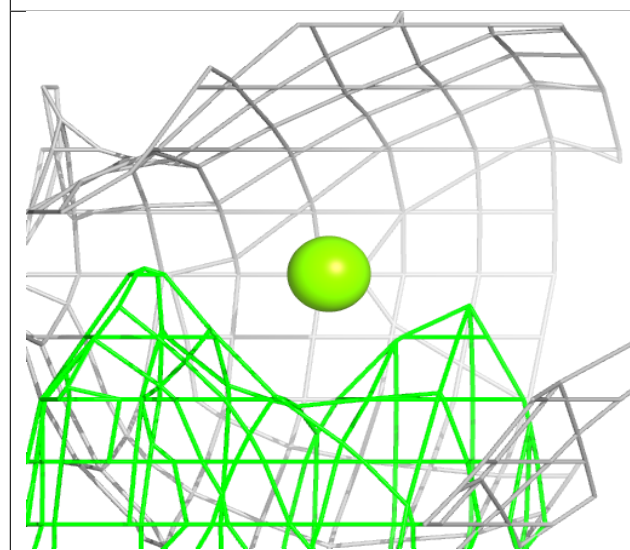
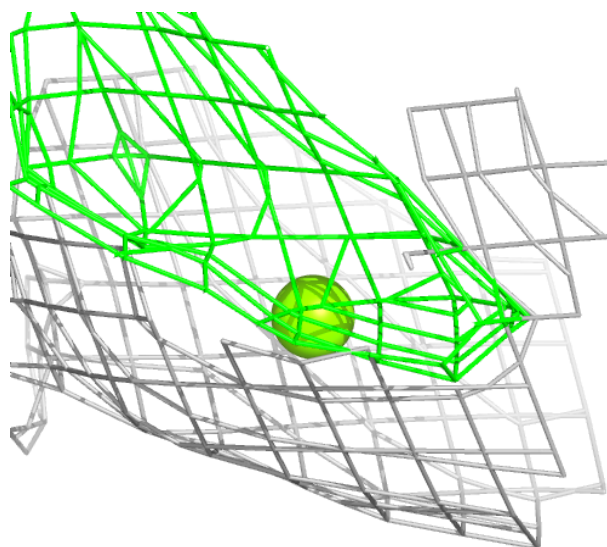
Electron density around MG I 602:

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



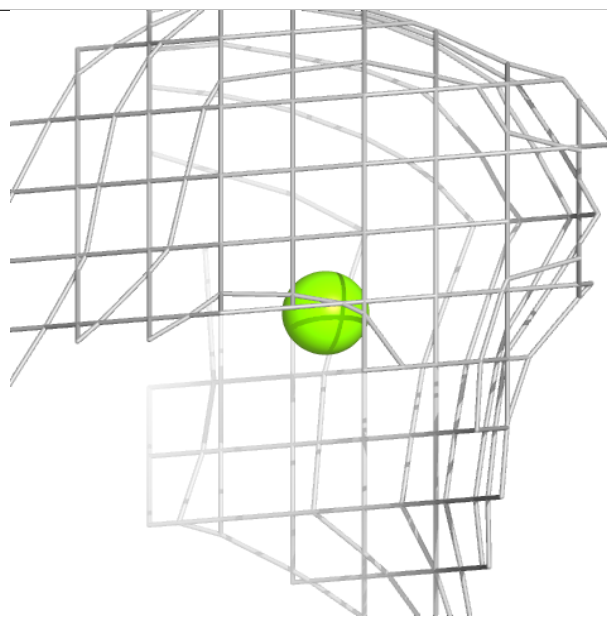
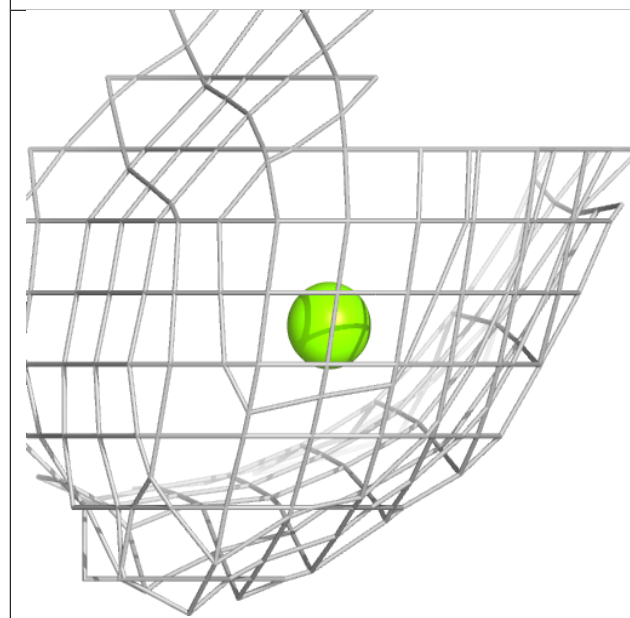
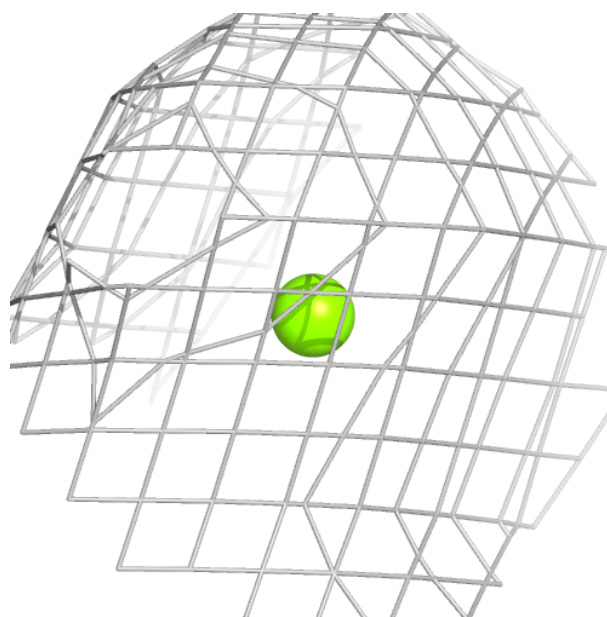
Electron density around MG E 602:

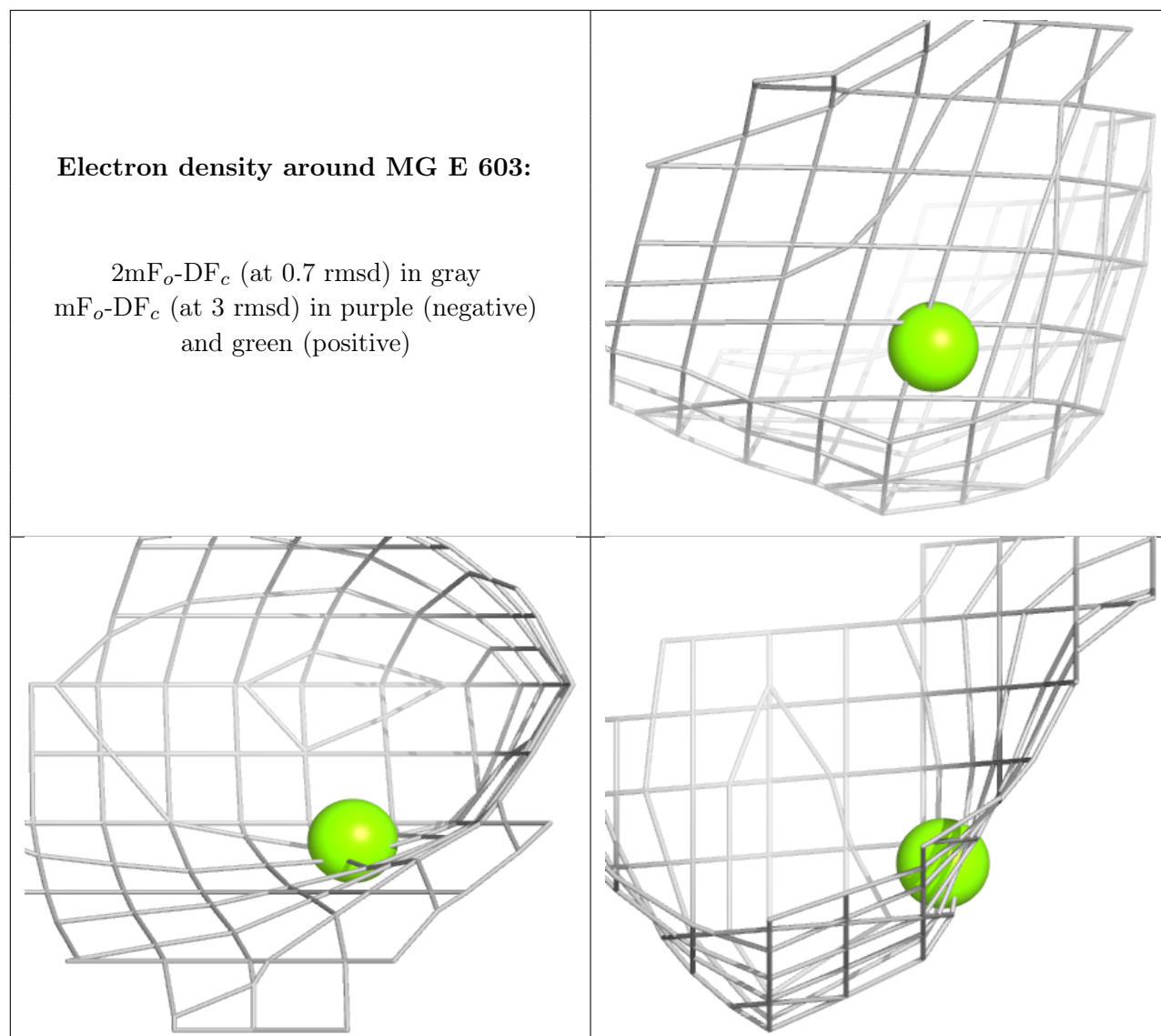
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.