



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2025 – 06:18 PM JST

PDB ID : 8ZN5 / pdb\_00008zn5  
Title : Crystal Structure of Designed Clock Protein KaiC  
Authors : Furuike, Y.; Akiyama, S.  
Deposited on : 2024-05-26  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

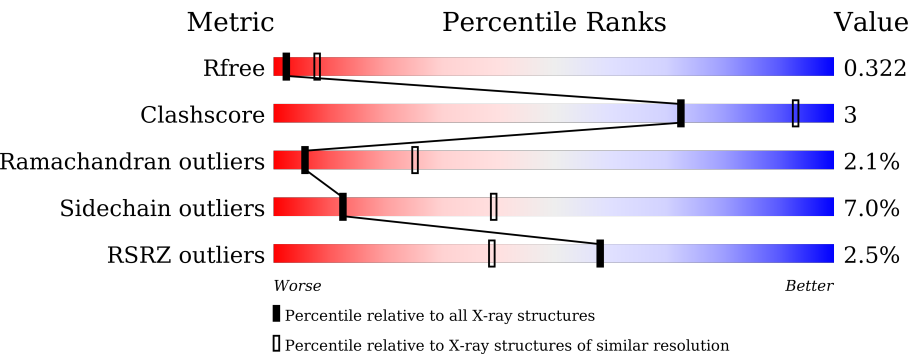
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

# 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 3.10 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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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  $\geq 3$ , 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	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%75%10%•14%</div>
1	B	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%77%9%•12%</div>
1	C	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%78%11%11%</div>
1	D	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%74%10%•14%</div>
1	E	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%78%9%•12%</div>
1	F	518	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%77%8%•14%</div>

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Mol	Chain	Length	Quality of chain
1	G	518	<div><div></div><div>3%</div><div>76%</div><div>9%</div><div>•</div><div>14%</div></div>
1	H	518	<div><div></div><div>6%</div><div>77%</div><div>6%</div><div>•</div><div>15%</div></div>
1	I	518	<div><div></div><div>3%</div><div>78%</div><div>8%</div><div>•</div><div>14%</div></div>
1	J	518	<div><div></div><div>2%</div><div>78%</div><div>7%</div><div>•</div><div>14%</div></div>
1	K	518	<div><div></div><div>2%</div><div>77%</div><div>7%</div><div>•</div><div>14%</div></div>
1	L	518	<div><div></div><div>2%</div><div>78%</div><div>6%</div><div>•</div><div>15%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36725 atoms, of which 0 are hydrogens and 0 are deuteriums.

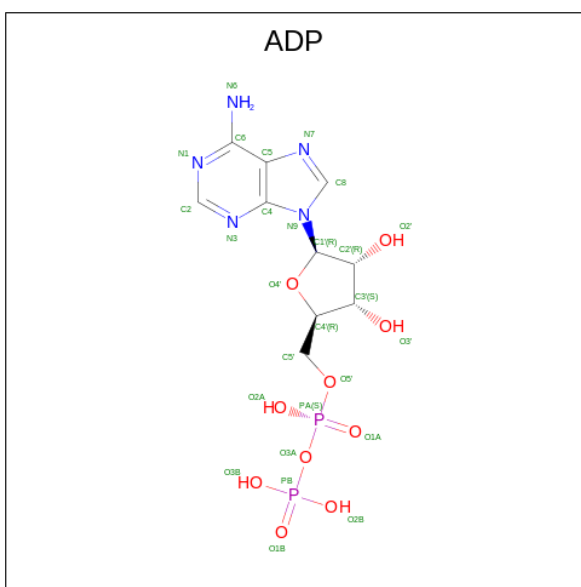
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	454	Total	C	N	O	S	0	0	0
			3201	2036	560	593	12			
1	C	463	Total	C	N	O	S	0	0	0
			3207	2025	572	599	11			
1	F	446	Total	C	N	O	S	0	0	0
			3100	1963	548	577	12			
1	A	446	Total	C	N	O	S	0	0	0
			3151	2002	555	582	12			
1	D	443	Total	C	N	O	S	0	0	0
			3002	1889	533	571	9			
1	E	456	Total	C	N	O	S	0	0	0
			3158	1997	553	596	12			
1	G	447	Total	C	N	O	S	0	0	0
			2853	1785	513	547	8			
1	H	439	Total	C	N	O	S	0	0	0
			2809	1747	513	540	9			
1	K	444	Total	C	N	O	S	0	0	0
			2865	1789	524	546	6			
1	L	439	Total	C	N	O	S	0	0	0
			2784	1738	518	519	9			
1	I	446	Total	C	N	O	S	0	0	0
			2918	1807	527	573	11			
1	J	447	Total	C	N	O	S	0	0	0
			2978	1871	532	568	7			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	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	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		
3	A	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	G	2	Total	Mg	0	0
			2	2		
3	H	2	Total	Mg	0	0
			2	2		
3	K	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	J	2	Total 2	Mg 2	0	0

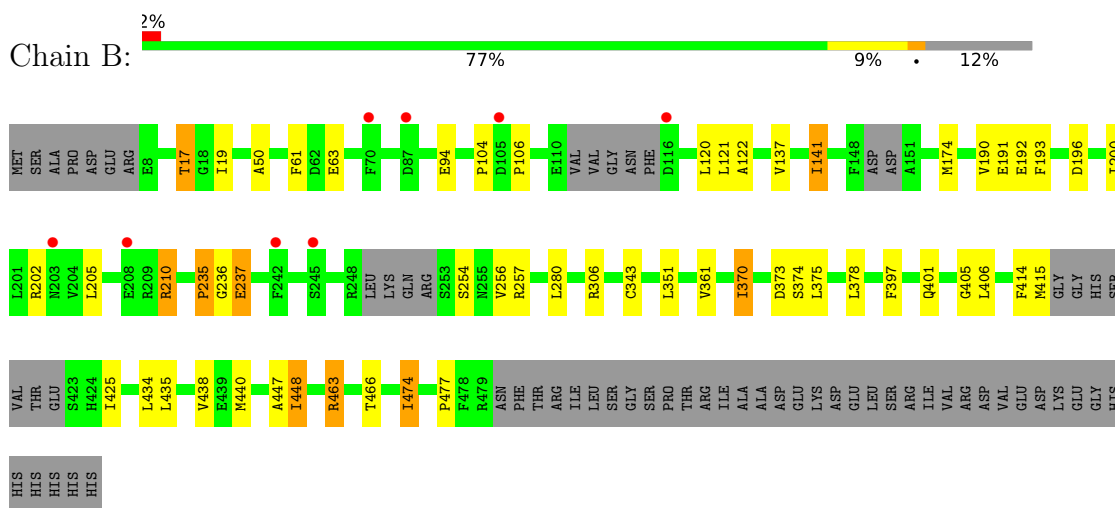
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	O 1	0	0
4	C	4	Total 4	O 4	0	0
4	F	2	Total 2	O 2	0	0
4	A	7	Total 7	O 7	0	0
4	D	2	Total 2	O 2	0	0
4	E	5	Total 5	O 5	0	0
4	K	2	Total 2	O 2	0	0
4	J	4	Total 4	O 4	0	0

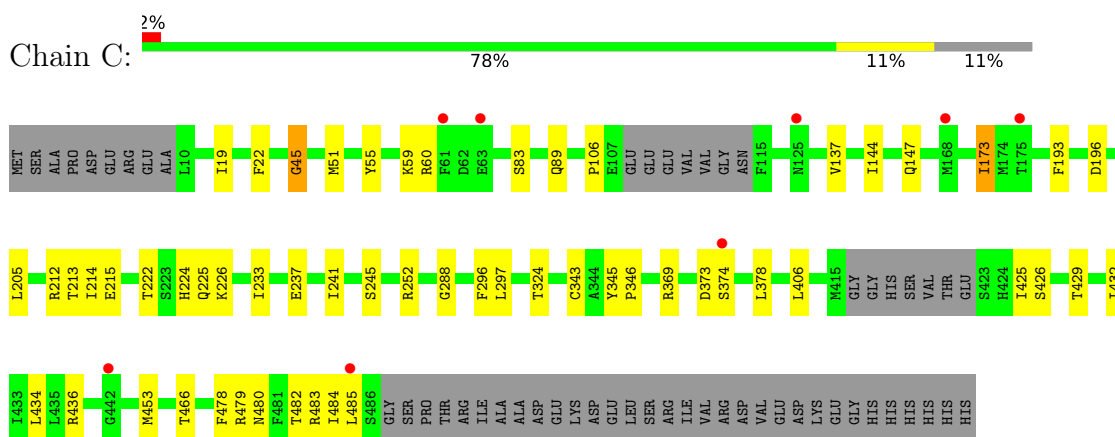
### 3 Residue-property plots [i](#)

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.

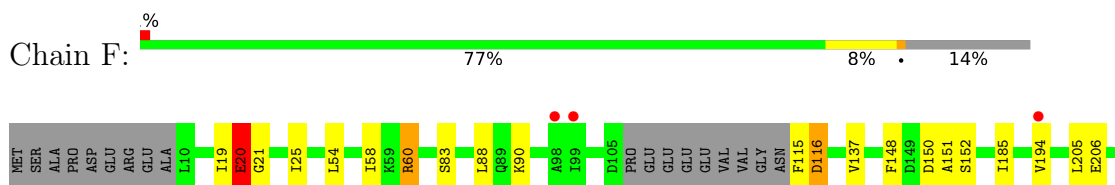
#### • Molecule 1: KaiC

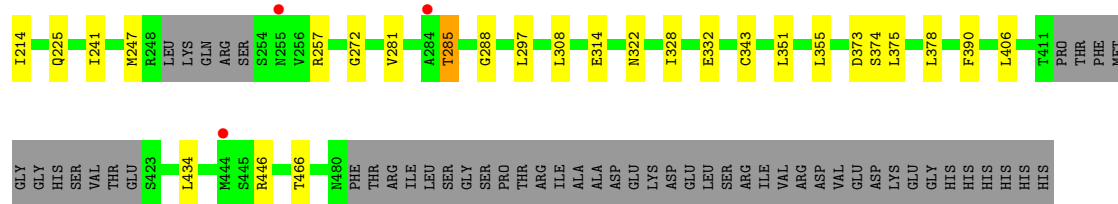


#### • Molecule 1: KaiC

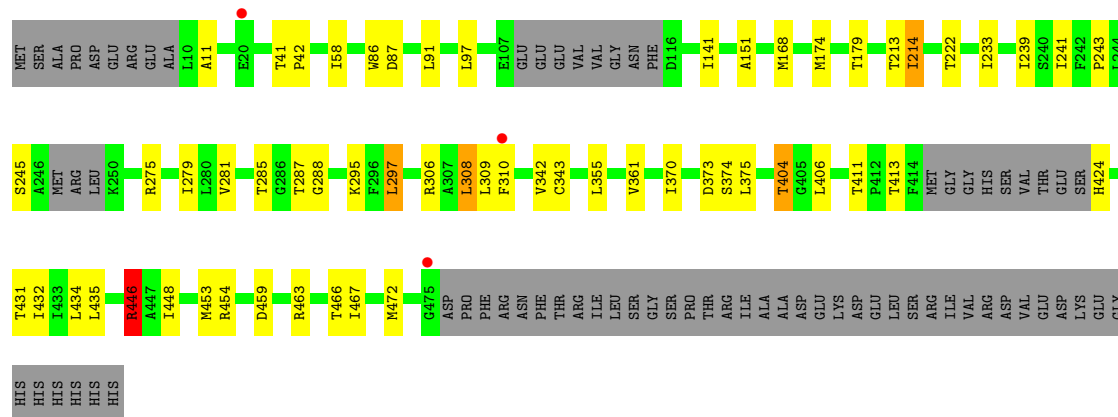
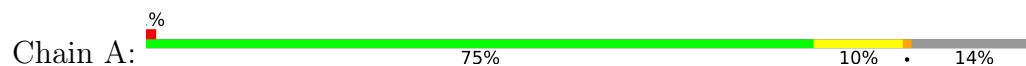


#### • Molecule 1: KaiC

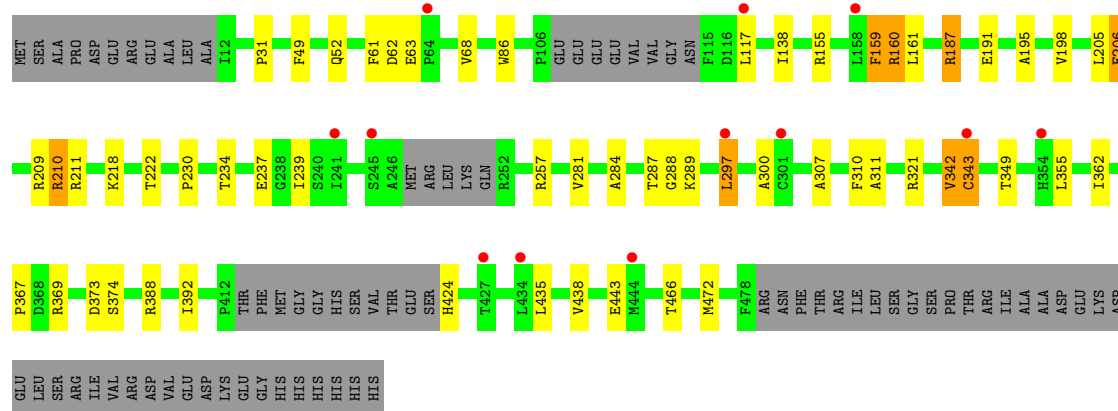
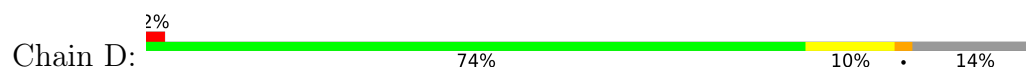




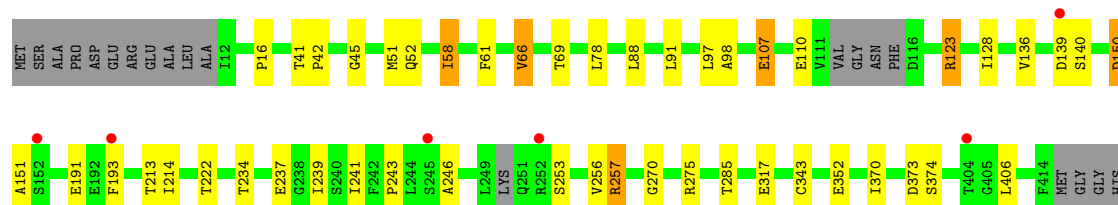
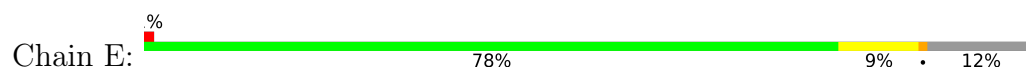
● Molecule 1: KaiC

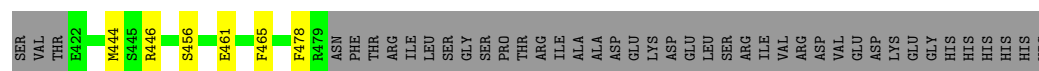


● Molecule 1: KaiC

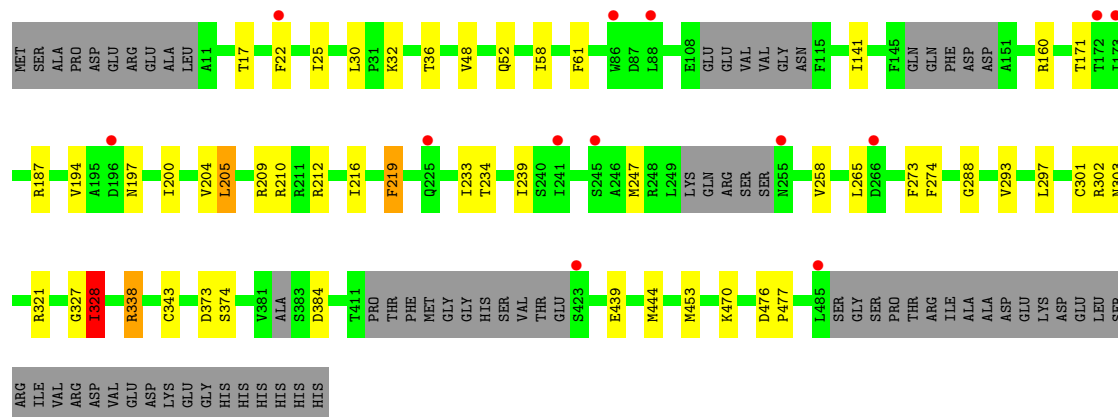
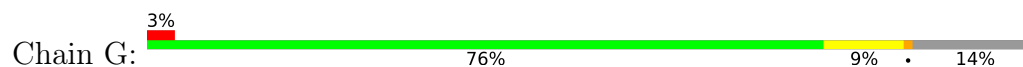


● Molecule 1: KaiC

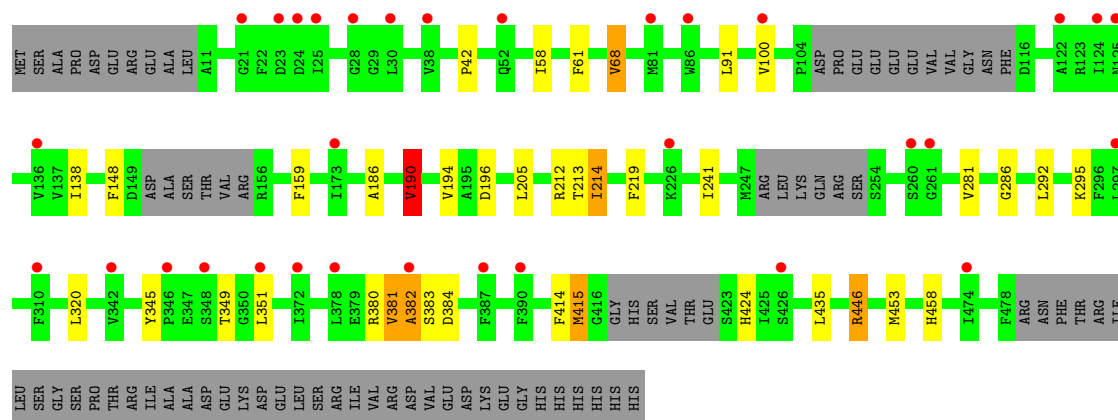
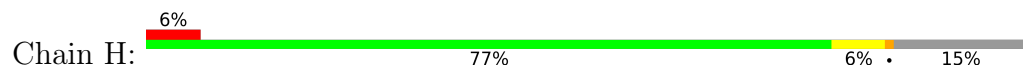




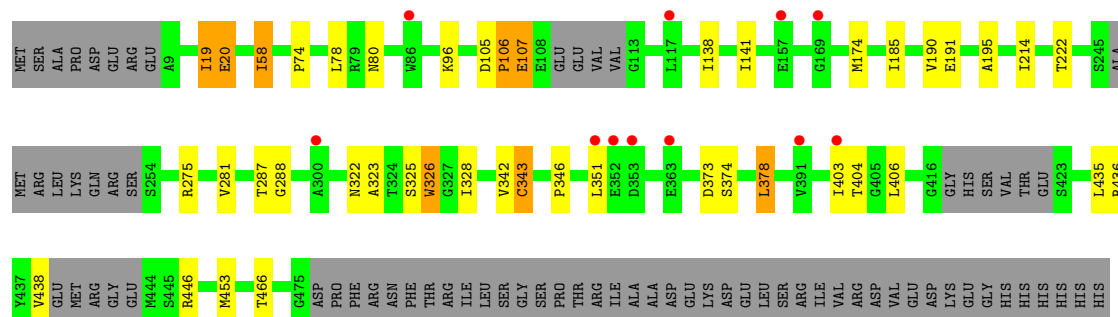
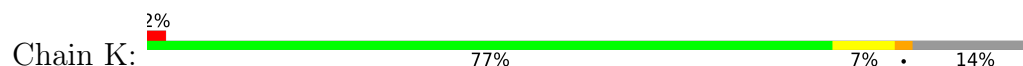
• Molecule 1: KaiC



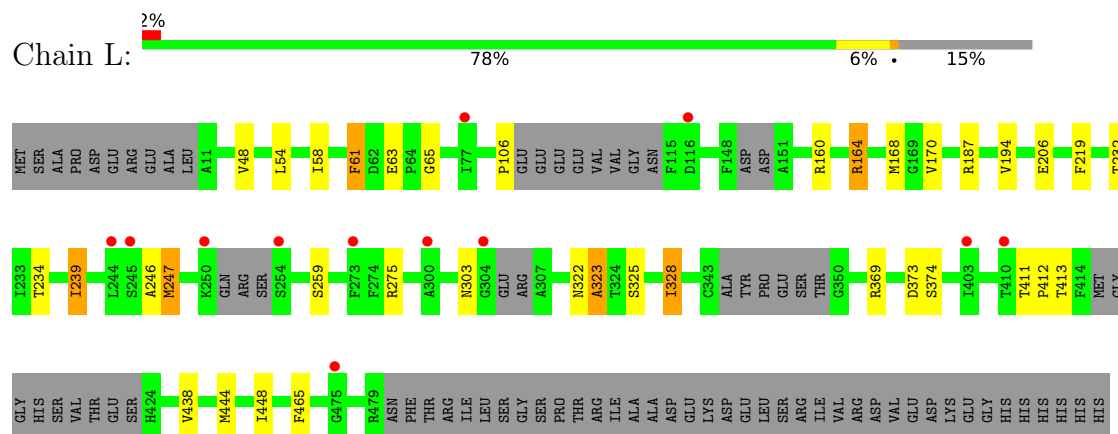
• Molecule 1: KaiC



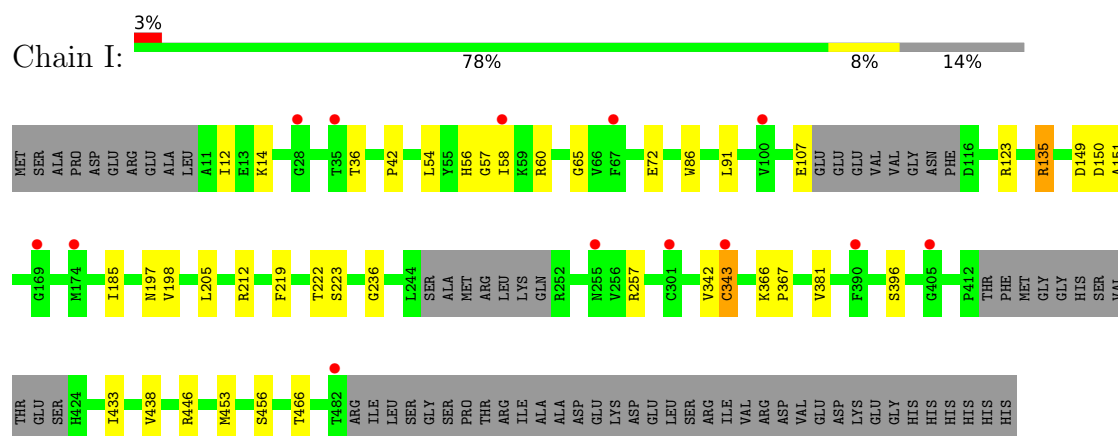
• Molecule 1: KaiC



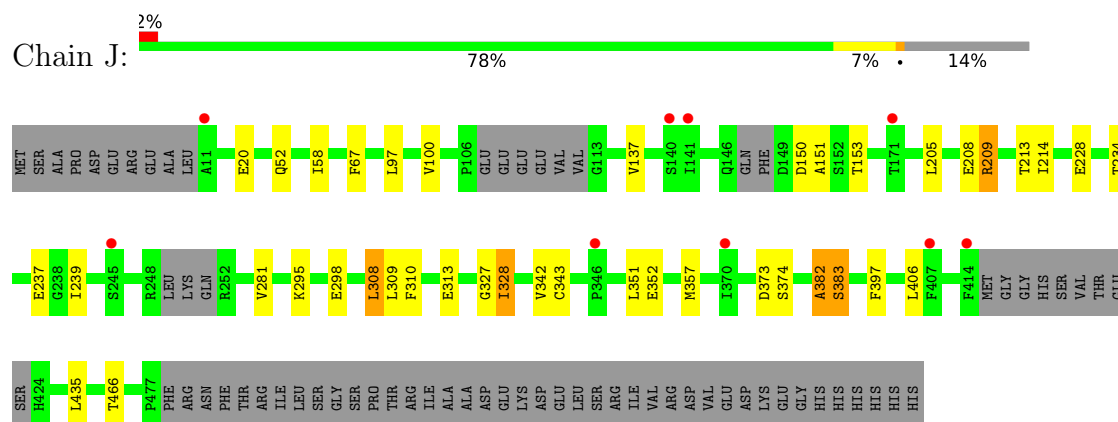
- Molecule 1: KaiC



- Molecule 1: KaiC



- Molecule 1: KaiC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.13Å 385.57Å 108.11Å 90.00° 113.15° 90.00°	Depositor
Resolution (Å)	49.35 – 3.10 49.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.35-3.10) 99.8 (49.35-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, $R_{free}$	0.280 , 0.329 0.278 , 0.322	Depositor DCC
$R_{free}$ test set	6299 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 104.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	36725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG

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	0/3206	0.44	0/4355
1	B	0.26	0/3259	0.44	0/4432
1	C	0.26	0/3262	0.44	0/4440
1	D	0.27	0/3055	0.45	0/4166
1	E	0.27	0/3214	0.45	0/4375
1	F	0.27	0/3151	0.44	0/4282
1	G	0.27	0/2895	0.45	0/3963
1	H	0.27	0/2854	0.44	0/3902
1	I	0.27	0/2967	0.44	0/4055
1	J	0.27	0/3029	0.44	0/4137
1	K	0.27	0/2909	0.44	0/3982
1	L	0.27	0/2824	0.45	0/3859
All	All	0.27	0/36625	0.44	0/49948

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	ARG	Sidechain
1	J	209	ARG	Sidechain

## 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	3151	0	2880	21	0
1	B	3201	0	2896	23	0
1	C	3207	0	2851	18	0
1	D	3002	0	2586	28	0
1	E	3158	0	2782	22	0
1	F	3100	0	2780	16	0
1	G	2853	0	2281	16	0
1	H	2809	0	2200	9	0
1	I	2918	0	2332	12	0
1	J	2978	0	2502	18	0
1	K	2865	0	2339	20	0
1	L	2784	0	2217	13	0
2	A	54	0	24	0	0
2	B	54	0	24	0	0
2	C	54	0	24	1	0
2	D	54	0	24	0	0
2	E	54	0	24	0	0
2	F	54	0	24	1	0
2	G	54	0	24	0	0
2	H	54	0	24	0	0
2	I	54	0	24	1	0
2	J	54	0	24	0	0
2	K	54	0	24	1	0
2	L	54	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
4	E	5	0	0	0	0
4	F	2	0	0	0	0
4	J	4	0	0	0	0
4	K	2	0	0	0	0
All	All	36725	0	30934	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (207) 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:A:141:ILE:HD11	1:A:174:MET:HB3	1.48	0.93
1:D:187:ARG:HH11	1:D:187:ARG:HB3	1.50	0.76
1:A:58:ILE:HD11	1:A:91:LEU:HD13	1.67	0.76
1:A:446:ARG:HH11	1:A:467:ILE:HD12	1.55	0.72
1:J:209:ARG:HH21	1:J:209:ARG:HG2	1.55	0.71
1:E:123:ARG:HH21	1:E:123:ARG:HB3	1.58	0.69
1:J:351:LEU:HD11	1:J:382:ALA:HB1	1.74	0.67
1:K:281:VAL:HG23	1:K:406:LEU:HD11	1.76	0.67
1:C:106:PRO:HB3	1:D:159:PHE:HA	1.79	0.64
1:A:141:ILE:HD11	1:A:174:MET:CB	2.27	0.62
1:F:83:SER:HG	2:F:601:ADP:HN62	1.46	0.62
1:H:68:VAL:HG22	1:H:138:ILE:HA	1.83	0.61
1:K:58:ILE:HG21	1:K:96:LYS:HB3	1.81	0.61
1:C:83:SER:OG	2:C:601:ADP:N6	2.33	0.61
1:K:342:VAL:O	1:K:343:CYS:SG	2.58	0.60
1:J:58:ILE:HD11	1:J:97:LEU:HD23	1.84	0.60
1:I:54:LEU:HD23	1:I:65:GLY:HA3	1.83	0.59
1:H:286:GLY:O	1:H:446:ARG:NH1	2.35	0.59
1:B:141:ILE:HD11	1:B:174:MET:HB3	1.83	0.58
1:J:281:VAL:HG23	1:J:406:LEU:HD11	1.84	0.58
1:D:209:ARG:HD2	1:D:349:THR:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:VAL:HG22	1:C:173:ILE:HG23	1.84	0.57
1:B:447:ALA:HA	1:B:463:ARG:O	2.05	0.57
1:K:275:ARG:O	1:K:404:THR:HG22	2.06	0.56
1:A:432:ILE:HG22	1:A:434:LEU:HD13	1.88	0.56
1:D:68:VAL:HG22	1:D:138:ILE:HA	1.88	0.55
1:D:61:PHE:O	1:D:63:GLU:N	2.39	0.55
1:F:351:LEU:HD21	1:F:378:LEU:HB3	1.88	0.55
1:F:150:ASP:O	1:F:152:SER:N	2.40	0.55
1:A:214:ILE:HG21	1:A:241:ILE:HD13	1.89	0.55
1:G:327:GLY:O	1:G:328:ILE:C	2.46	0.54
1:J:52:GLN:HE22	1:J:239:ILE:H	1.54	0.54
1:G:293:VAL:O	1:G:297:LEU:HB2	2.08	0.54
1:G:52:GLN:HE22	1:G:239:ILE:H	1.55	0.53
1:J:208:GLU:O	1:J:209:ARG:NH2	2.41	0.53
1:K:105:ASP:O	1:K:107:GLU:N	2.41	0.53
1:K:185:ILE:HB	1:K:191:GLU:HG2	1.90	0.53
1:H:186:ALA:HB1	1:H:190:VAL:H	1.74	0.53
1:F:83:SER:HB3	1:A:11:ALA:HB2	1.92	0.52
1:F:115:PHE:O	1:F:116:ASP:C	2.48	0.52
1:H:214:ILE:HG21	1:H:241:ILE:HD13	1.93	0.51
1:B:50:ALA:HB1	1:B:137:VAL:HG11	1.92	0.51
1:D:187:ARG:HH11	1:D:187:ARG:CB	2.19	0.51
1:B:463:ARG:HA	1:B:477:PRO:HA	1.92	0.51
1:E:41:THR:HB	1:E:42:PRO:HD2	1.93	0.51
1:L:48:VAL:HG23	2:L:602:ADP:O1A	2.11	0.50
1:A:281:VAL:HG23	1:A:406:LEU:HD11	1.93	0.50
1:B:235:PRO:O	1:B:237:GLU:N	2.44	0.50
1:K:191:GLU:O	1:K:195:ALA:HB2	2.11	0.50
1:B:414:PHE:O	1:B:415:MET:CB	2.60	0.49
1:H:281:VAL:HG13	1:H:435:LEU:CD1	2.40	0.49
1:L:246:ALA:O	1:L:247:MET:C	2.50	0.49
1:G:301:CYS:SG	1:G:302:ARG:N	2.86	0.49
1:I:56:HIS:O	1:I:60:ARG:N	2.45	0.49
1:I:446:ARG:NH1	2:I:601:ADP:O2'	2.44	0.49
1:K:80:ASN:O	2:K:602:ADP:N6	2.46	0.49
1:K:323:ALA:O	1:K:326:TRP:N	2.44	0.49
1:F:314:GLU:OE1	1:F:322:ASN:ND2	2.46	0.48
1:L:322:ASN:O	1:L:323:ALA:C	2.51	0.48
1:L:48:VAL:HG12	1:L:239:ILE:HD11	1.95	0.48
1:E:66:VAL:HG21	1:E:128:ILE:HG12	1.95	0.48
1:L:259:SER:O	1:L:369:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:HG22	1:D:218:LYS:HB3	1.96	0.48
1:C:478:PHE:O	1:C:480:ASN:N	2.47	0.48
1:B:370:ILE:HG22	1:B:405:GLY:HA2	1.96	0.47
1:E:257:ARG:NH2	1:E:270:GLY:O	2.46	0.47
1:F:19:ILE:O	1:F:20:GLU:C	2.51	0.47
1:C:426:SER:HA	1:C:429:THR:HG22	1.96	0.47
1:D:211:ARG:HH21	1:D:230:PRO:HG3	1.79	0.47
1:K:343:CYS:SG	1:K:343:CYS:O	2.73	0.47
1:D:205:LEU:HA	1:D:210:ARG:HG3	1.97	0.47
1:G:301:CYS:O	1:G:338:ARG:NH2	2.48	0.47
1:J:67:PHE:CE2	1:J:137:VAL:HG11	2.50	0.47
1:E:257:ARG:HH12	1:E:456:SER:CB	2.27	0.46
1:E:16:PRO:HB2	1:E:61:PHE:CZ	2.50	0.46
1:C:51:MET:O	1:C:55:TYR:N	2.41	0.46
1:I:36:THR:HA	1:I:197:ASN:HB2	1.97	0.46
1:B:254:SER:HB2	1:B:256:VAL:HG12	1.97	0.46
1:B:373:ASP:HA	1:B:374:SER:HA	1.74	0.46
1:J:327:GLY:O	1:J:328:ILE:C	2.52	0.46
1:C:373:ASP:HA	1:C:374:SER:HA	1.73	0.46
1:E:58:ILE:HD11	1:E:91:LEU:HD22	1.97	0.46
1:G:32:LYS:HA	1:G:171:THR:HG22	1.97	0.46
1:K:325:SER:O	1:K:326:TRP:C	2.53	0.46
1:I:12:ILE:HB	1:I:222:THR:HG23	1.96	0.46
1:F:54:LEU:HD13	1:F:137:VAL:HG23	1.96	0.46
1:I:54:LEU:HA	1:I:135:ARG:HD3	1.98	0.46
1:B:61:PHE:HB2	1:B:63:GLU:HG3	1.97	0.46
1:C:225:GLN:HE22	1:C:245:SER:CB	2.29	0.46
1:F:281:VAL:HG23	1:F:406:LEU:HD11	1.97	0.46
1:B:210:ARG:NE	1:C:215:GLU:OE2	2.47	0.46
1:C:224:HIS:O	1:C:226:LYS:NZ	2.43	0.46
1:E:150:ASP:O	1:E:151:ALA:HB3	2.16	0.46
1:E:446:ARG:HB3	1:E:465:PHE:CZ	2.50	0.46
1:F:257:ARG:NH2	1:F:272:GLY:O	2.49	0.45
1:K:106:PRO:HB3	1:L:160:ARG:HA	1.98	0.45
1:B:435:LEU:CD2	1:B:448:ILE:HG12	2.46	0.45
1:D:297:LEU:HD12	1:D:307:ALA:HB1	1.97	0.45
1:L:164:ARG:O	1:L:168:MET:HG2	2.16	0.45
1:B:463:ARG:HB2	1:B:474:ILE:HD11	1.98	0.45
1:E:66:VAL:HG12	1:E:98:ALA:HB3	1.97	0.45
1:A:308:LEU:HD21	1:A:361:VAL:HG12	1.98	0.45
1:I:58:ILE:HD11	1:I:91:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:PRO:HB2	1:E:246:ALA:HB3	1.98	0.45
1:G:205:LEU:HG	1:G:210:ARG:HG2	1.98	0.45
1:K:141:ILE:HD11	1:K:190:VAL:HG11	1.98	0.45
1:K:346:PRO:HB3	1:K:378:LEU:HD12	1.98	0.45
1:J:308:LEU:HD22	1:J:310:PHE:CE2	2.52	0.45
1:L:322:ASN:O	1:L:325:SER:N	2.50	0.45
1:H:381:VAL:O	1:H:382:ALA:C	2.54	0.45
1:K:19:ILE:HG22	1:K:20:GLU:H	1.82	0.45
1:B:463:ARG:NH1	1:B:474:ILE:HG13	2.31	0.45
1:F:373:ASP:HA	1:F:374:SER:HA	1.78	0.45
1:D:443:GLU:HA	1:E:461:GLU:HA	1.99	0.45
1:C:482:THR:O	1:C:484:ILE:N	2.50	0.44
1:F:322:ASN:HD21	1:A:454:ARG:HB3	1.83	0.44
1:L:373:ASP:HA	1:L:374:SER:HA	1.67	0.44
1:A:275:ARG:O	1:A:404:THR:HG22	2.17	0.44
1:A:297:LEU:HD21	1:A:309:LEU:HB2	2.00	0.44
1:G:17:THR:HG21	1:G:22:PHE:CD2	2.53	0.44
1:J:382:ALA:O	1:J:383:SER:CB	2.66	0.44
1:B:17:THR:HG23	1:B:19:ILE:HG22	2.00	0.43
1:J:373:ASP:HA	1:J:374:SER:HA	1.74	0.43
1:K:141:ILE:HD13	1:K:174:MET:HB3	2.01	0.43
1:J:151:ALA:O	1:J:153:THR:N	2.51	0.43
1:B:280:LEU:HD13	1:B:425:ILE:HG21	2.01	0.43
1:D:187:ARG:HH11	1:D:187:ARG:CG	2.30	0.43
1:K:373:ASP:HA	1:K:374:SER:HA	1.74	0.43
1:I:57:GLY:HA3	1:I:135:ARG:HD2	1.99	0.43
1:F:54:LEU:CD1	1:F:137:VAL:HG23	2.49	0.43
1:D:321:ARG:HD3	1:E:253:SER:HB2	1.98	0.43
1:E:373:ASP:HA	1:E:374:SER:HA	1.82	0.43
1:C:22:PHE:HB2	1:C:241:ILE:HD12	1.99	0.43
1:D:52:GLN:HG2	1:D:86:TRP:CH2	2.54	0.43
1:G:30:LEU:HD22	1:G:36:THR:HG21	2.00	0.43
1:L:239:ILE:HD12	1:L:239:ILE:H	1.83	0.43
1:G:373:ASP:HA	1:G:374:SER:HA	1.69	0.43
1:K:74:PRO:O	1:K:78:LEU:HG	2.19	0.43
1:B:351:LEU:HD21	1:B:378:LEU:HB3	2.01	0.43
1:D:281:VAL:HG23	1:D:435:LEU:HD13	2.01	0.43
1:D:284:ALA:O	1:D:289:LYS:NZ	2.52	0.43
1:B:190:VAL:C	1:B:192:GLU:H	2.23	0.42
1:F:19:ILE:O	1:F:21:GLY:N	2.52	0.42
1:F:21:GLY:HA3	1:F:241:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HB2	1:I:257:ARG:HB2	2.01	0.42
1:D:388:ARG:O	1:D:392:ILE:HG12	2.19	0.42
1:L:54:LEU:HG	1:L:65:GLY:HA3	2.01	0.42
1:D:373:ASP:HA	1:D:374:SER:HA	1.75	0.42
1:E:52:GLN:OE1	1:E:239:ILE:N	2.48	0.42
1:G:439:GLU:HG2	1:G:444:MET:SD	2.59	0.42
1:J:209:ARG:HA	1:J:209:ARG:HD3	1.86	0.42
1:E:58:ILE:HD11	1:E:91:LEU:HD13	2.00	0.42
1:B:435:LEU:HD22	1:B:448:ILE:HG12	2.01	0.42
1:C:212:ARG:HG2	1:C:212:ARG:HH11	1.84	0.42
1:C:346:PRO:HB3	1:C:378:LEU:HD23	2.02	0.42
1:G:258:VAL:N	1:G:273:PHE:O	2.50	0.42
1:K:138:ILE:HB	1:K:174:MET:HG2	2.01	0.42
1:J:281:VAL:HG13	1:J:435:LEU:HD13	2.01	0.42
1:I:342:VAL:O	1:I:343:CYS:SG	2.76	0.42
1:J:52:GLN:HE21	1:J:52:GLN:HB2	1.65	0.42
1:G:160:ARG:HA	1:L:106:PRO:HB3	2.01	0.42
1:B:120:LEU:O	1:B:122:ALA:N	2.52	0.42
1:B:397:PHE:O	1:B:401:GLN:HG2	2.20	0.42
1:D:362:ILE:O	1:D:367:PRO:HD3	2.19	0.42
1:H:186:ALA:HB1	1:H:190:VAL:N	2.34	0.42
1:D:311:ALA:HB3	1:D:343:CYS:HA	2.01	0.41
1:C:45:GLY:HA3	1:C:233:ILE:HD11	2.01	0.41
1:A:233:ILE:HG12	1:A:239:ILE:HD13	2.02	0.41
1:E:123:ARG:HH21	1:E:123:ARG:CB	2.29	0.41
1:E:256:VAL:HG13	1:E:275:ARG:HB3	2.02	0.41
1:G:476:ASP:HB3	1:G:477:PRO:HD2	2.02	0.41
1:H:292:LEU:HD23	1:H:292:LEU:HA	1.93	0.41
1:C:296:PHE:O	1:C:369:ARG:NH1	2.53	0.41
1:E:66:VAL:HG23	1:E:136:VAL:HG13	2.02	0.41
1:H:414:PHE:O	1:H:415:MET:HB2	2.20	0.41
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.89	0.41
1:D:310:PHE:HA	1:D:342:VAL:HG13	2.02	0.41
1:E:241:ILE:O	1:E:243:PRO:HD3	2.21	0.41
1:I:257:ARG:HH22	1:I:456:SER:CB	2.33	0.41
1:A:373:ASP:HA	1:A:374:SER:HA	1.81	0.41
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.88	0.41
1:C:432:ILE:HG22	1:C:434:LEU:CD1	2.50	0.41
1:A:87:ASP:O	1:A:91:LEU:HG	2.21	0.41
1:A:279:ILE:HG23	1:A:431:THR:HB	2.03	0.41
1:A:310:PHE:CE1	1:A:342:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASP:OD2	1:A:463:ARG:NE	2.51	0.41
1:D:49:PHE:HA	1:D:239:ILE:HD12	2.02	0.41
1:D:155:ARG:O	1:D:159:PHE:HB2	2.20	0.41
1:G:22:PHE:HA	1:G:25:ILE:HG12	2.03	0.41
1:L:61:PHE:HB2	1:L:63:GLU:HG3	2.02	0.41
1:I:14:LYS:NZ	1:I:223:SER:O	2.54	0.41
1:E:69:THR:HA	1:E:139:ASP:HB3	2.04	0.41
1:G:197:ASN:HD22	1:G:219:PHE:HA	1.86	0.41
1:J:209:ARG:HG2	1:J:209:ARG:NH2	2.27	0.41
1:J:213:THR:HB	1:J:228:GLU:HB3	2.03	0.41
1:D:160:ARG:O	1:D:161:LEU:C	2.59	0.40
1:D:300:ALA:HB2	1:D:369:ARG:HD2	2.01	0.40
1:K:287:THR:HA	1:K:446:ARG:HD2	2.03	0.40
1:B:190:VAL:HA	1:B:193:PHE:CD1	2.56	0.40
1:C:436:ARG:HD2	1:C:485:LEU:HA	2.03	0.40
1:A:287:THR:HB	1:A:435:LEU:HB3	2.03	0.40
1:D:191:GLU:O	1:D:195:ALA:HB2	2.22	0.40
1:D:287:THR:HB	1:D:435:LEU:HB3	2.04	0.40
1:E:214:ILE:HG21	1:E:241:ILE:HD13	2.04	0.40
1:J:310:PHE:CD1	1:J:342:VAL:HG21	2.56	0.40
1:F:25:ILE:HG23	1:F:225:GLN:HB2	2.03	0.40
1:A:41:THR:HB	1:A:42:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/518 (85%)	405 (92%)	27 (6%)	6 (1%)	9	34
1	B	444/518 (86%)	401 (90%)	34 (8%)	9 (2%)	6	26
1	C	457/518 (88%)	412 (90%)	35 (8%)	10 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	435/518 (84%)	391 (90%)	37 (8%)	7 (2%)	8	31
1	E	448/518 (86%)	409 (91%)	30 (7%)	9 (2%)	6	26
1	F	438/518 (85%)	398 (91%)	28 (6%)	12 (3%)	4	21
1	G	435/518 (84%)	373 (86%)	54 (12%)	8 (2%)	7	29
1	H	429/518 (83%)	365 (85%)	52 (12%)	12 (3%)	4	20
1	I	438/518 (85%)	393 (90%)	35 (8%)	10 (2%)	5	23
1	J	437/518 (84%)	391 (90%)	38 (9%)	8 (2%)	7	29
1	K	434/518 (84%)	379 (87%)	47 (11%)	8 (2%)	7	29
1	L	425/518 (82%)	373 (88%)	43 (10%)	9 (2%)	5	25
All	All	5258/6216 (85%)	4690 (89%)	460 (9%)	108 (2%)	5	25

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	PRO
1	F	20	GLU
1	F	116	ASP
1	F	151	ALA
1	A	413	THR
1	D	62	ASP
1	G	328	ILE
1	H	194	VAL
1	H	382	ALA
1	L	247	MET
1	L	275	ARG
1	L	328	ILE
1	L	412	PRO
1	B	121	LEU
1	B	196	ASP
1	B	237	GLU
1	C	483	ARG
1	F	194	VAL
1	A	245	SER
1	D	160	ARG
1	D	237	GLU
1	E	237	GLU
1	H	381	VAL
1	H	383	SER
1	K	107	GLU

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Mol	Chain	Res	Type
1	K	328	ILE
1	L	194	VAL
1	L	303	ASN
1	L	323	ALA
1	I	381	VAL
1	J	237	GLU
1	J	313	GLU
1	J	328	ILE
1	B	236	GLY
1	C	60	ARG
1	C	147	GLN
1	C	237	GLU
1	C	343	CYS
1	F	148	PHE
1	F	247	MET
1	A	151	ALA
1	A	343	CYS
1	E	107	GLU
1	E	150	ASP
1	E	343	CYS
1	G	384	ASP
1	H	61	PHE
1	H	424	HIS
1	K	288	GLY
1	K	322	ASN
1	I	150	ASP
1	J	150	ASP
1	J	383	SER
1	B	94	GLU
1	B	104	PRO
1	B	343	CYS
1	C	193	PHE
1	C	479	ARG
1	F	205	LEU
1	F	285	THR
1	F	343	CYS
1	D	206	GLU
1	E	88	LEU
1	E	110	GLU
1	E	478	PHE
1	G	247	MET
1	G	274	PHE

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Mol	Chain	Res	Type
1	G	303	ASN
1	G	343	CYS
1	H	148	PHE
1	H	196	ASP
1	H	415	MET
1	I	236	GLY
1	I	396	SER
1	J	20	GLU
1	J	343	CYS
1	B	106	PRO
1	F	60	ARG
1	D	343	CYS
1	E	140	SER
1	G	470	LYS
1	H	384	ASP
1	K	106	PRO
1	K	326	TRP
1	K	343	CYS
1	K	403	ILE
1	L	413	THR
1	I	149	ASP
1	I	151	ALA
1	I	366	LYS
1	J	382	ALA
1	F	206	GLU
1	A	288	GLY
1	D	31	PRO
1	I	343	CYS
1	C	45	GLY
1	A	243	PRO
1	H	190	VAL
1	I	42	PRO
1	F	288	GLY
1	L	239	ILE
1	E	45	GLY
1	H	42	PRO
1	C	19	ILE
1	C	288	GLY
1	G	288	GLY
1	I	367	PRO
1	D	288	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/442 (64%)	260 (92%)	22 (8%)	10	35
1	B	285/442 (64%)	266 (93%)	19 (7%)	13	40
1	C	275/442 (62%)	258 (94%)	17 (6%)	15	43
1	D	248/442 (56%)	234 (94%)	14 (6%)	17	46
1	E	272/442 (62%)	253 (93%)	19 (7%)	12	39
1	F	267/442 (60%)	249 (93%)	18 (7%)	13	40
1	G	201/442 (46%)	181 (90%)	20 (10%)	6	24
1	H	193/442 (44%)	173 (90%)	20 (10%)	5	22
1	I	219/442 (50%)	205 (94%)	14 (6%)	14	42
1	J	235/442 (53%)	223 (95%)	12 (5%)	20	49
1	K	208/442 (47%)	196 (94%)	12 (6%)	17	45
1	L	186/442 (42%)	171 (92%)	15 (8%)	9	33
All	All	2871/5304 (54%)	2669 (93%)	202 (7%)	12	39

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	141	ILE
1	B	191	GLU
1	B	200	ILE
1	B	202	ARG
1	B	205	LEU
1	B	210	ARG
1	B	257	ARG
1	B	306	ARG
1	B	361	VAL
1	B	370	ILE
1	B	406	LEU
1	B	434	LEU
1	B	438	VAL

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Mol	Chain	Res	Type
1	B	440	MET
1	B	448	ILE
1	B	463	ARG
1	B	466	THR
1	B	474	ILE
1	C	59	LYS
1	C	89	GLN
1	C	144	ILE
1	C	173	ILE
1	C	196	ASP
1	C	205	LEU
1	C	213	THR
1	C	214	ILE
1	C	222	THR
1	C	252	ARG
1	C	297	LEU
1	C	324	THR
1	C	345	TYR
1	C	406	LEU
1	C	425	ILE
1	C	453	MET
1	C	466	THR
1	F	20	GLU
1	F	58	ILE
1	F	60	ARG
1	F	88	LEU
1	F	90	LYS
1	F	185	ILE
1	F	214	ILE
1	F	285	THR
1	F	297	LEU
1	F	308	LEU
1	F	328	ILE
1	F	332	GLU
1	F	355	LEU
1	F	375	LEU
1	F	390	PHE
1	F	434	LEU
1	F	446	ARG
1	F	466	THR
1	A	86	TRP
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	168	MET
1	A	179	THR
1	A	213	THR
1	A	214	ILE
1	A	222	THR
1	A	285	THR
1	A	295	LYS
1	A	297	LEU
1	A	306	ARG
1	A	308	LEU
1	A	370	ILE
1	A	375	LEU
1	A	404	THR
1	A	411	THR
1	A	424	HIS
1	A	446	ARG
1	A	448	ILE
1	A	453	MET
1	A	466	THR
1	A	472	MET
1	D	117	LEU
1	D	159	PHE
1	D	187	ARG
1	D	206	GLU
1	D	210	ARG
1	D	222	THR
1	D	234	THR
1	D	297	LEU
1	D	342	VAL
1	D	355	LEU
1	D	424	HIS
1	D	438	VAL
1	D	466	THR
1	D	472	MET
1	E	51	MET
1	E	58	ILE
1	E	66	VAL
1	E	78	LEU
1	E	97	LEU
1	E	107	GLU
1	E	123	ARG
1	E	191	GLU

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Mol	Chain	Res	Type
1	E	193	PHE
1	E	213	THR
1	E	222	THR
1	E	234	THR
1	E	257	ARG
1	E	285	THR
1	E	317	GLU
1	E	352	GLU
1	E	370	ILE
1	E	406	LEU
1	E	444	MET
1	G	48	VAL
1	G	58	ILE
1	G	61	PHE
1	G	141	ILE
1	G	187	ARG
1	G	194	VAL
1	G	200	ILE
1	G	204	VAL
1	G	205	LEU
1	G	209	ARG
1	G	212	ARG
1	G	216	ILE
1	G	219	PHE
1	G	233	ILE
1	G	234	THR
1	G	265	LEU
1	G	321	ARG
1	G	328	ILE
1	G	338	ARG
1	G	453	MET
1	H	58	ILE
1	H	68	VAL
1	H	91	LEU
1	H	100	VAL
1	H	159	PHE
1	H	190	VAL
1	H	205	LEU
1	H	212	ARG
1	H	213	THR
1	H	214	ILE
1	H	219	PHE

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Mol	Chain	Res	Type
1	H	295	LYS
1	H	320	LEU
1	H	345	TYR
1	H	349	THR
1	H	351	LEU
1	H	380	ARG
1	H	446	ARG
1	H	453	MET
1	H	458	HIS
1	K	19	ILE
1	K	20	GLU
1	K	58	ILE
1	K	214	ILE
1	K	222	THR
1	K	351	LEU
1	K	378	LEU
1	K	435	LEU
1	K	436	ARG
1	K	438	VAL
1	K	453	MET
1	K	466	THR
1	L	58	ILE
1	L	61	PHE
1	L	164	ARG
1	L	170	VAL
1	L	187	ARG
1	L	206	GLU
1	L	219	PHE
1	L	232	THR
1	L	234	THR
1	L	328	ILE
1	L	411	THR
1	L	438	VAL
1	L	444	MET
1	L	448	ILE
1	L	465	PHE
1	I	72	GLU
1	I	86	TRP
1	I	107	GLU
1	I	123	ARG
1	I	135	ARG
1	I	185	ILE

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Mol	Chain	Res	Type
1	I	198	VAL
1	I	205	LEU
1	I	212	ARG
1	I	219	PHE
1	I	433	ILE
1	I	438	VAL
1	I	453	MET
1	I	466	THR
1	J	100	VAL
1	J	205	LEU
1	J	214	ILE
1	J	234	THR
1	J	295	LYS
1	J	298	GLU
1	J	308	LEU
1	J	309	LEU
1	J	352	GLU
1	J	357	MET
1	J	397	PHE
1	J	466	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	400	GLN
1	B	458	HIS
1	C	197	ASN
1	C	225	GLN
1	F	197	ASN
1	A	147	GLN
1	A	322	ASN
1	D	458	HIS
1	E	56	HIS
1	E	197	ASN
1	E	255	ASN
1	G	52	GLN
1	G	197	ASN
1	G	225	GLN
1	H	197	ASN
1	K	303	ASN
1	K	322	ASN
1	L	146	GLN

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Mol	Chain	Res	Type
1	I	303	ASN
1	J	52	GLN
1	J	303	ASN
1	J	318	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 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	C	602	3	24,29,29	0.64	0	29,45,45	0.78	1 (3%)
2	ADP	L	601	3	24,29,29	0.64	0	29,45,45	0.69	1 (3%)
2	ADP	G	601	3	24,29,29	0.65	0	29,45,45	0.70	1 (3%)
2	ADP	G	602	3	24,29,29	0.65	0	29,45,45	0.67	1 (3%)
2	ADP	I	602	3	24,29,29	0.64	0	29,45,45	0.73	1 (3%)
2	ADP	A	602	3	24,29,29	0.64	0	29,45,45	0.73	1 (3%)
2	ADP	C	601	3	24,29,29	0.64	0	29,45,45	0.77	1 (3%)
2	ADP	E	601	3	24,29,29	0.64	0	29,45,45	0.75	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	K	602	3	24,29,29	0.64	0	29,45,45	0.72	1 (3%)
2	ADP	D	601	3	24,29,29	0.66	0	29,45,45	0.70	1 (3%)
2	ADP	F	601	3	24,29,29	0.66	0	29,45,45	0.74	1 (3%)
2	ADP	L	602	3	24,29,29	0.65	0	29,45,45	0.69	1 (3%)
2	ADP	B	601	3	24,29,29	0.65	0	29,45,45	0.72	1 (3%)
2	ADP	F	602	3	24,29,29	0.64	0	29,45,45	0.72	1 (3%)
2	ADP	H	602	3	24,29,29	0.64	0	29,45,45	0.74	1 (3%)
2	ADP	J	602	3	24,29,29	0.66	0	29,45,45	0.68	1 (3%)
2	ADP	B	602	3	24,29,29	0.66	0	29,45,45	0.70	1 (3%)
2	ADP	H	601	3	24,29,29	0.64	0	29,45,45	0.70	1 (3%)
2	ADP	J	601	3	24,29,29	0.65	0	29,45,45	0.74	1 (3%)
2	ADP	E	602	-	24,29,29	0.65	0	29,45,45	0.69	1 (3%)
2	ADP	A	601	3	24,29,29	0.65	0	29,45,45	0.71	1 (3%)
2	ADP	I	601	3	24,29,29	0.65	0	29,45,45	0.67	1 (3%)
2	ADP	D	602	3	24,29,29	0.66	0	29,45,45	0.75	1 (3%)
2	ADP	K	601	3	24,29,29	0.66	0	29,45,45	0.71	1 (3%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	F	602	3	-	7/12/32/32	0/3/3/3
2	ADP	H	602	3	-	2/12/32/32	0/3/3/3
2	ADP	J	602	3	-	3/12/32/32	0/3/3/3
2	ADP	B	602	3	-	5/12/32/32	0/3/3/3
2	ADP	H	601	3	-	1/12/32/32	0/3/3/3
2	ADP	J	601	3	-	3/12/32/32	0/3/3/3
2	ADP	E	602	-	-	0/12/32/32	0/3/3/3
2	ADP	A	601	3	-	5/12/32/32	0/3/3/3
2	ADP	I	601	3	-	8/12/32/32	0/3/3/3
2	ADP	D	602	3	-	2/12/32/32	0/3/3/3
2	ADP	K	601	3	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	ADP	C5-C6-N6	2.29	123.83	120.35
2	L	601	ADP	C5-C6-N6	2.26	123.78	120.35
2	I	602	ADP	C5-C6-N6	2.25	123.78	120.35
2	C	602	ADP	C5-C6-N6	2.25	123.77	120.35
2	D	602	ADP	C5-C6-N6	2.24	123.76	120.35
2	K	601	ADP	C5-C6-N6	2.23	123.75	120.35
2	L	602	ADP	C5-C6-N6	2.23	123.75	120.35
2	H	602	ADP	C5-C6-N6	2.23	123.74	120.35
2	J	601	ADP	C5-C6-N6	2.21	123.72	120.35
2	A	601	ADP	C5-C6-N6	2.21	123.71	120.35
2	E	602	ADP	C5-C6-N6	2.21	123.71	120.35
2	B	601	ADP	C5-C6-N6	2.21	123.70	120.35
2	F	602	ADP	C5-C6-N6	2.19	123.69	120.35
2	H	601	ADP	C5-C6-N6	2.19	123.67	120.35
2	G	601	ADP	C5-C6-N6	2.18	123.67	120.35
2	G	602	ADP	C5-C6-N6	2.17	123.64	120.35
2	B	602	ADP	C5-C6-N6	2.16	123.64	120.35
2	J	602	ADP	C5-C6-N6	2.15	123.63	120.35
2	C	601	ADP	C5-C6-N6	2.15	123.62	120.35
2	E	601	ADP	C5-C6-N6	2.14	123.61	120.35
2	D	601	ADP	C5-C6-N6	2.14	123.60	120.35
2	K	602	ADP	C5-C6-N6	2.12	123.57	120.35
2	F	601	ADP	C5-C6-N6	2.10	123.54	120.35
2	I	601	ADP	C5-C6-N6	2.05	123.46	120.35

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O3A
2	B	602	ADP	C5'-O5'-PA-O1A
2	B	602	ADP	O4'-C4'-C5'-O5'
2	F	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	C5'-O5'-PA-O2A
2	F	601	ADP	C5'-O5'-PA-O3A
2	F	601	ADP	O4'-C4'-C5'-O5'
2	F	602	ADP	C5'-O5'-PA-O1A
2	F	602	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	C5'-O5'-PA-O2A
2	A	602	ADP	C5'-O5'-PA-O3A
2	A	602	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	C3'-C4'-C5'-O5'
2	G	602	ADP	O4'-C4'-C5'-O5'
2	G	602	ADP	C3'-C4'-C5'-O5'
2	H	601	ADP	PA-O3A-PB-O2B
2	K	601	ADP	C5'-O5'-PA-O2A
2	K	601	ADP	C5'-O5'-PA-O3A
2	K	601	ADP	O4'-C4'-C5'-O5'
2	K	602	ADP	C5'-O5'-PA-O1A
2	K	602	ADP	C5'-O5'-PA-O3A
2	L	602	ADP	C5'-O5'-PA-O2A
2	I	601	ADP	PA-O3A-PB-O2B
2	I	601	ADP	C5'-O5'-PA-O3A
2	I	602	ADP	C5'-O5'-PA-O1A
2	I	602	ADP	C5'-O5'-PA-O2A
2	I	602	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	O4'-C4'-C5'-O5'
2	F	601	ADP	C3'-C4'-C5'-O5'
2	K	601	ADP	C3'-C4'-C5'-O5'
2	J	601	ADP	O4'-C4'-C5'-O5'
2	J	602	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
2	A	602	ADP	C3'-C4'-C5'-O5'
2	D	602	ADP	O4'-C4'-C5'-O5'
2	D	602	ADP	C3'-C4'-C5'-O5'
2	H	602	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	I	602	ADP	O4'-C4'-C5'-O5'
2	J	601	ADP	C3'-C4'-C5'-O5'
2	J	602	ADP	O4'-C4'-C5'-O5'
2	H	602	ADP	C3'-C4'-C5'-O5'
2	L	602	ADP	C3'-C4'-C5'-O5'
2	I	601	ADP	C3'-C4'-C5'-O5'
2	D	601	ADP	C3'-C4'-C5'-O5'
2	L	602	ADP	O4'-C4'-C5'-O5'
2	I	602	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	C3'-C4'-C5'-O5'
2	K	602	ADP	O4'-C4'-C5'-O5'
2	C	602	ADP	PA-O3A-PB-O1B
2	I	602	ADP	PA-O3A-PB-O1B
2	D	601	ADP	O4'-C4'-C5'-O5'
2	I	601	ADP	PB-O3A-PA-O5'
2	G	602	ADP	PA-O3A-PB-O2B
2	I	601	ADP	PA-O3A-PB-O3B
2	J	601	ADP	PA-O3A-PB-O2B
2	B	602	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	C5'-O5'-PA-O3A
2	F	602	ADP	C5'-O5'-PA-O3A
2	A	601	ADP	C5'-O5'-PA-O3A
2	L	602	ADP	C5'-O5'-PA-O3A
2	J	602	ADP	PB-O3A-PA-O1A
2	B	602	ADP	C5'-O5'-PA-O2A
2	F	602	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	C5'-O5'-PA-O1A
2	A	602	ADP	C5'-O5'-PA-O2A
2	K	602	ADP	C5'-O5'-PA-O2A
2	I	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	O4'-C4'-C5'-O5'
2	I	601	ADP	O4'-C4'-C5'-O5'
2	F	602	ADP	C3'-C4'-C5'-O5'
2	F	602	ADP	PB-O3A-PA-O2A
2	K	602	ADP	C3'-C4'-C5'-O5'
2	I	601	ADP	PA-O3A-PB-O1B
2	B	602	ADP	C3'-C4'-C5'-O5'
2	G	601	ADP	PA-O3A-PB-O3B
2	I	602	ADP	PA-O3A-PB-O3B
2	F	602	ADP	PB-O3A-PA-O1A
2	L	602	ADP	PB-O3A-PA-O2A
2	C	601	ADP	C5'-O5'-PA-O1A

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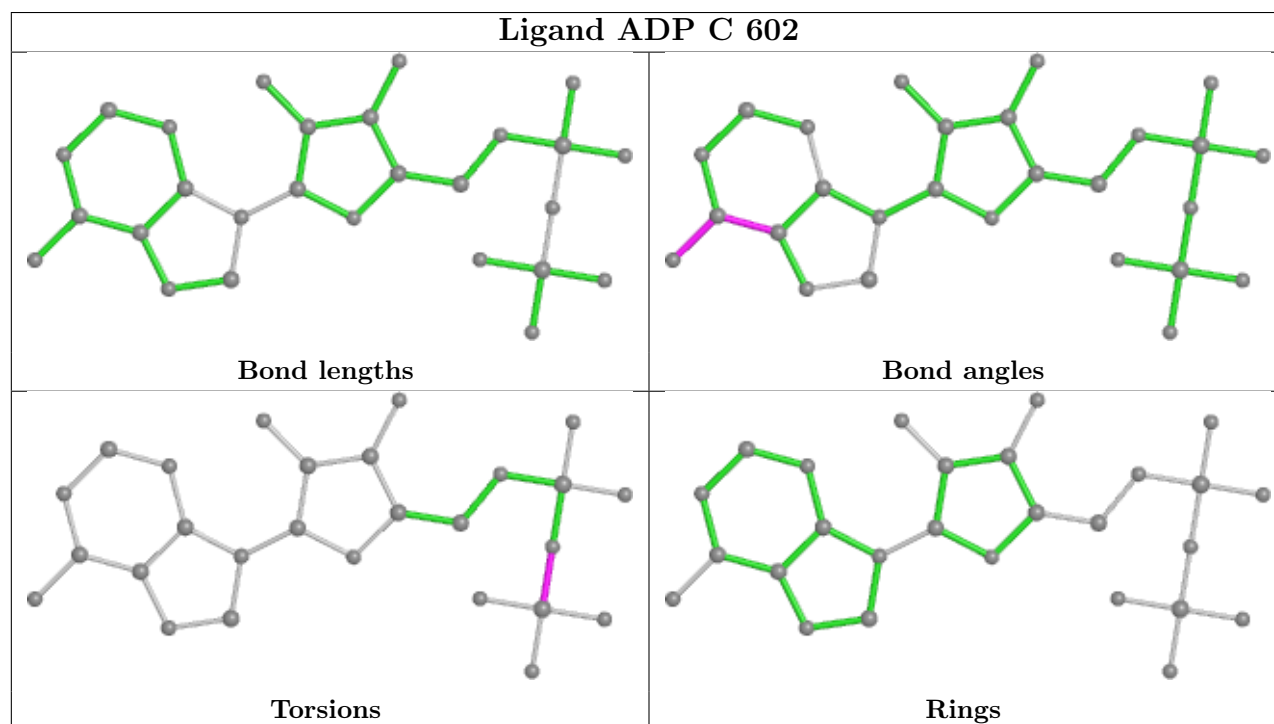
Mol	Chain	Res	Type	Atoms
2	L	602	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

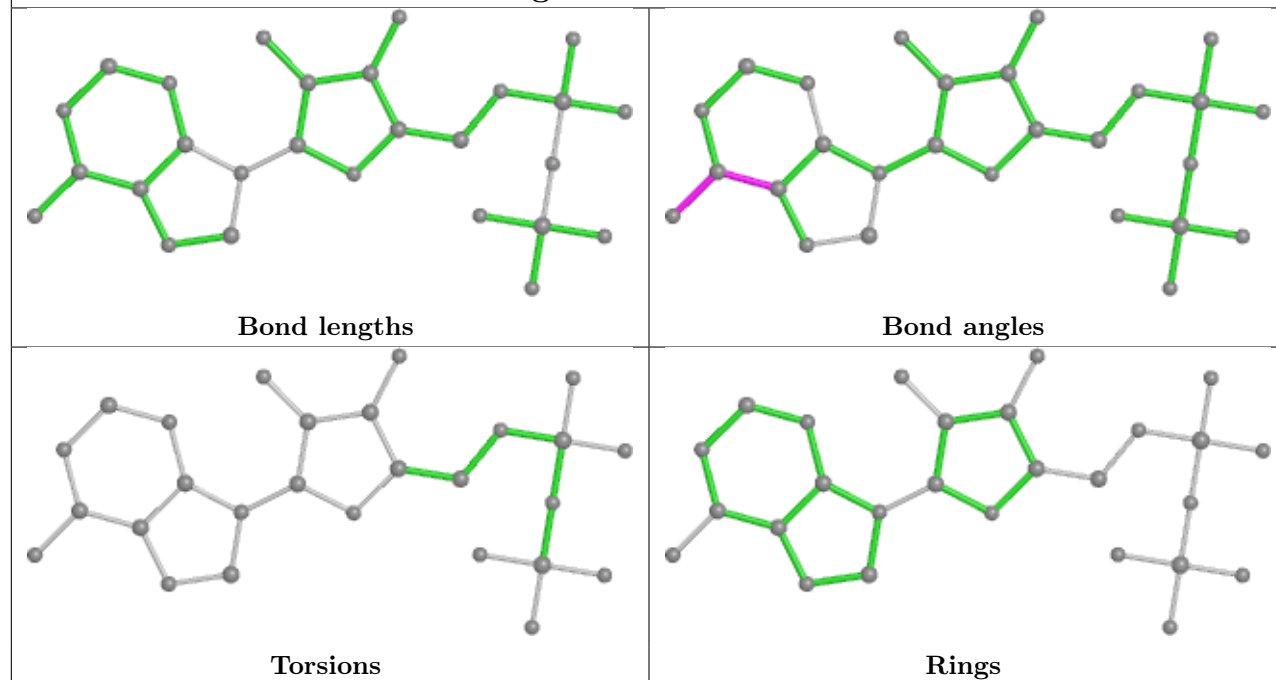
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	ADP	1	0
2	K	602	ADP	1	0
2	F	601	ADP	1	0
2	L	602	ADP	1	0
2	I	601	ADP	1	0

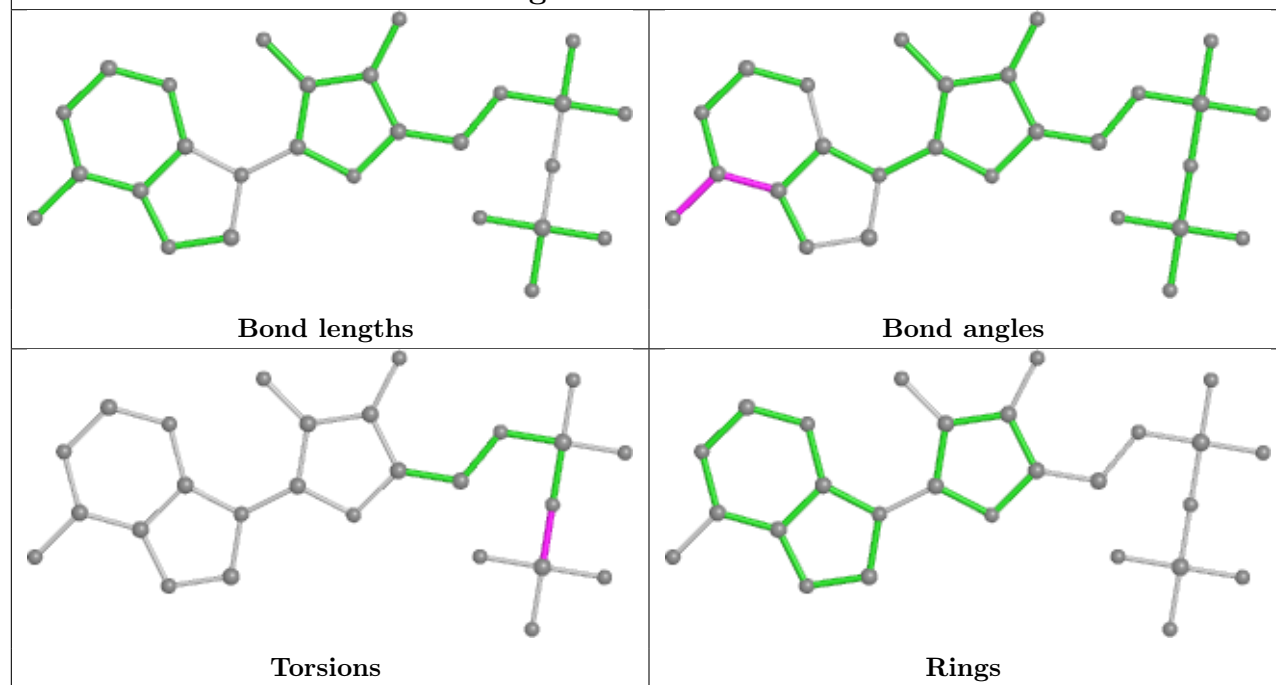
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



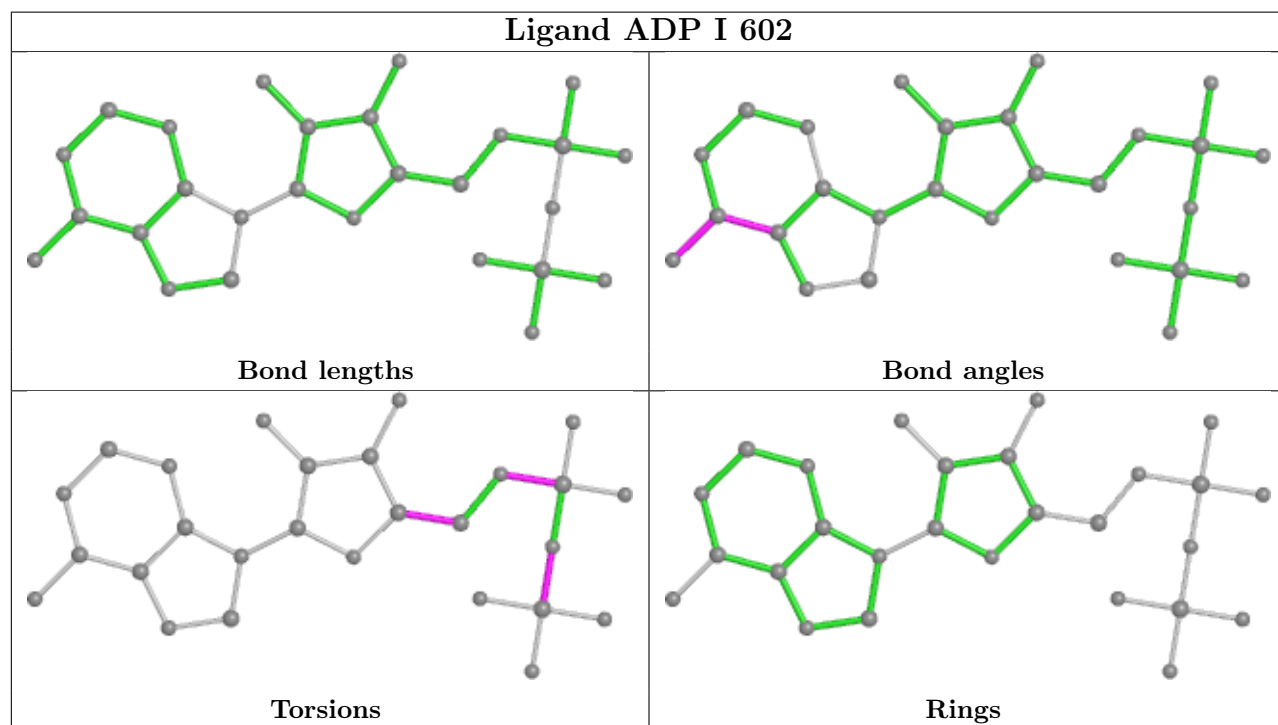
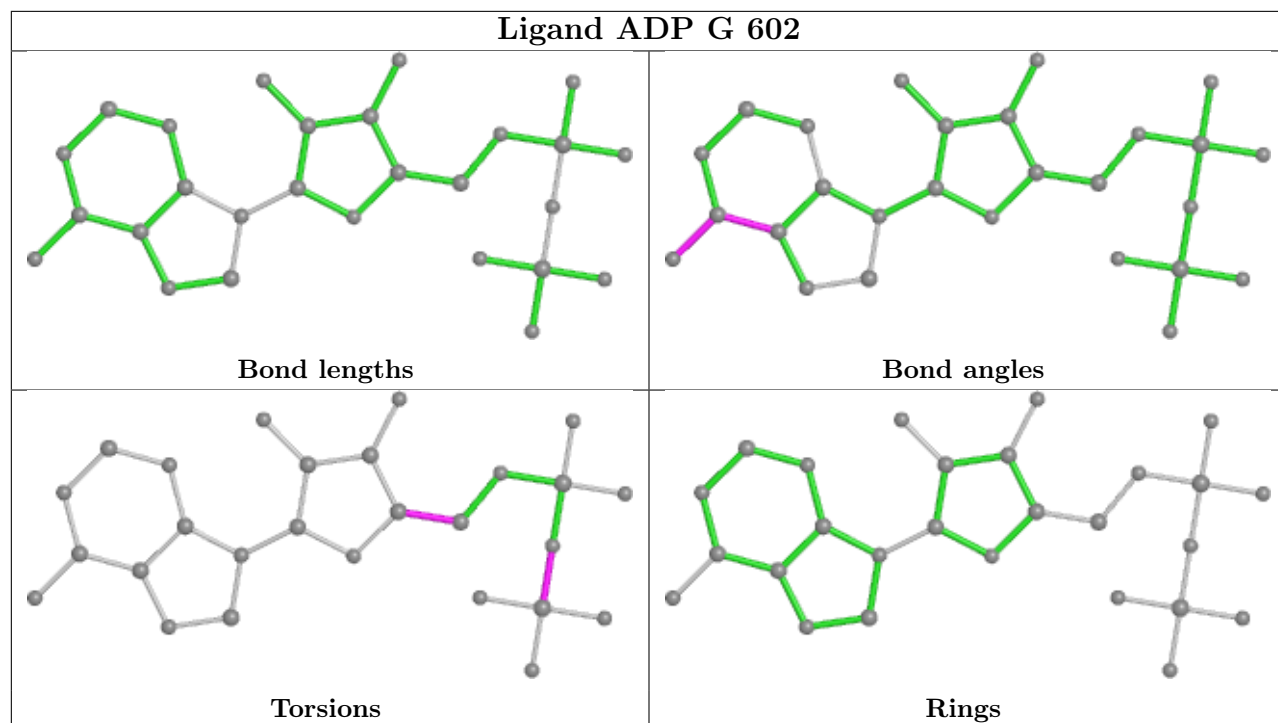
## Ligand ADP L 601

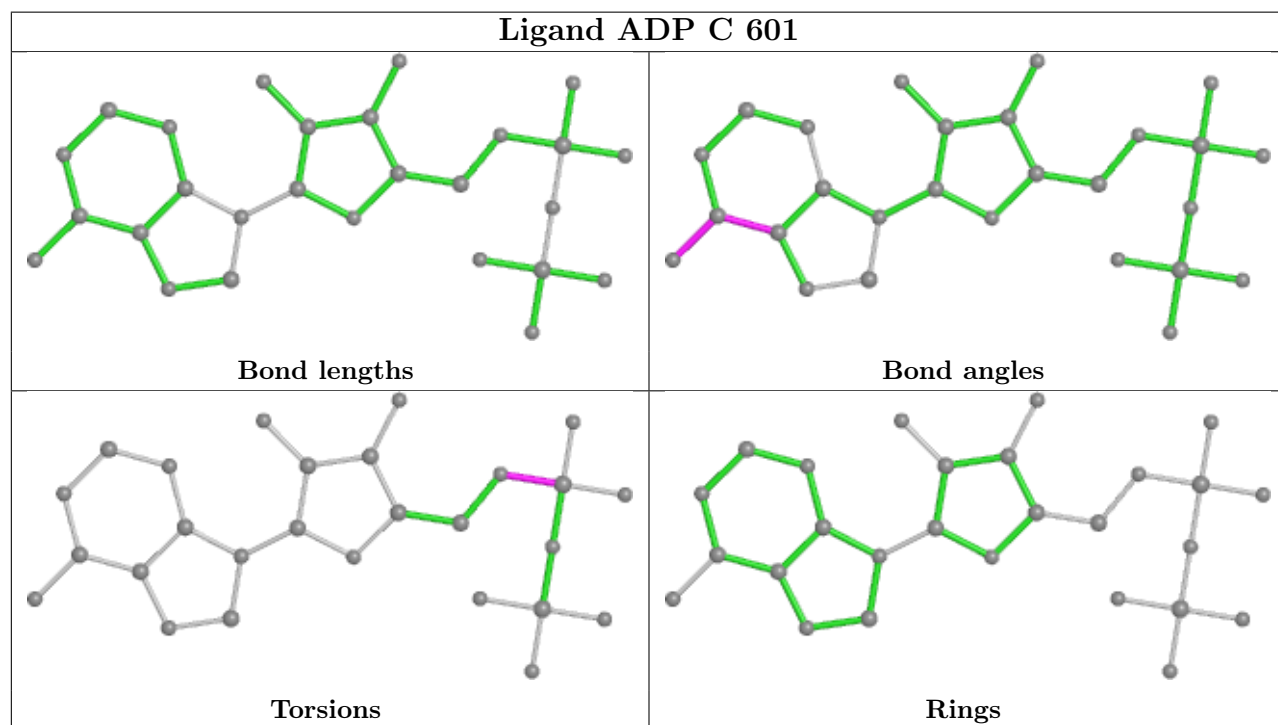
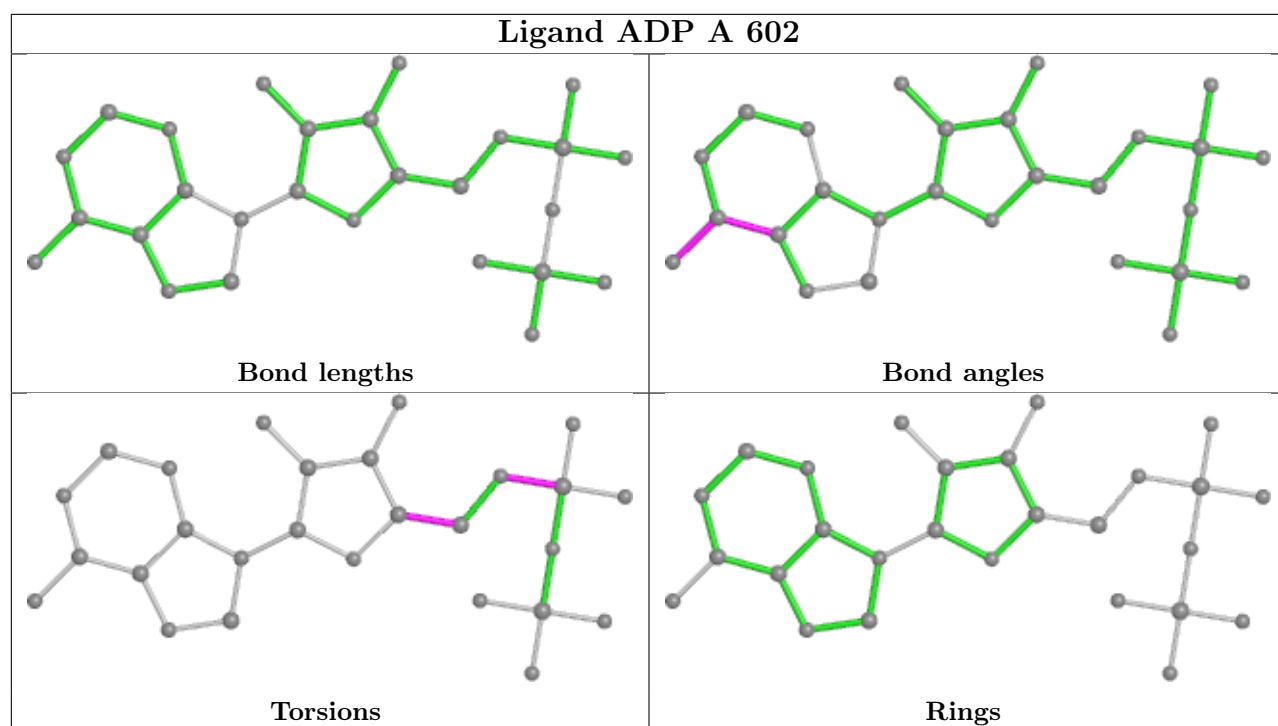


## Ligand ADP G 601

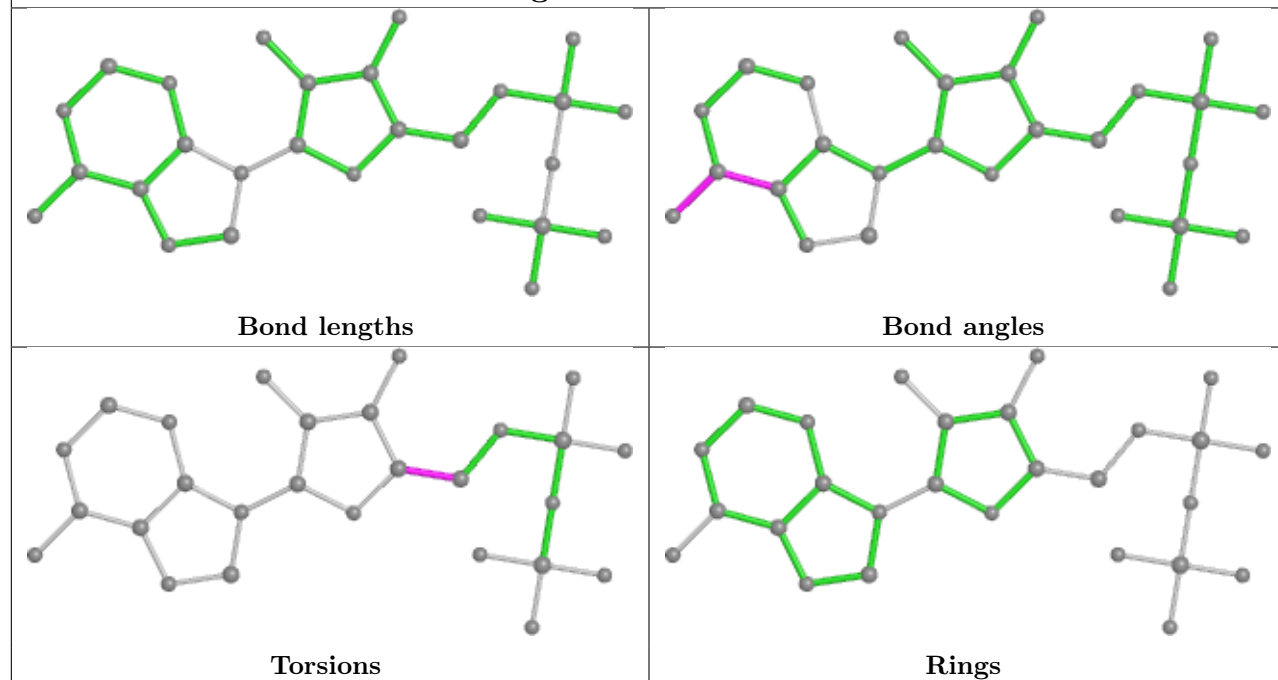




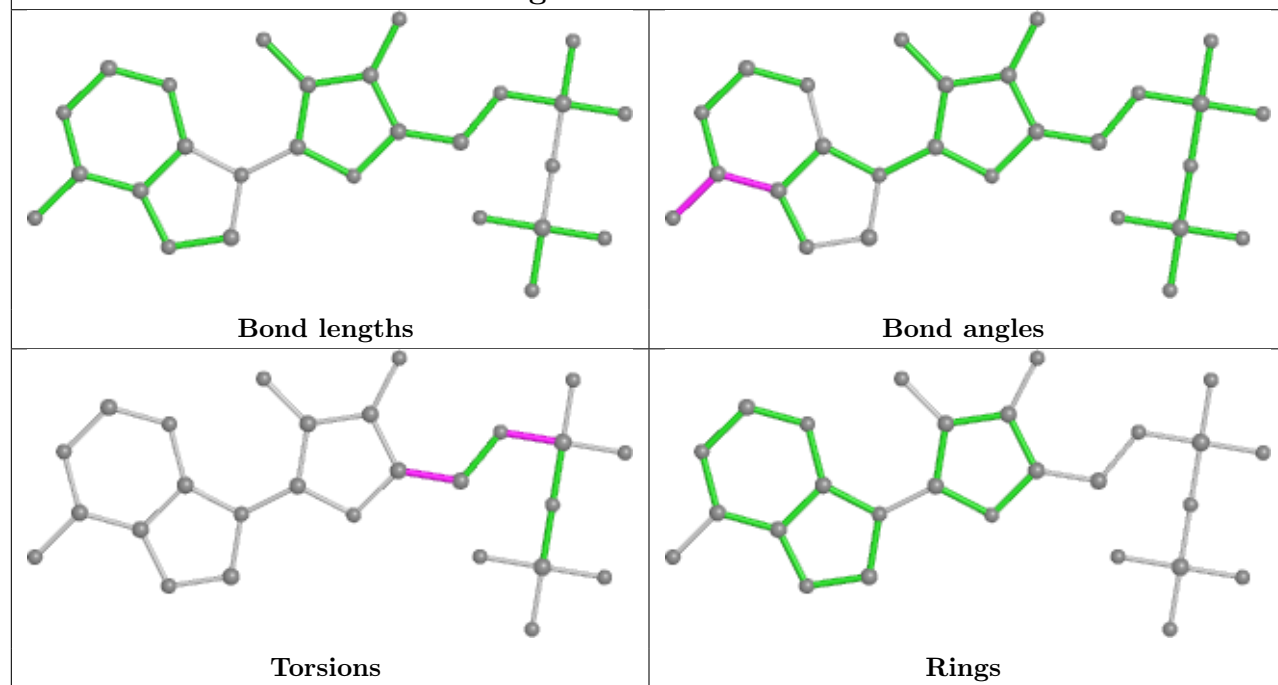


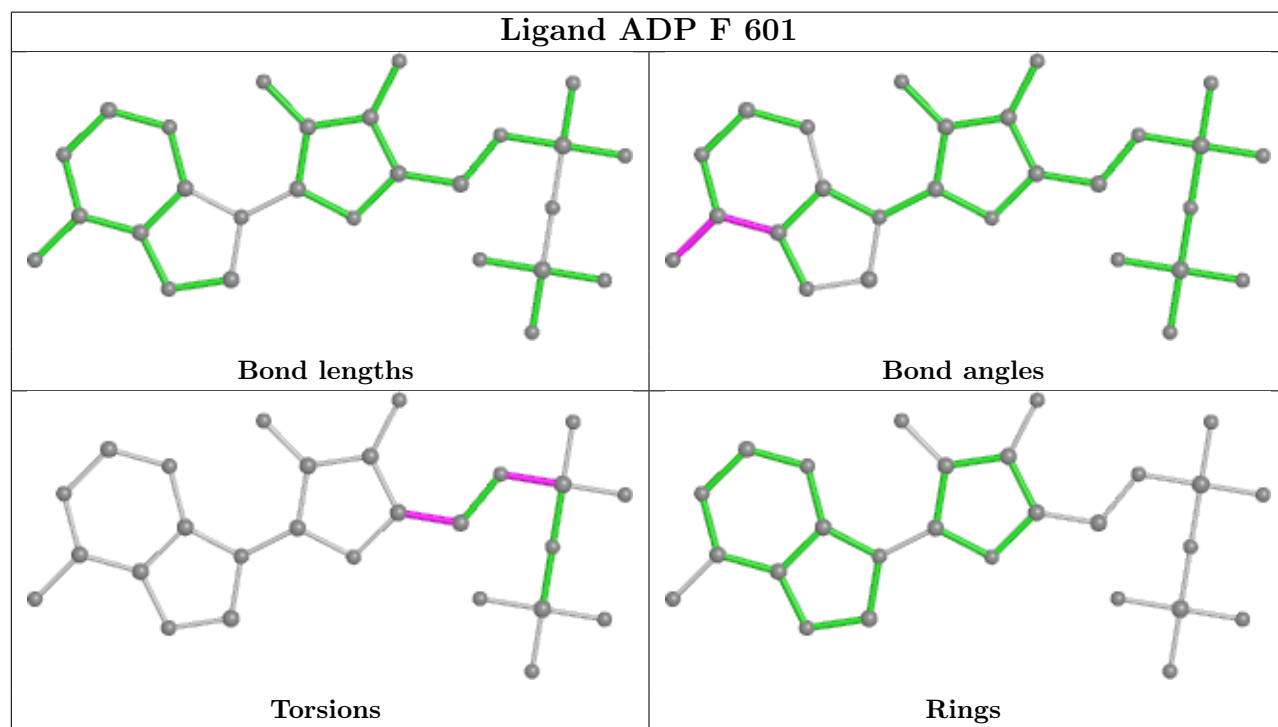
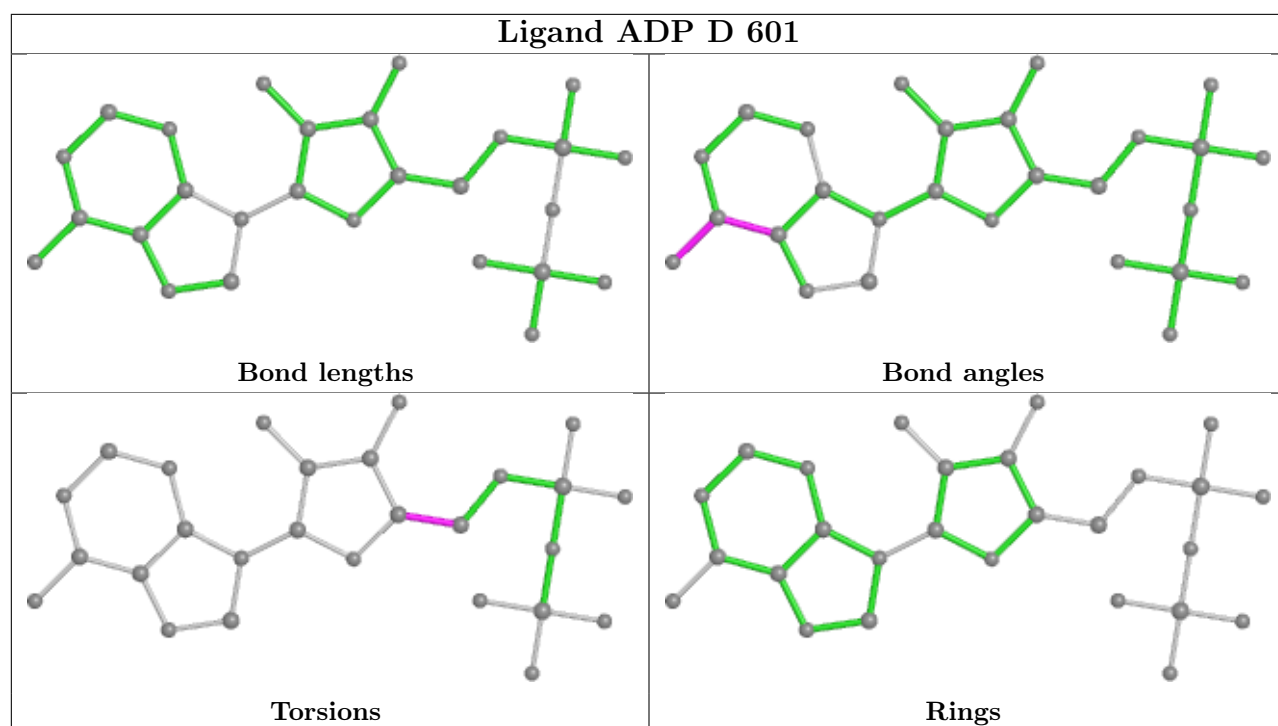


## Ligand ADP E 601

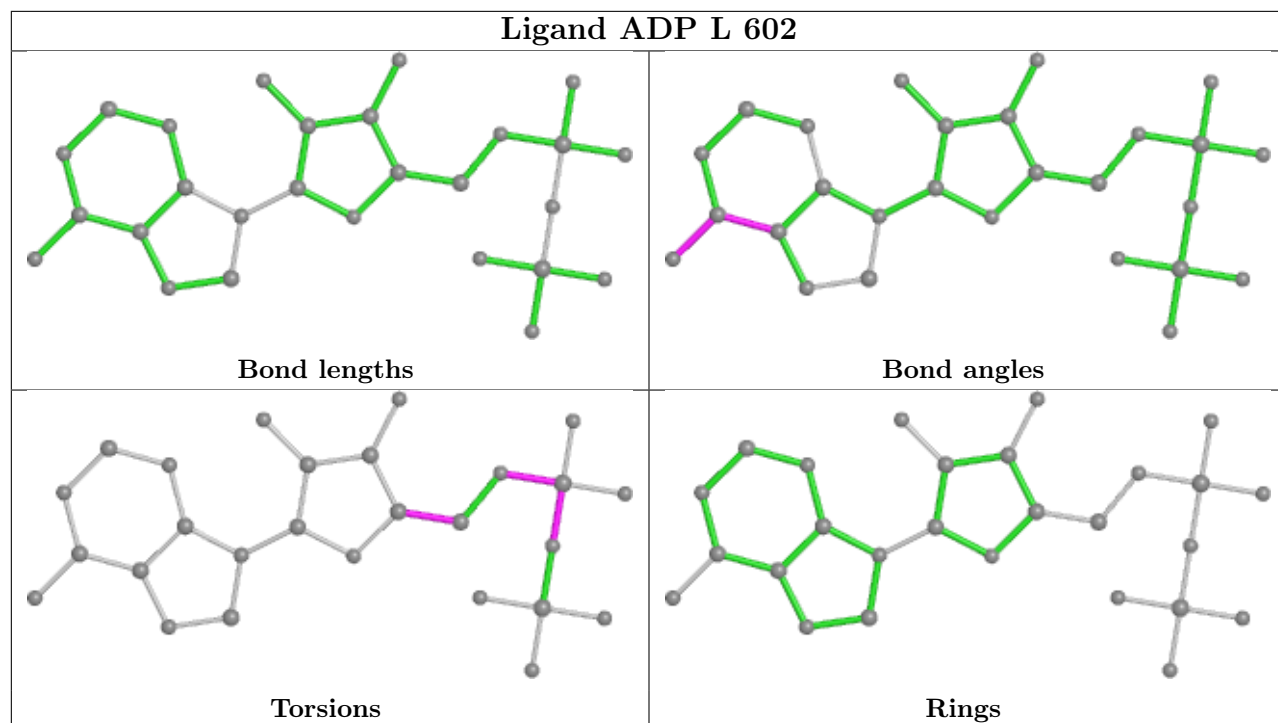


## Ligand ADP K 602

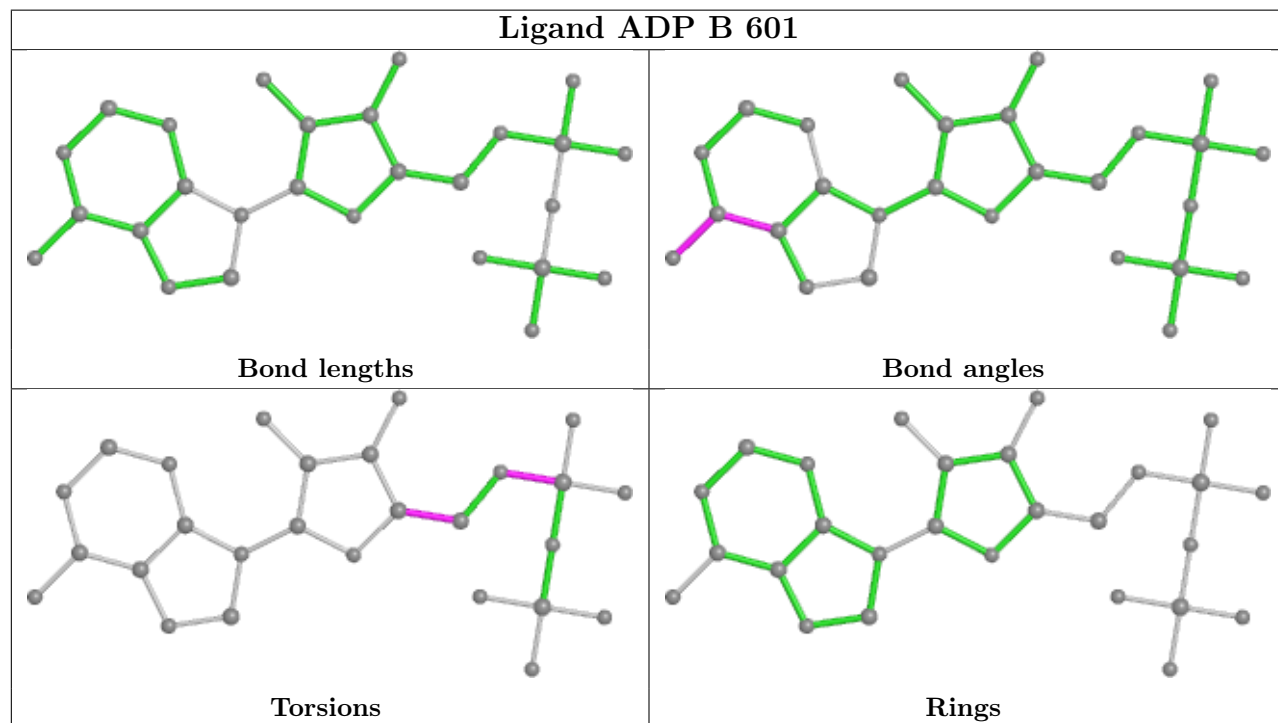




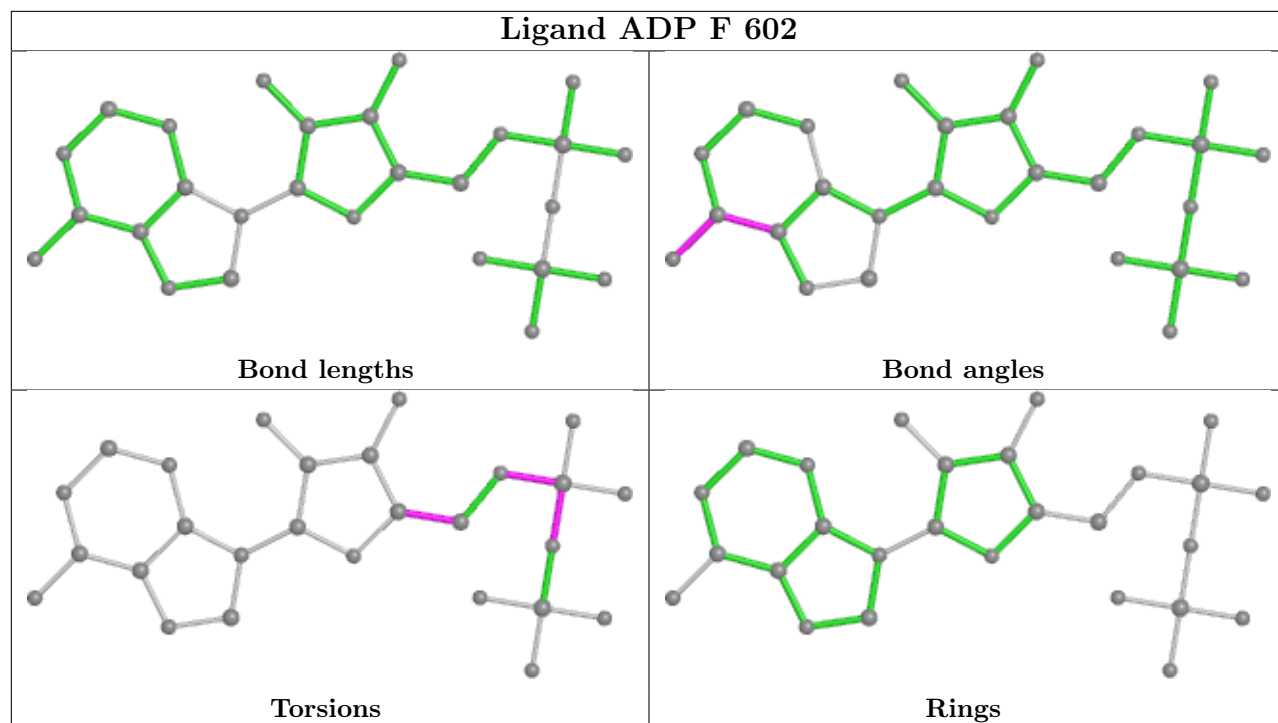
## Ligand ADP L 602



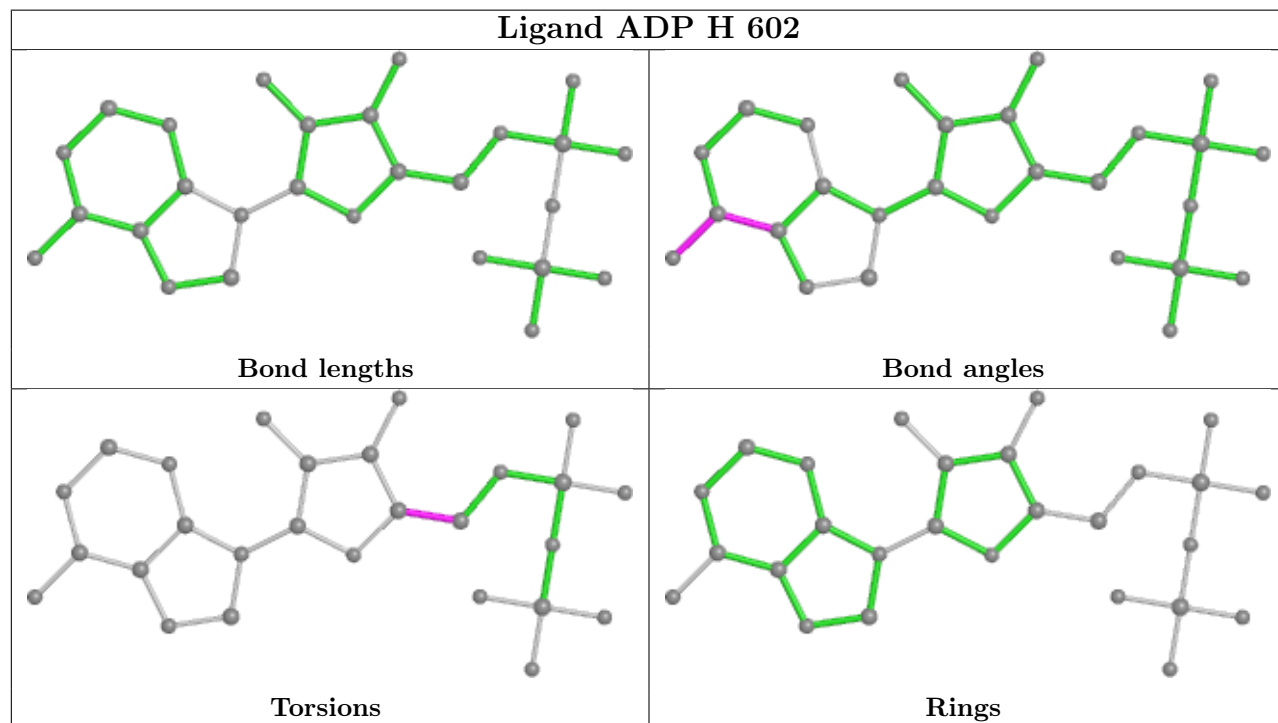
## Ligand ADP B 601



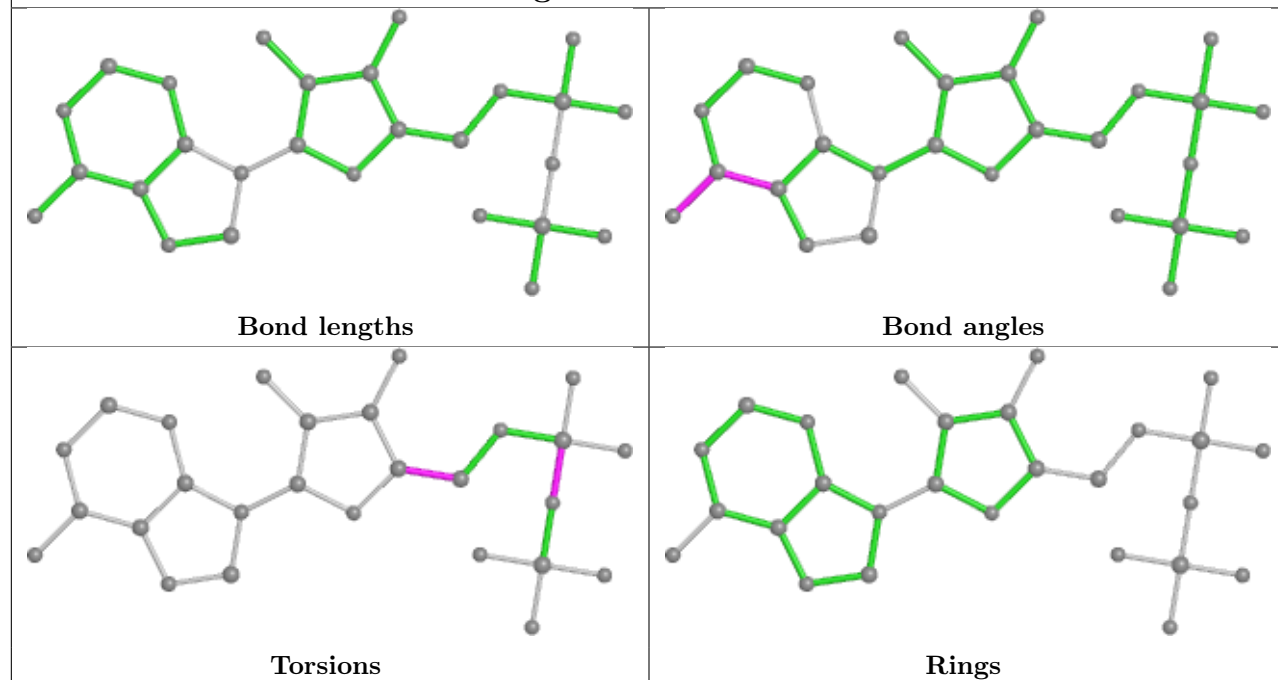
## Ligand ADP F 602



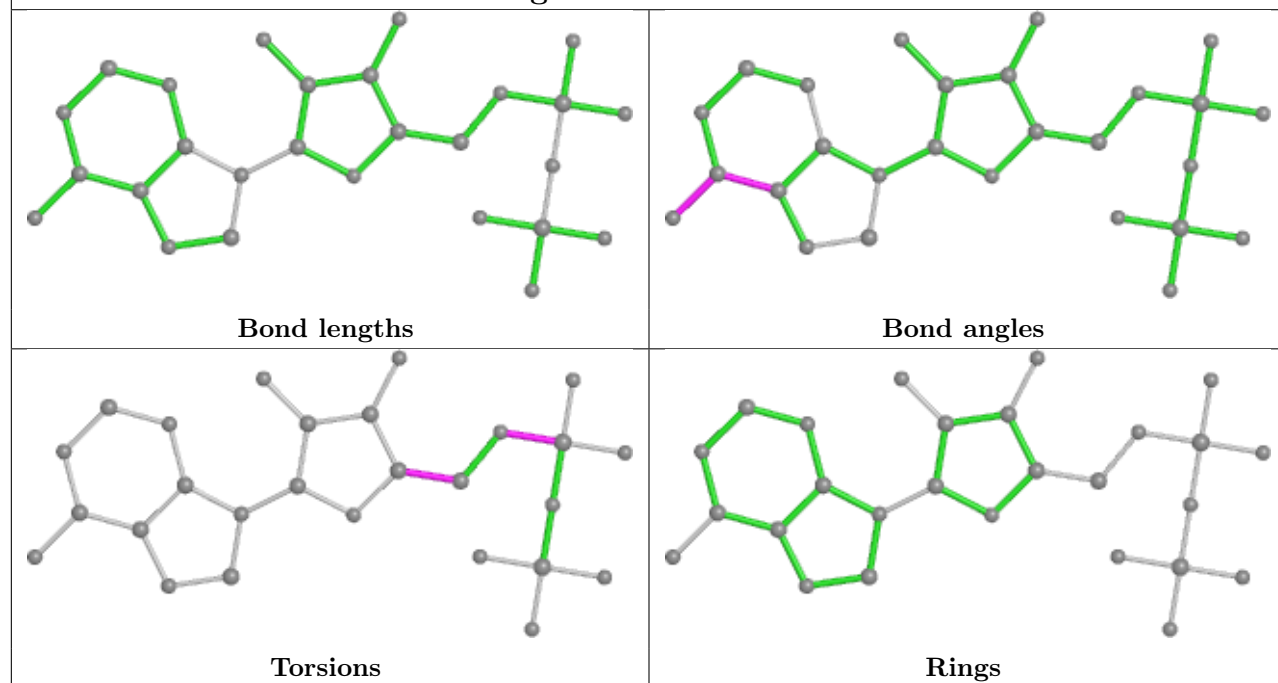
## Ligand ADP H 602

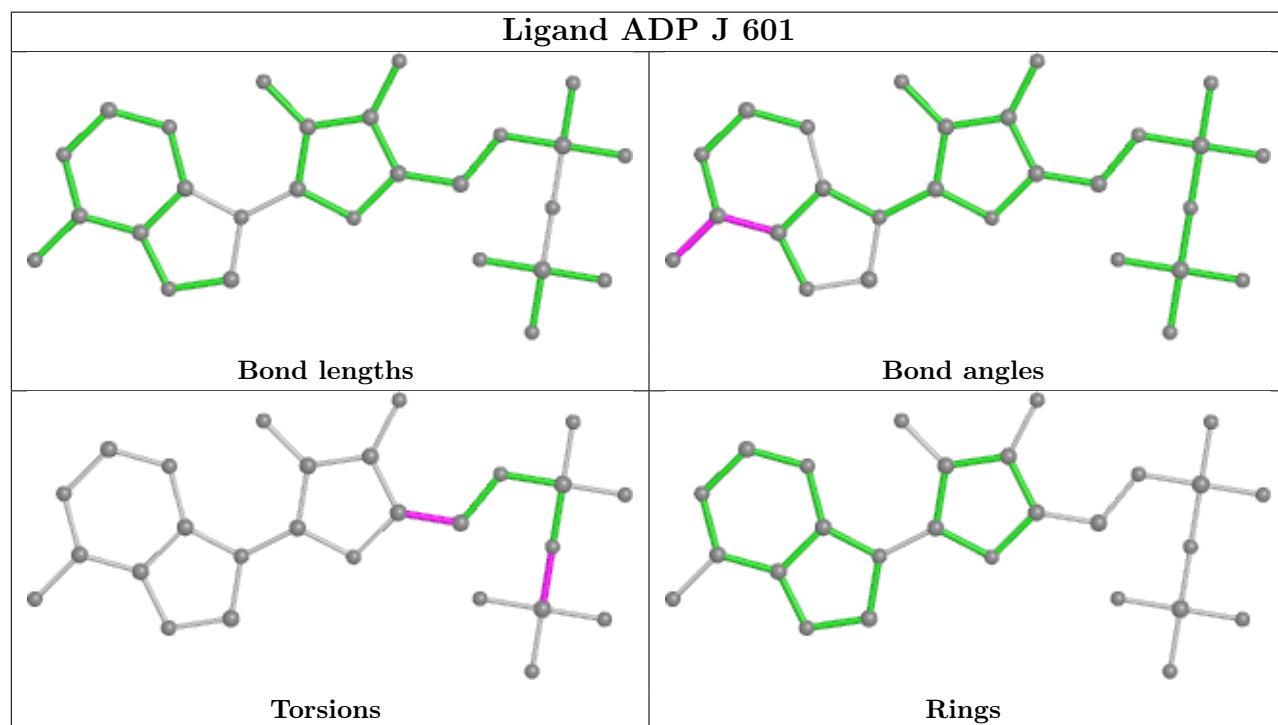
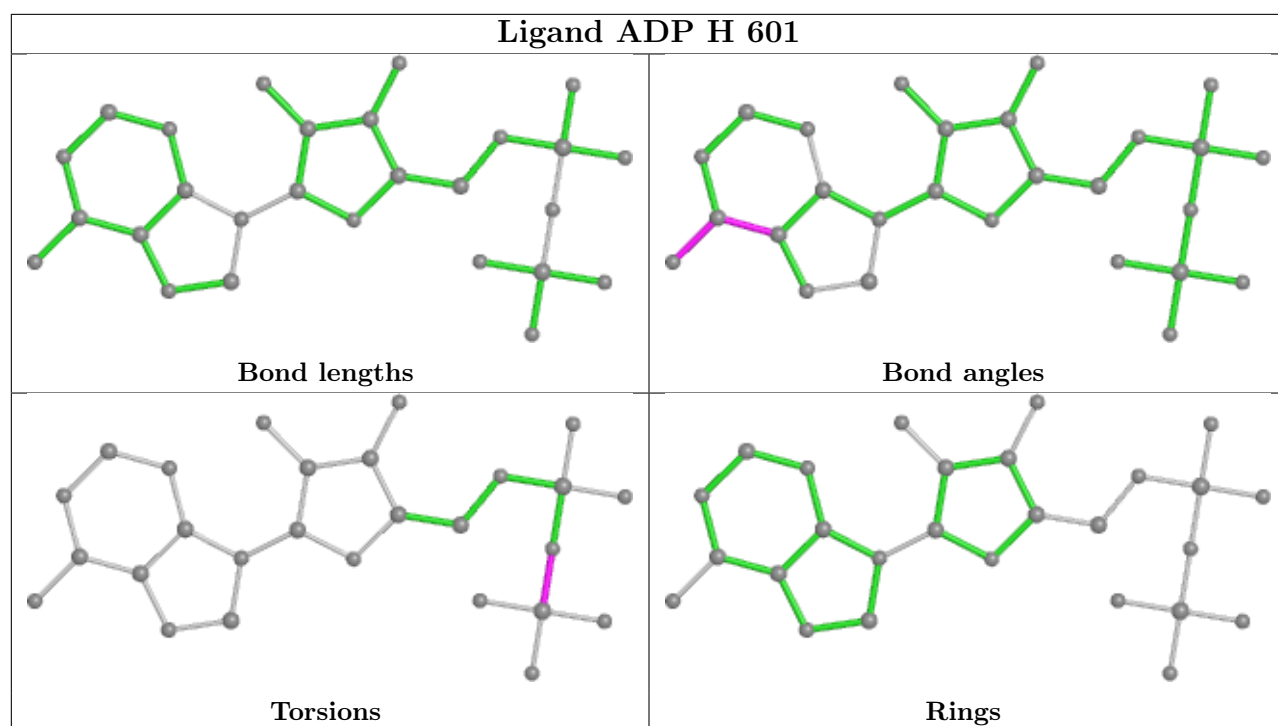


## Ligand ADP J 602



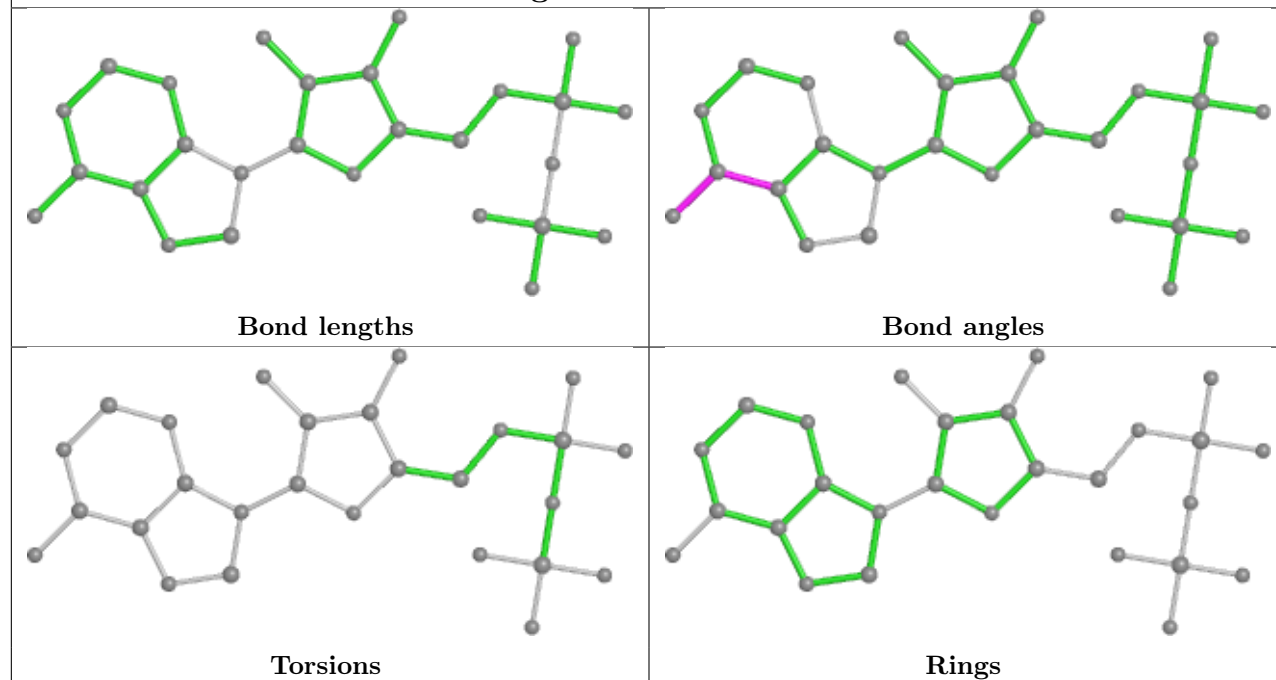
## Ligand ADP B 602



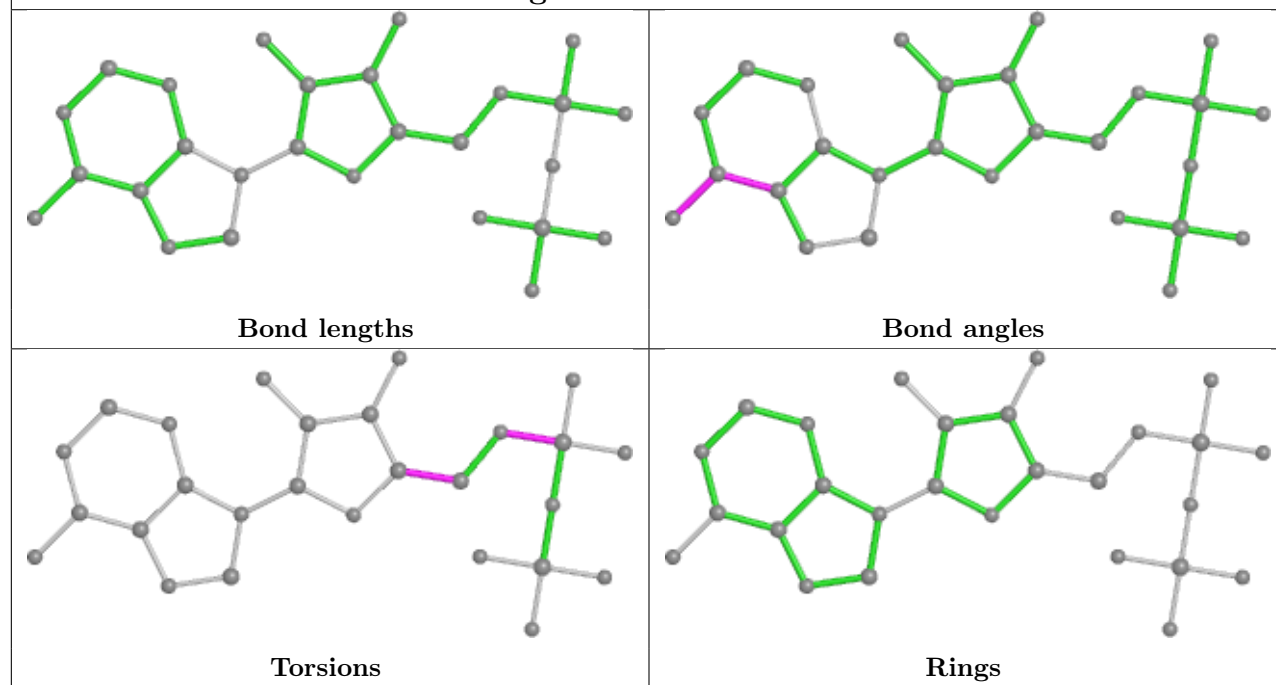




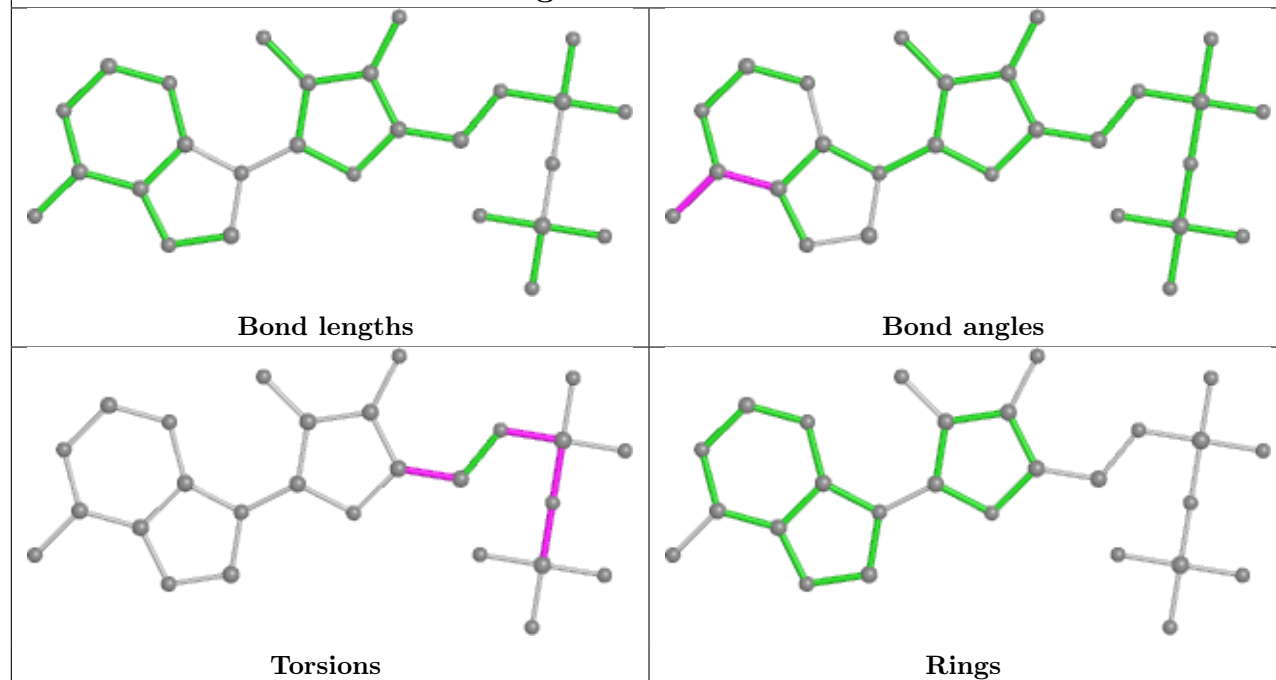
## Ligand ADP E 602



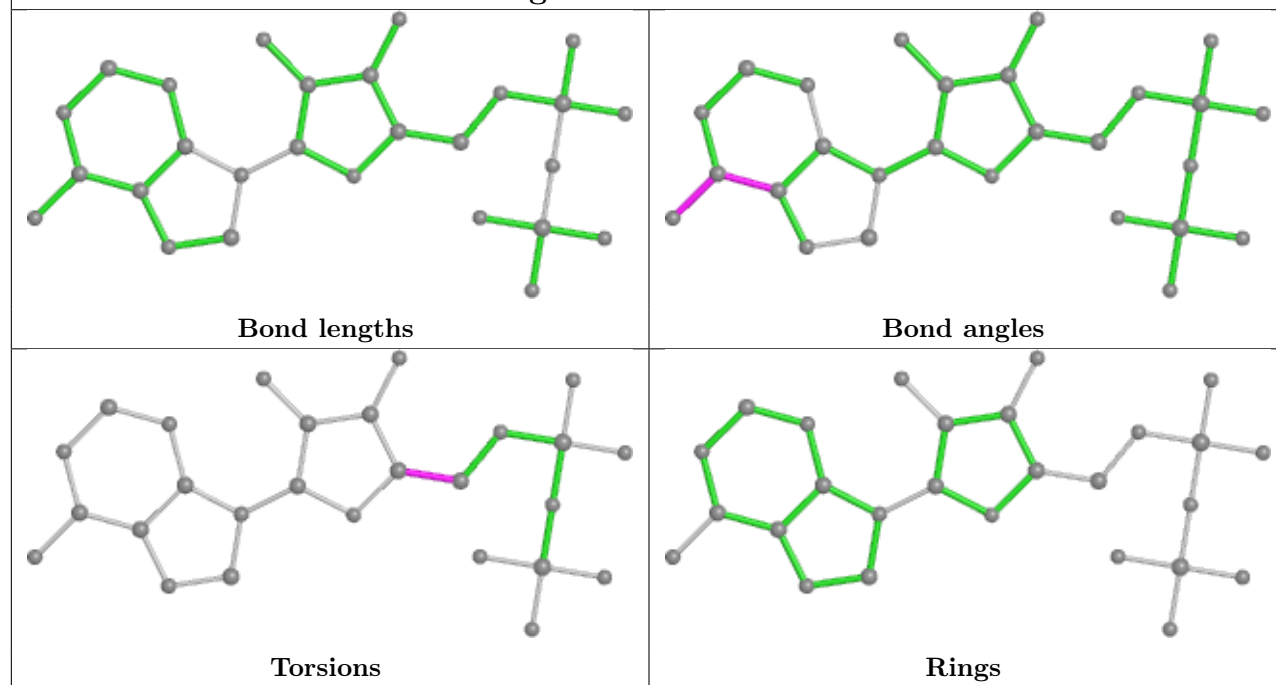
## Ligand ADP A 601

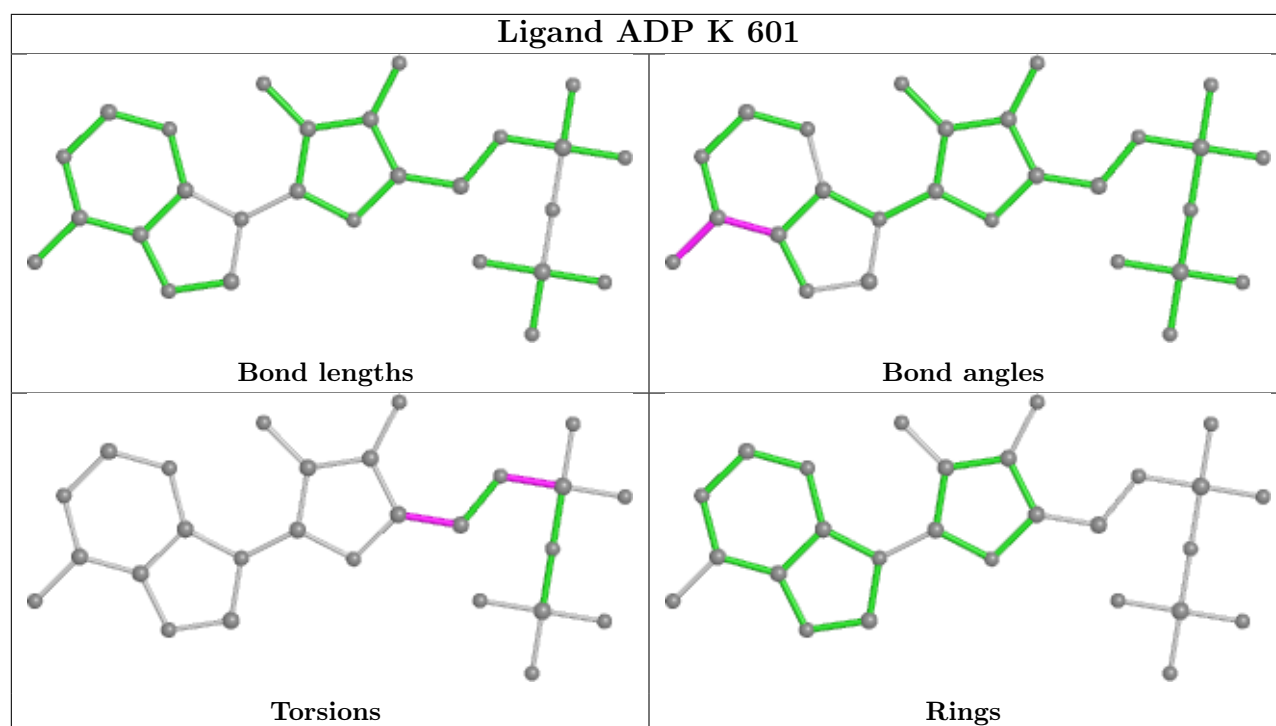


## Ligand ADP I 601



## Ligand ADP D 602





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	446/518 (86%)	0.10	3 (0%) 84 70	46, 68, 95, 120	0
1	B	454/518 (87%)	0.20	8 (1%) 67 49	42, 67, 116, 147	0
1	C	463/518 (89%)	0.32	8 (1%) 69 50	49, 80, 108, 130	0
1	D	443/518 (85%)	0.48	12 (2%) 56 36	54, 88, 131, 152	0
1	E	456/518 (88%)	0.18	6 (1%) 74 58	44, 72, 107, 152	0
1	F	446/518 (86%)	0.18	6 (1%) 74 58	45, 74, 100, 119	0
1	G	447/518 (86%)	0.47	13 (2%) 54 34	72, 108, 137, 151	0
1	H	439/518 (84%)	0.63	32 (7%) 22 13	69, 107, 141, 155	0
1	I	446/518 (86%)	0.49	13 (2%) 54 34	63, 97, 125, 138	0
1	J	447/518 (86%)	0.28	9 (2%) 64 45	53, 88, 123, 136	0
1	K	444/518 (85%)	0.39	11 (2%) 58 39	50, 89, 147, 161	0
1	L	439/518 (84%)	0.47	12 (2%) 56 36	61, 96, 141, 176	0
All	All	5370/6216 (86%)	0.35	133 (2%) 58 39	42, 86, 129, 176	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	245	SER	4.5
1	H	173	ILE	4.1
1	D	297	LEU	3.9
1	H	346	PRO	3.8
1	I	67	PHE	3.8
1	H	86	TRP	3.8
1	G	245	SER	3.7
1	H	372	ILE	3.6
1	G	255	ASN	3.6
1	H	124	ILE	3.5
1	C	442	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	35	THR	3.4
1	H	382	ALA	3.3
1	I	100	VAL	3.2
1	I	482	THR	3.2
1	F	284	ALA	3.2
1	E	245	SER	3.1
1	H	125	ASN	3.1
1	L	403	ILE	3.1
1	L	116	ASP	3.0
1	H	348	SER	3.0
1	B	245	SER	3.0
1	C	175	THR	2.9
1	J	245	SER	2.9
1	F	99	ILE	2.9
1	J	407	PHE	2.9
1	K	351	LEU	2.9
1	C	125	ASN	2.9
1	F	255	ASN	2.9
1	H	226	LYS	2.8
1	H	390	PHE	2.8
1	G	485	LEU	2.8
1	L	475	GLY	2.8
1	B	87	ASP	2.8
1	D	434	LEU	2.8
1	K	391	VAL	2.7
1	B	116	ASP	2.7
1	L	244	LEU	2.7
1	H	81	MET	2.7
1	H	297	LEU	2.6
1	G	225	GLN	2.6
1	G	172	THR	2.6
1	L	250	LYS	2.6
1	K	352	GLU	2.6
1	H	426	SER	2.6
1	G	88	LEU	2.5
1	H	378	LEU	2.5
1	H	21	GLY	2.5
1	H	28	GLY	2.5
1	I	343	CYS	2.5
1	D	158	LEU	2.5
1	H	30	LEU	2.5
1	B	208	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	63	GLU	2.5
1	D	301	CYS	2.5
1	H	136	VAL	2.5
1	H	24	ASP	2.5
1	I	255	ASN	2.5
1	F	194	VAL	2.5
1	J	346	PRO	2.5
1	D	343	CYS	2.4
1	G	173	ILE	2.4
1	H	122	ALA	2.4
1	E	152	SER	2.4
1	G	266	ASP	2.4
1	B	242	PHE	2.4
1	K	363	GLU	2.4
1	H	52	GLN	2.4
1	D	245	SER	2.4
1	H	351	LEU	2.4
1	D	354	HIS	2.4
1	G	423	SER	2.3
1	L	77	ILE	2.3
1	I	58	ILE	2.3
1	E	193	PHE	2.3
1	L	254	SER	2.3
1	K	86	TRP	2.3
1	K	300	ALA	2.3
1	I	169	GLY	2.3
1	D	117	LEU	2.3
1	J	11	ALA	2.3
1	L	273	PHE	2.3
1	J	140	SER	2.3
1	H	25	ILE	2.2
1	J	370	ILE	2.2
1	C	61	PHE	2.2
1	D	64	PRO	2.2
1	D	444	MET	2.2
1	H	38	VAL	2.2
1	J	141	ILE	2.2
1	H	23	ASP	2.2
1	J	171	THR	2.2
1	I	301	CYS	2.2
1	I	390	PHE	2.2
1	G	196	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	98	ALA	2.2
1	K	169	GLY	2.2
1	H	260	SER	2.2
1	I	174	MET	2.2
1	C	485	LEU	2.2
1	D	427	THR	2.2
1	A	310	PHE	2.1
1	H	310	PHE	2.1
1	C	374	SER	2.1
1	B	105	ASP	2.1
1	E	252	ARG	2.1
1	H	387	PHE	2.1
1	K	157	GLU	2.1
1	H	100	VAL	2.1
1	E	139	ASP	2.1
1	G	241	ILE	2.1
1	K	403	ILE	2.1
1	I	405	GLY	2.1
1	G	22	PHE	2.1
1	K	353	ASP	2.1
1	B	70	PHE	2.1
1	E	404	THR	2.1
1	L	304	GLY	2.1
1	I	28	GLY	2.1
1	B	203	ASN	2.1
1	K	117	LEU	2.1
1	D	241	ILE	2.0
1	L	410	THR	2.0
1	J	414	PHE	2.0
1	H	342	VAL	2.0
1	A	20	GLU	2.0
1	G	86	TRP	2.0
1	C	168	MET	2.0
1	F	444	MET	2.0
1	H	474	ILE	2.0
1	L	300	ALA	2.0
1	A	475	GLY	2.0
1	H	261	GLY	2.0

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

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

## 6.3 Carbohydrates [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	G	604	1/1	0.83	0.18	70,70,70,70	0
3	MG	H	603	1/1	0.85	0.15	97,97,97,97	0
2	ADP	H	602	27/27	0.86	0.13	105,110,115,116	0
3	MG	B	603	1/1	0.86	0.21	61,61,61,61	0
3	MG	L	604	1/1	0.87	0.25	94,94,94,94	0
3	MG	D	604	1/1	0.88	0.17	67,67,67,67	0
2	ADP	G	602	27/27	0.88	0.10	100,103,105,106	0
3	MG	G	603	1/1	0.89	0.16	62,62,62,62	0
2	ADP	K	601	27/27	0.89	0.12	75,100,114,115	0
3	MG	J	604	1/1	0.89	0.15	54,54,54,54	0
2	ADP	L	601	27/27	0.90	0.10	96,99,104,106	0
2	ADP	G	601	27/27	0.90	0.09	72,75,76,77	0
3	MG	F	604	1/1	0.90	0.14	41,41,41,41	0
3	MG	L	603	1/1	0.91	0.25	97,97,97,97	0
2	ADP	L	602	27/27	0.91	0.10	74,79,83,84	0
3	MG	H	604	1/1	0.91	0.08	82,82,82,82	0
3	MG	F	603	1/1	0.92	0.22	69,69,69,69	0
2	ADP	D	602	27/27	0.92	0.09	70,72,73,75	0
2	ADP	I	602	27/27	0.92	0.10	72,79,81,81	0
2	ADP	B	601	27/27	0.92	0.10	62,65,72,73	0
3	MG	B	604	1/1	0.92	0.08	49,49,49,49	0
2	ADP	H	601	27/27	0.93	0.08	76,79,82,83	0
2	ADP	I	601	27/27	0.93	0.09	73,75,76,76	0
2	ADP	C	601	27/27	0.93	0.10	65,69,75,77	0
2	ADP	F	602	27/27	0.93	0.08	57,60,61,63	0
3	MG	I	603	1/1	0.93	0.13	54,54,54,54	0
3	MG	I	604	1/1	0.93	0.07	82,82,82,82	0
2	ADP	A	601	27/27	0.93	0.09	68,70,72,73	0
2	ADP	K	602	27/27	0.94	0.10	60,65,71,71	0
3	MG	C	603	1/1	0.94	0.08	61,61,61,61	0
2	ADP	E	602	27/27	0.94	0.10	64,70,77,78	0
2	ADP	D	601	27/27	0.94	0.09	58,62,64,64	0

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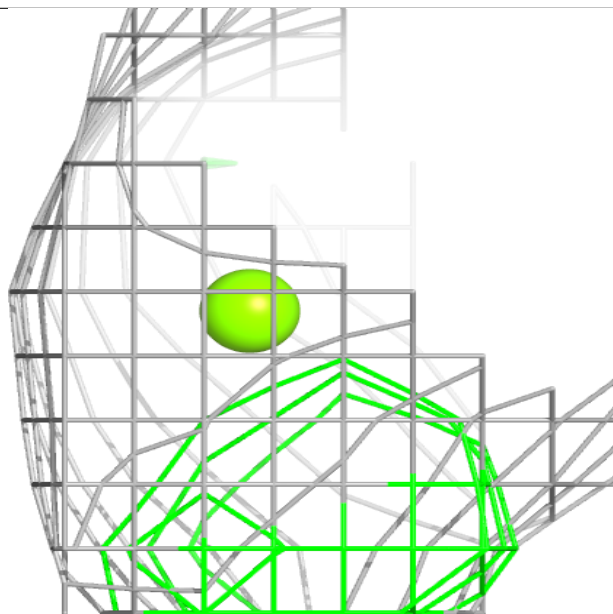
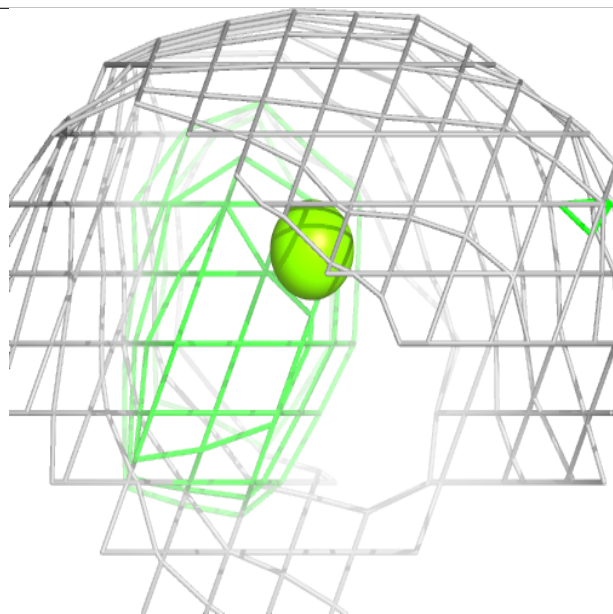
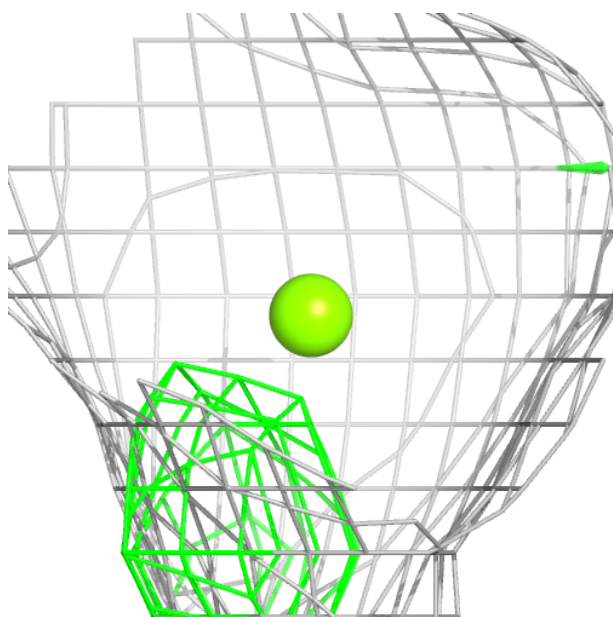
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	603	1/1	0.94	0.13	53,53,53,53	0
2	ADP	F	601	27/27	0.95	0.09	53,55,58,58	0
2	ADP	J	601	27/27	0.95	0.08	67,80,88,89	0
2	ADP	J	602	27/27	0.95	0.09	55,61,67,69	0
2	ADP	B	602	27/27	0.95	0.08	46,51,54,54	0
3	MG	E	603	1/1	0.95	0.14	61,61,61,61	0
2	ADP	C	602	27/27	0.95	0.08	60,68,72,73	0
2	ADP	A	602	27/27	0.95	0.07	52,54,55,56	0
2	ADP	E	601	27/27	0.96	0.08	46,53,59,60	0
3	MG	E	604	1/1	0.96	0.11	71,71,71,71	0
3	MG	A	603	1/1	0.96	0.05	70,70,70,70	0
3	MG	K	603	1/1	0.96	0.16	38,38,38,38	0
3	MG	K	604	1/1	0.96	0.13	66,66,66,66	0
3	MG	J	603	1/1	0.98	0.10	38,38,38,38	0
3	MG	C	604	1/1	0.98	0.07	71,71,71,71	0
3	MG	A	604	1/1	0.99	0.06	37,37,37,37	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.

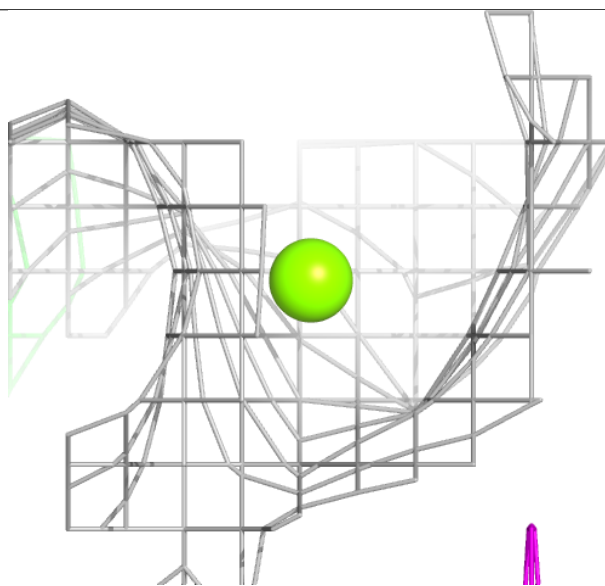
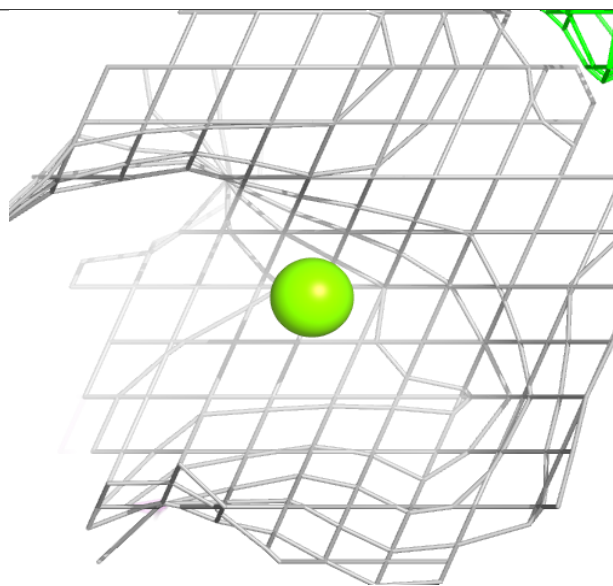
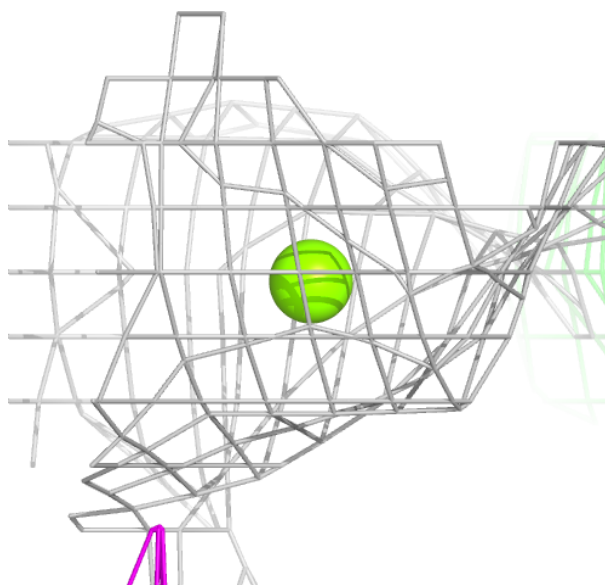
**Electron density around MG G 604:**

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



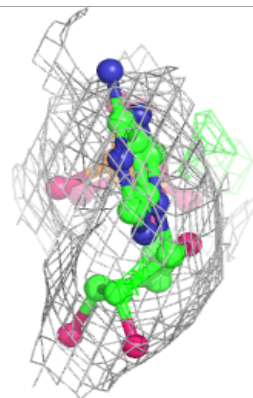
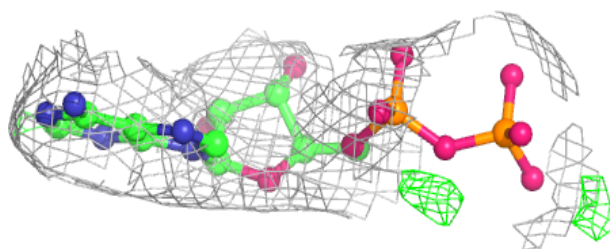
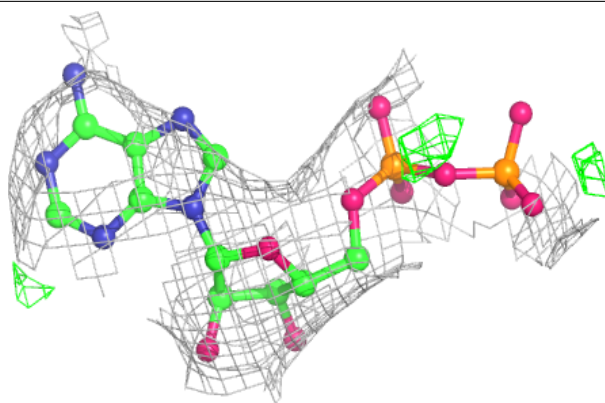
**Electron density around MG H 603:**

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



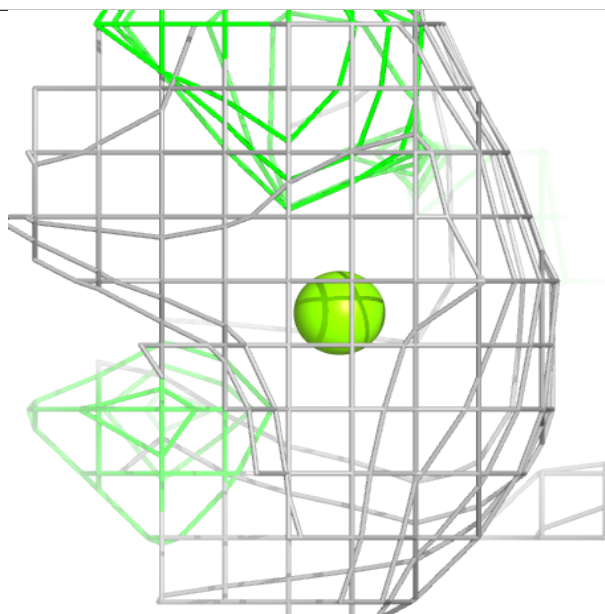
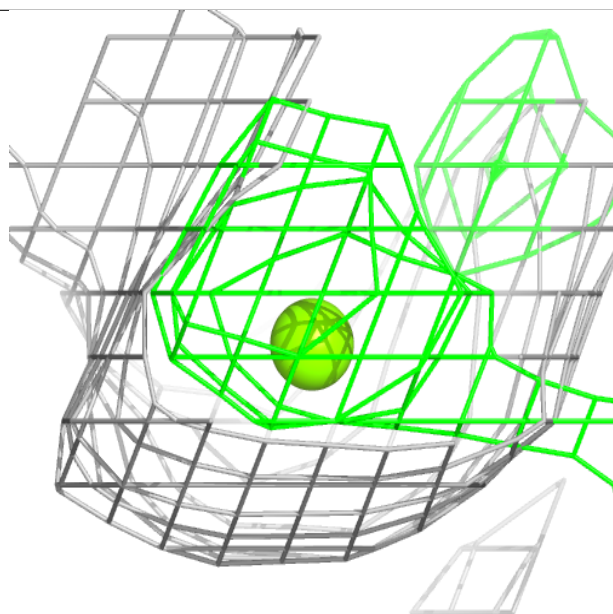
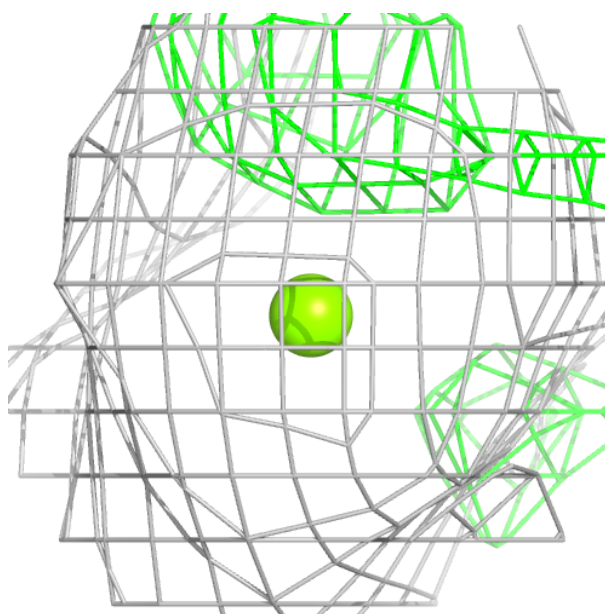
**Electron density around ADP H 602:**

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



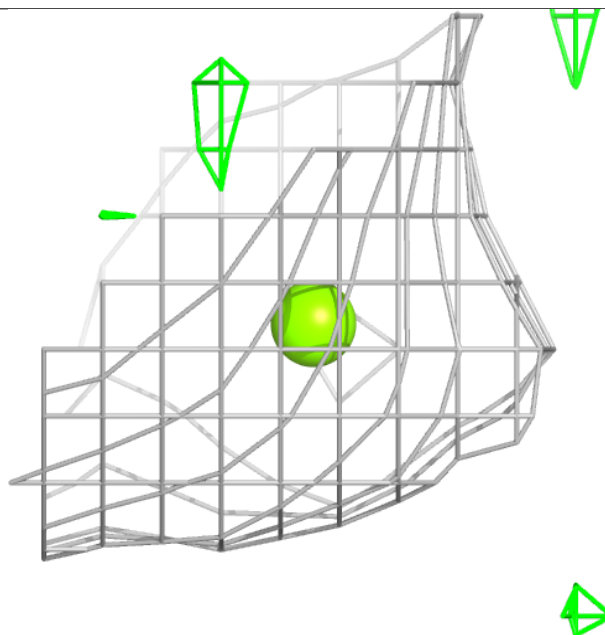
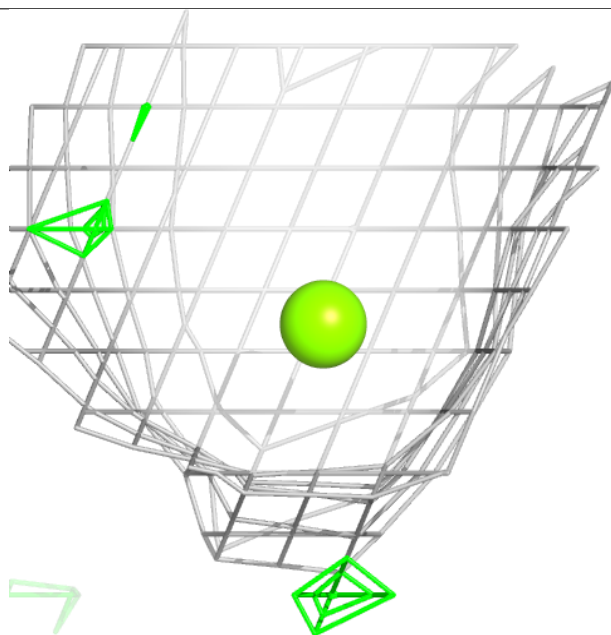
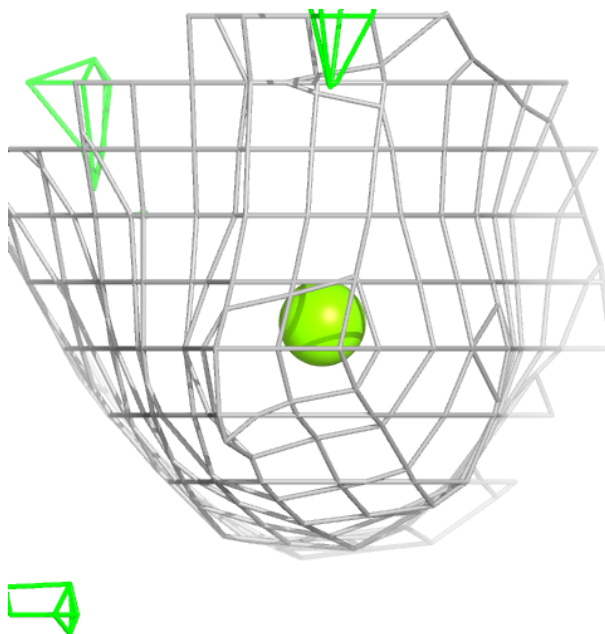
**Electron density around MG B 603:**

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



**Electron density around MG L 604:**

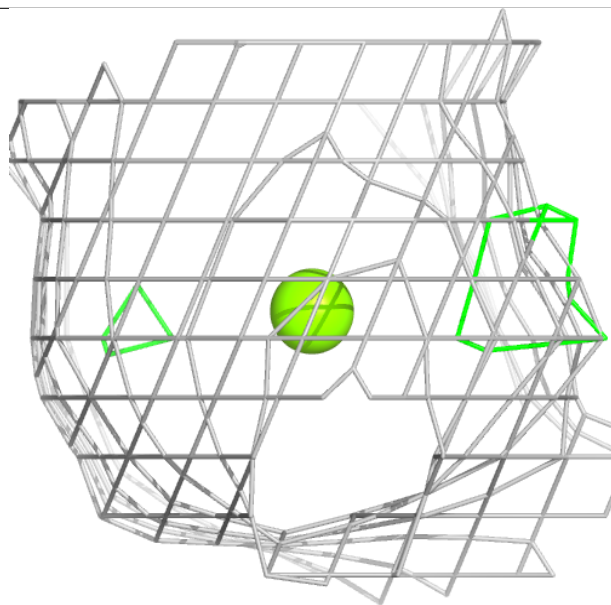
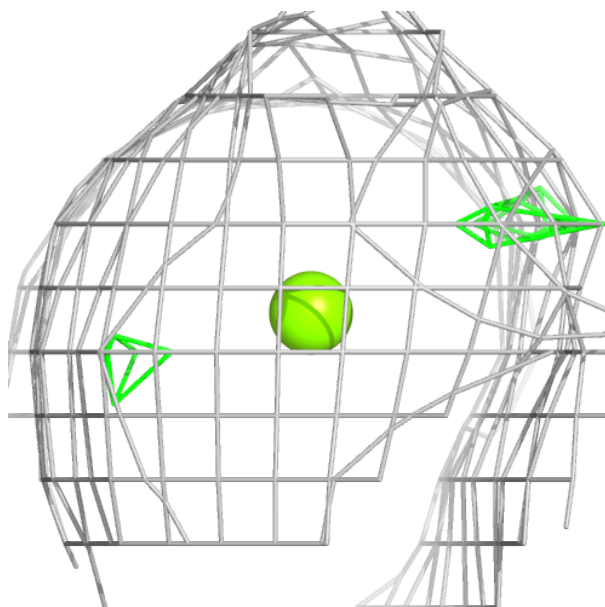
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





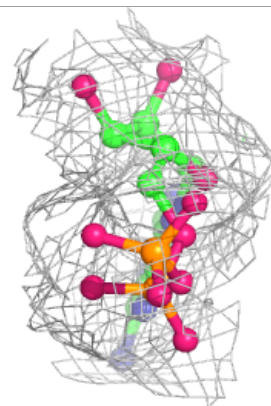
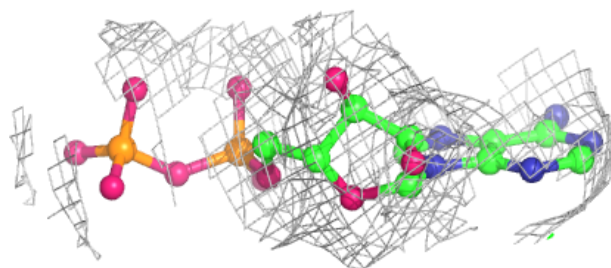
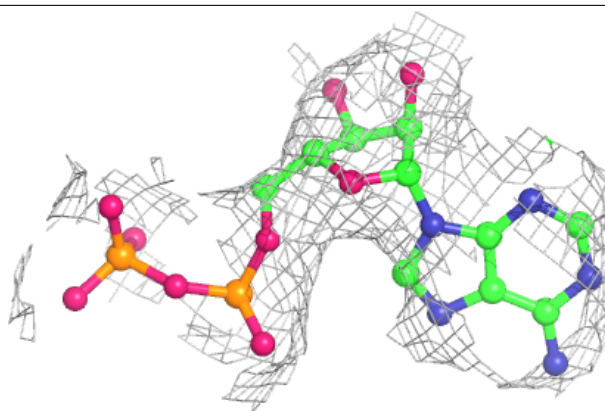
**Electron density around MG D 604:**

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



**Electron density around ADP G 602:**

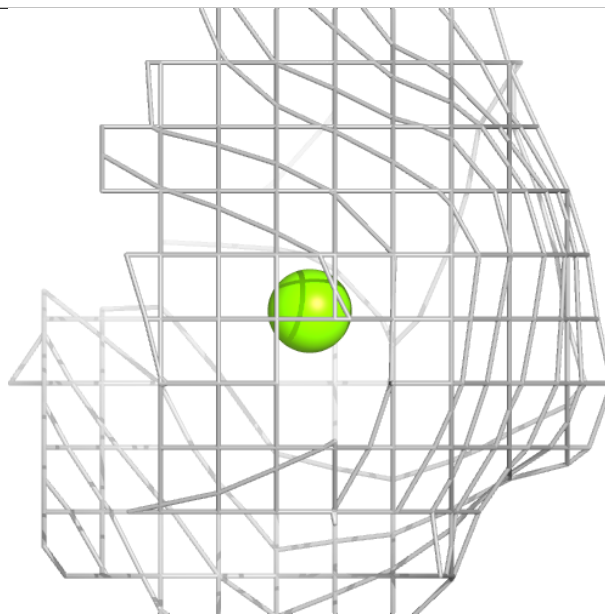
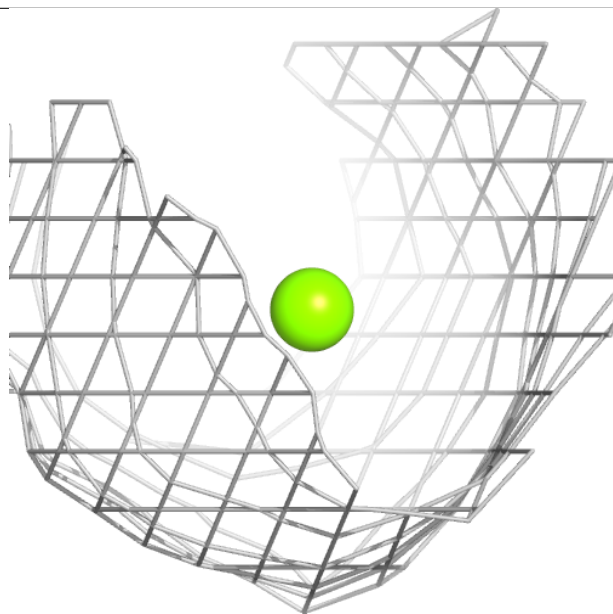
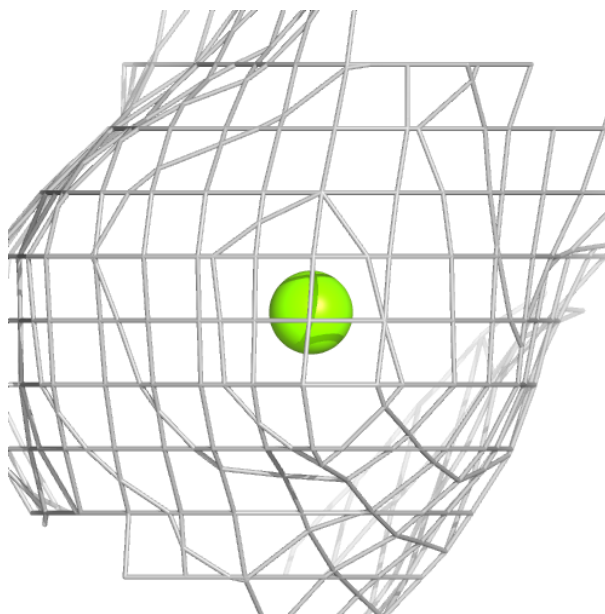
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





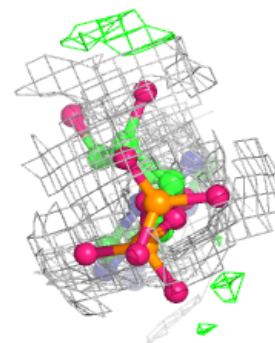
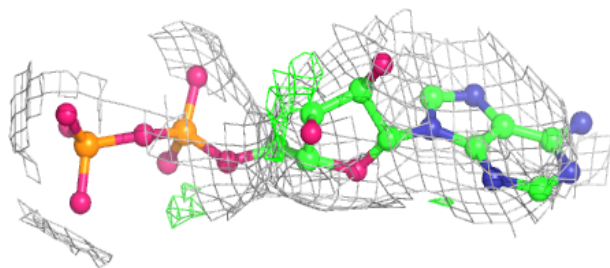
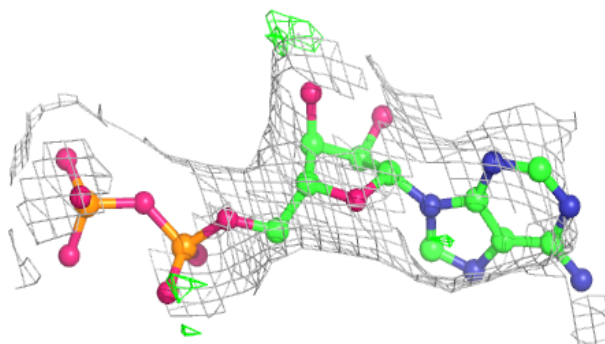
**Electron density around MG G 603:**

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



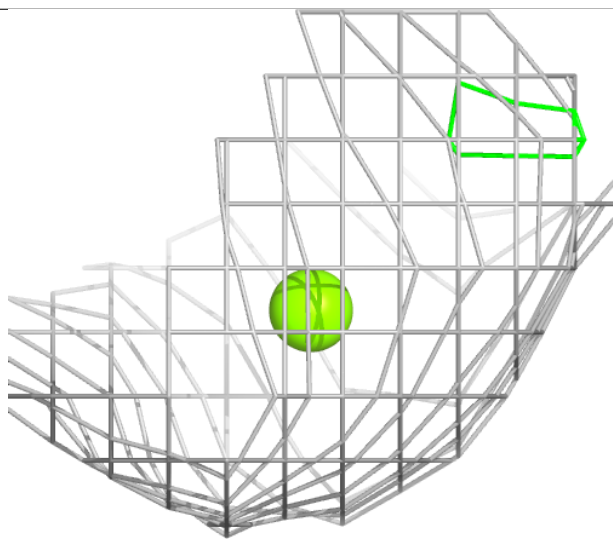
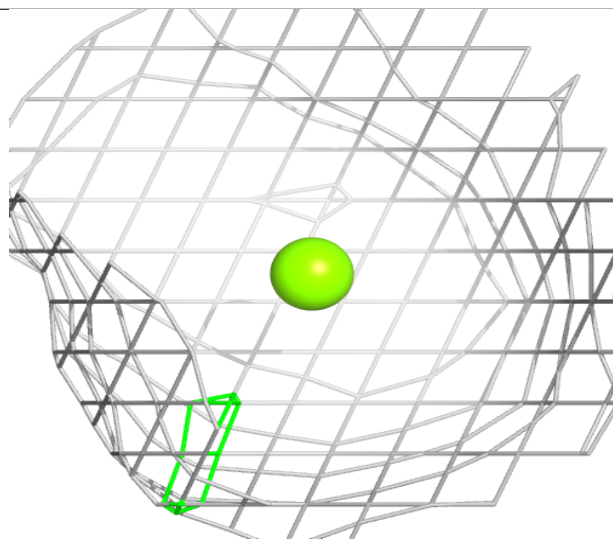
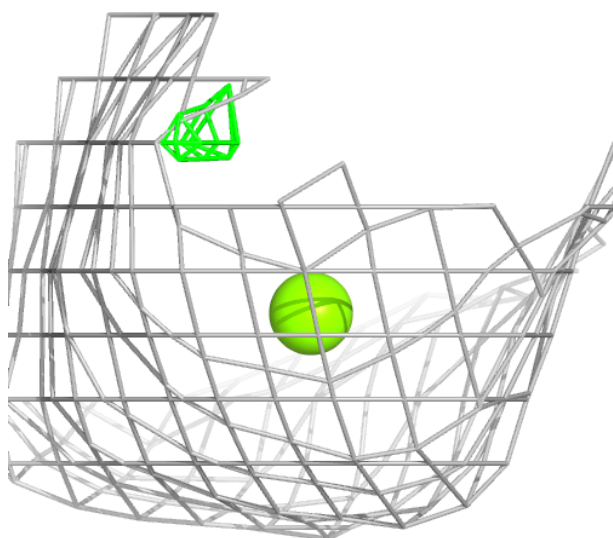
**Electron density around ADP K 601:**

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



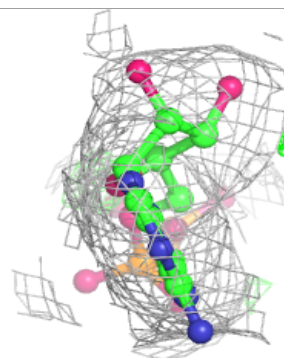
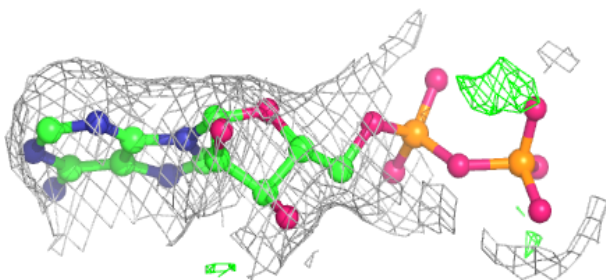
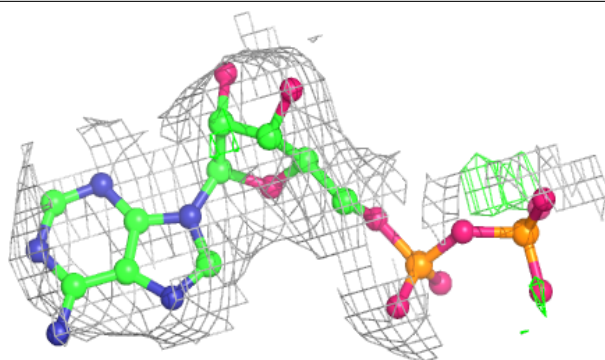
**Electron density around MG J 604:**

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

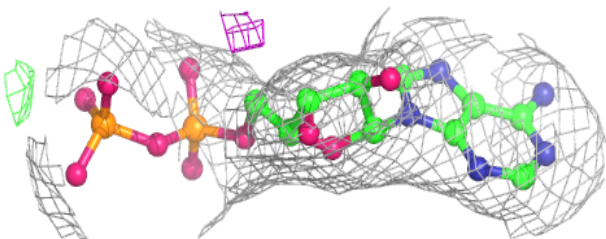
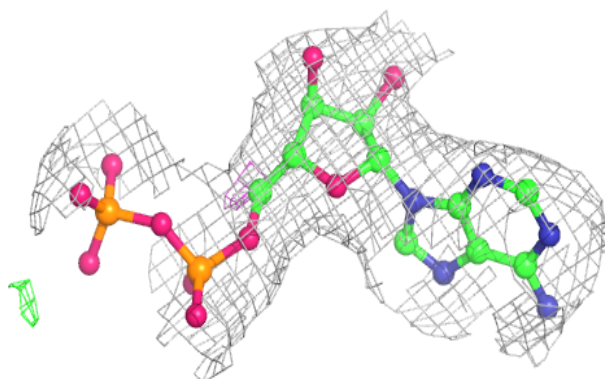


**Electron density around ADP L 601:**

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

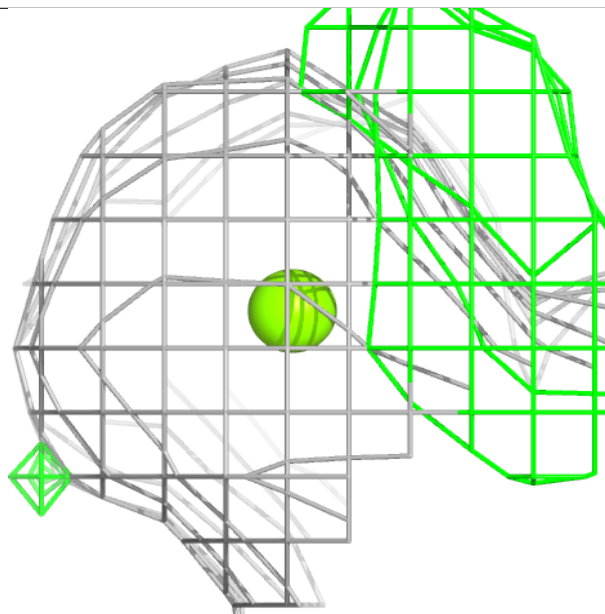
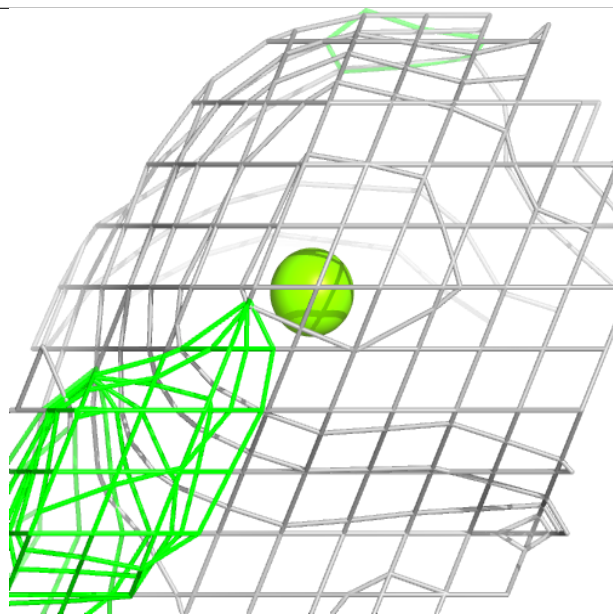
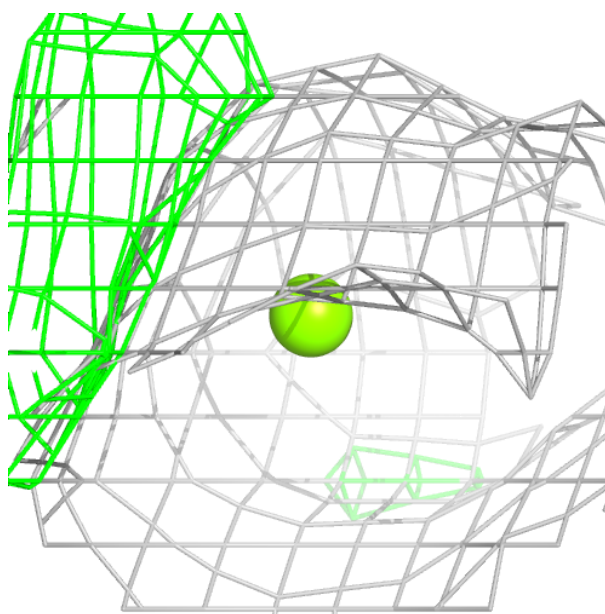
**Electron density around ADP G 601:**

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



**Electron density around MG F 604:**

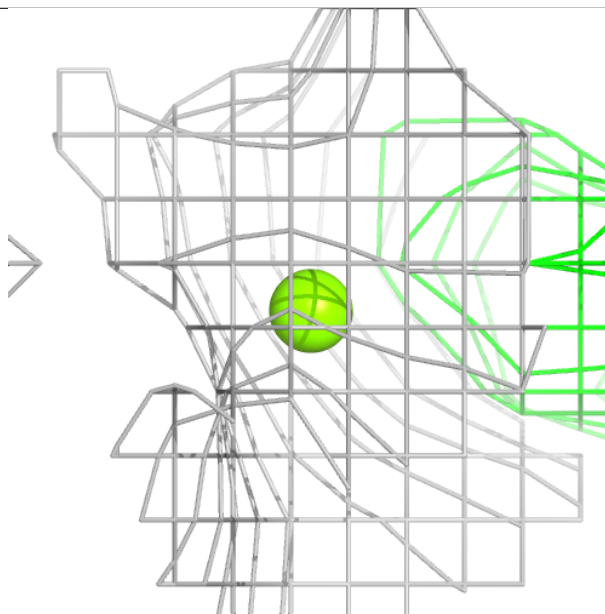
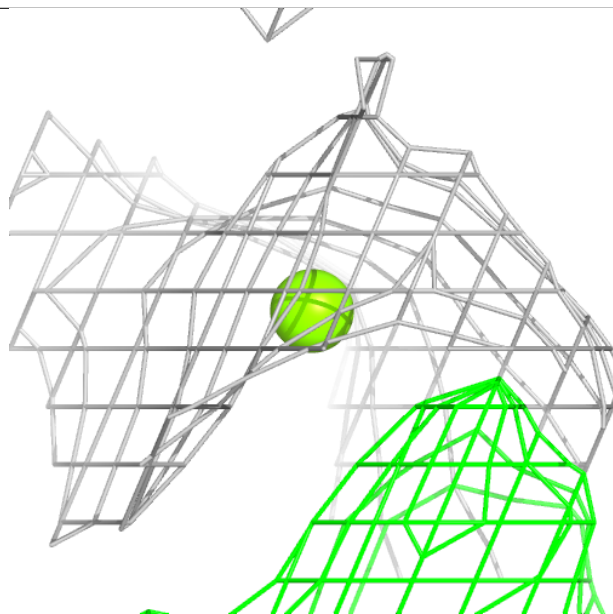
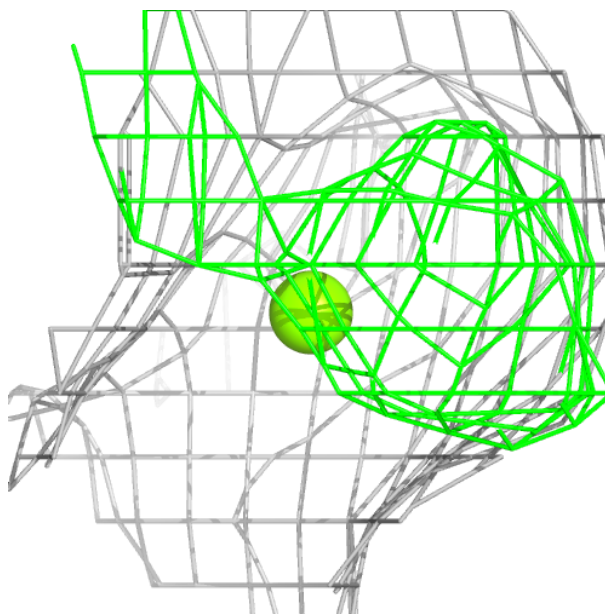
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





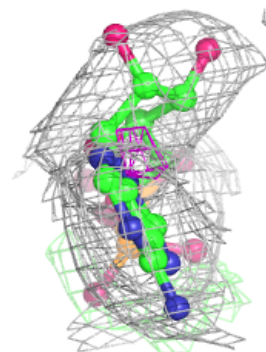
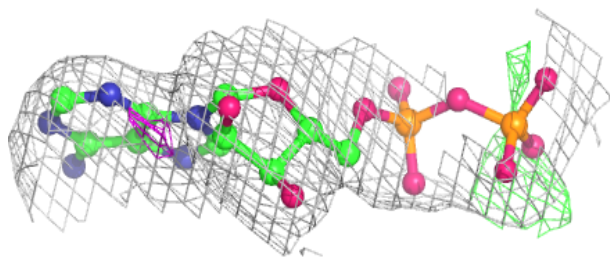
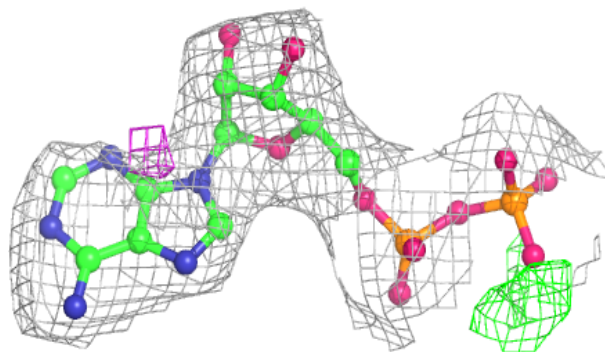
**Electron density around MG L 603:**

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



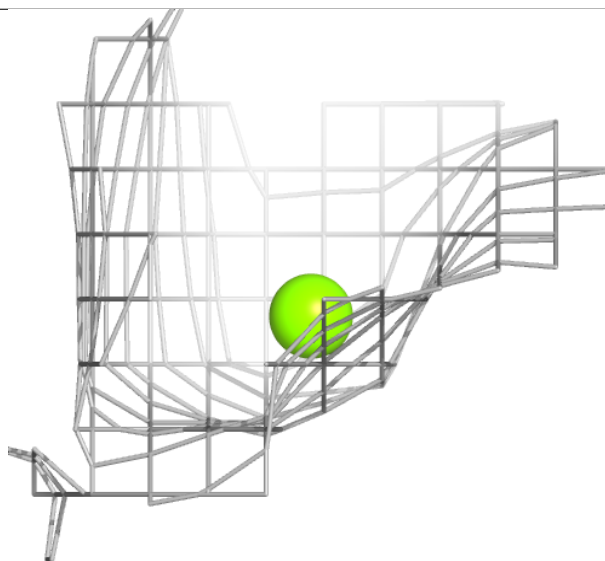
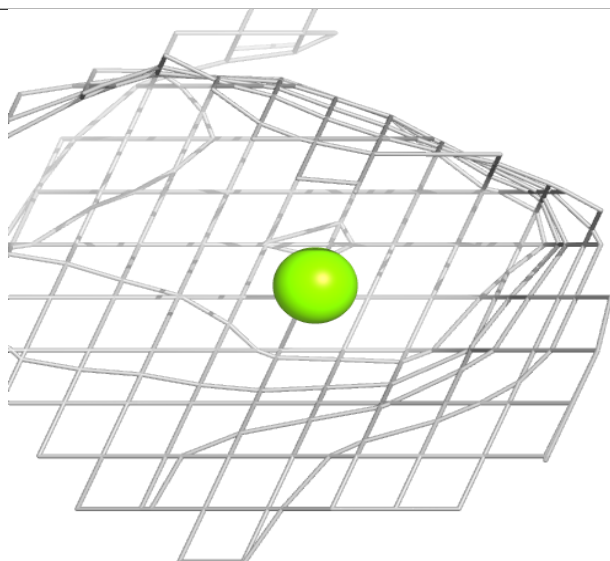
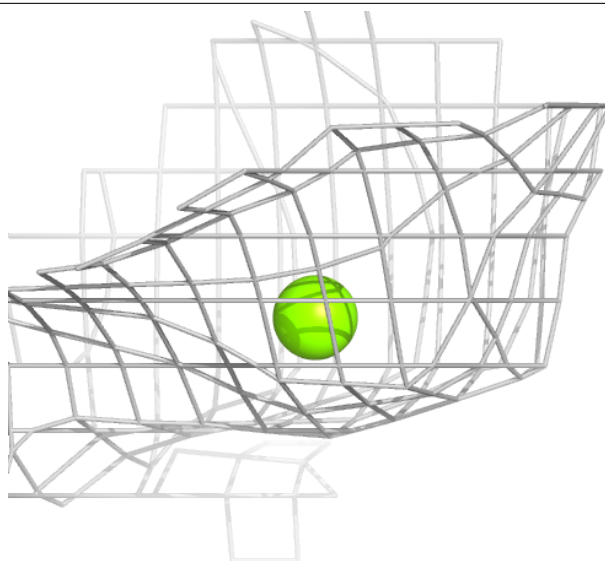
**Electron density around ADP L 602:**

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



**Electron density around MG H 604:**

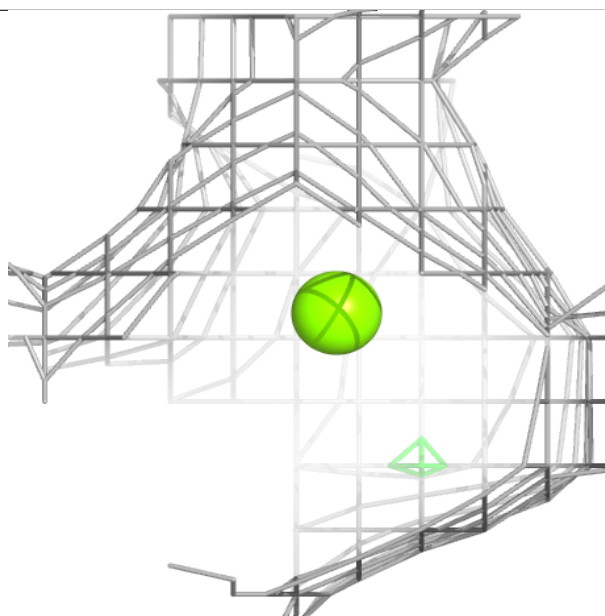
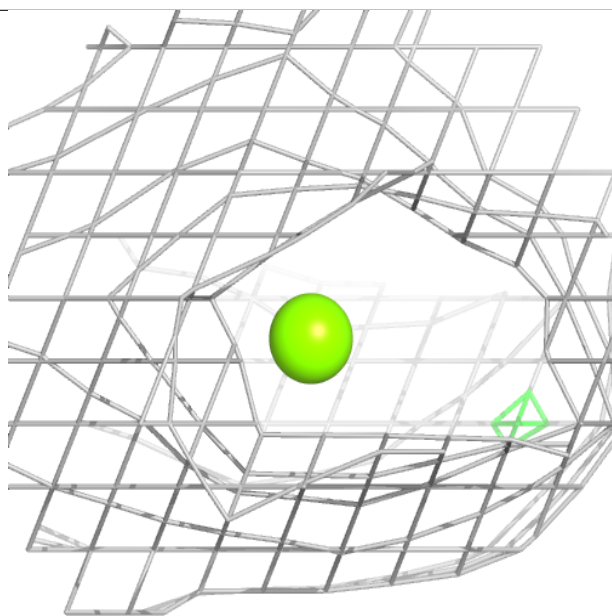
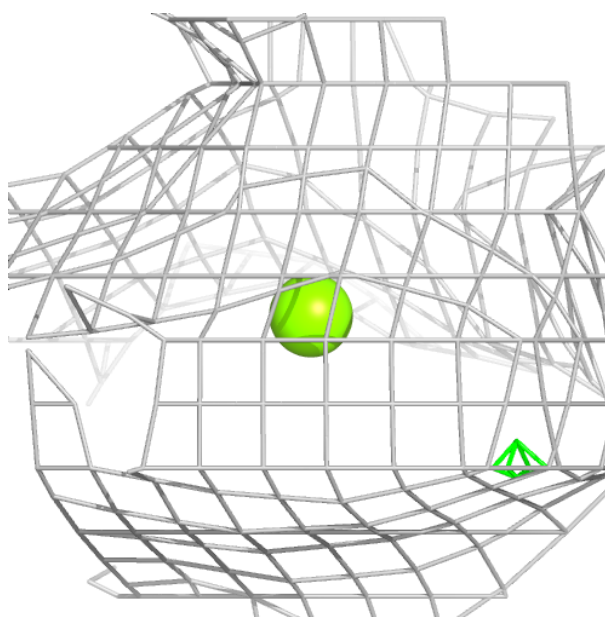
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





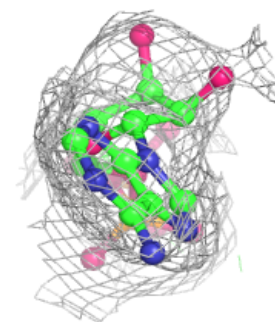
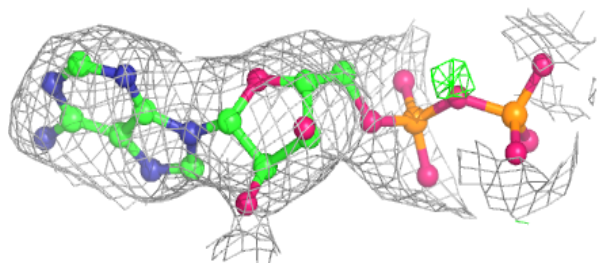
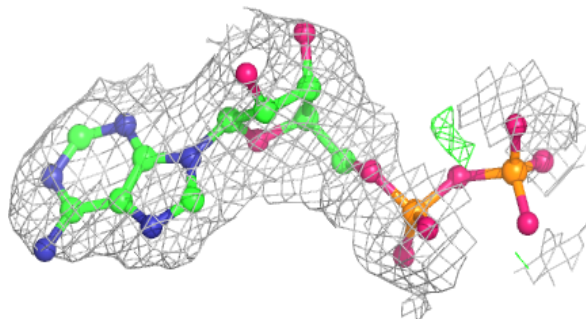
**Electron density around MG F 603:**

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

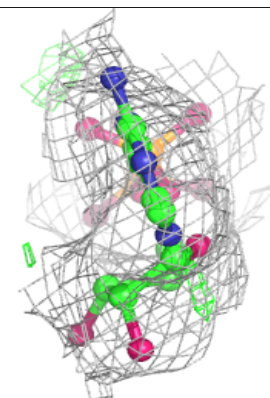
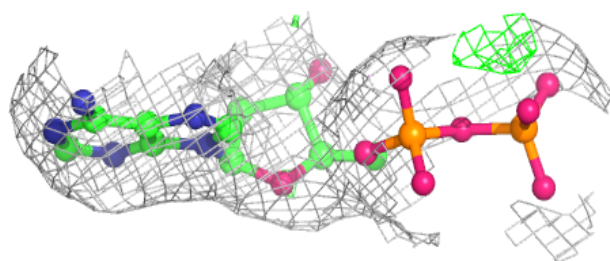
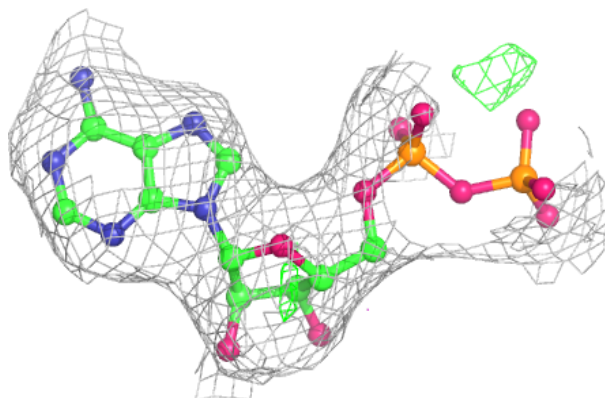


**Electron density around ADP D 602:**

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

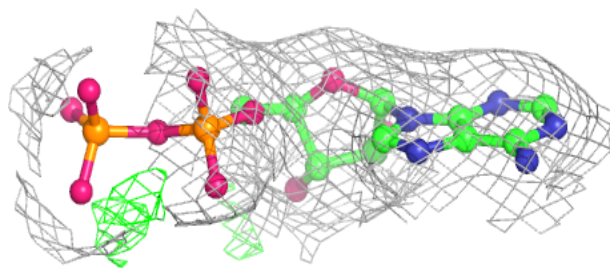
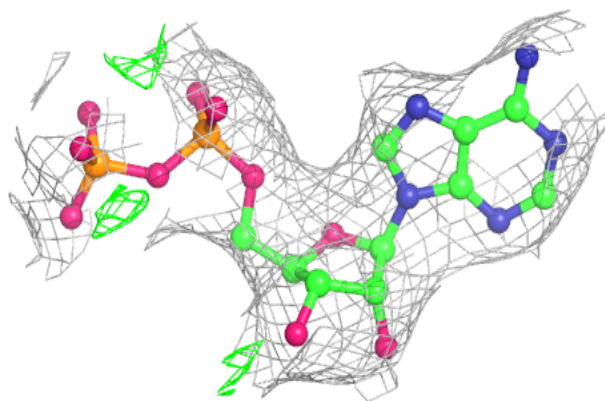
**Electron density around ADP I 602:**

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



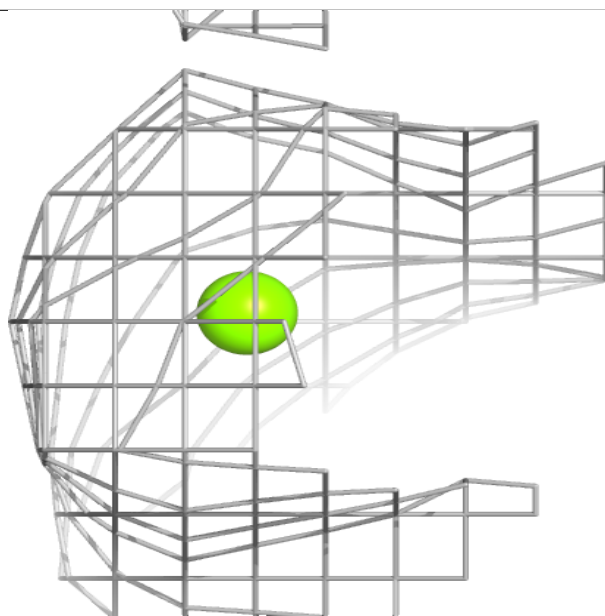
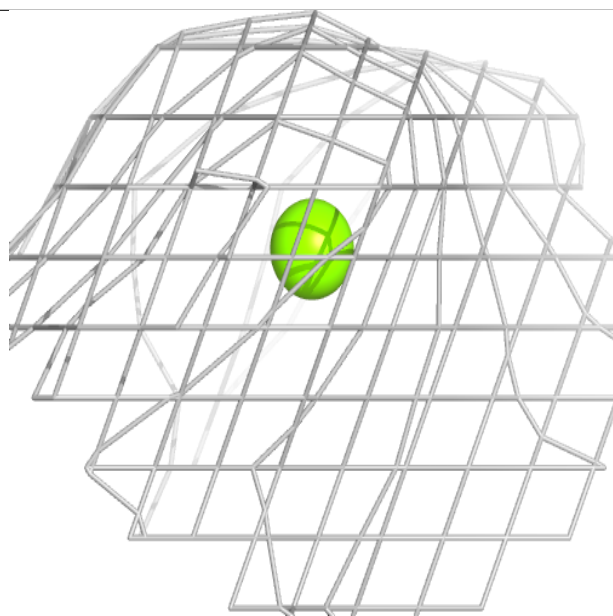
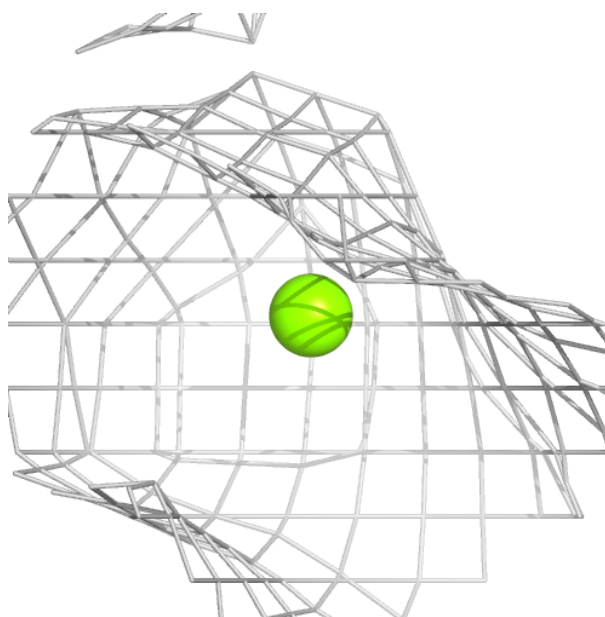
**Electron density around ADP B 601:**

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



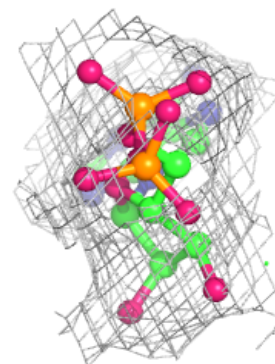
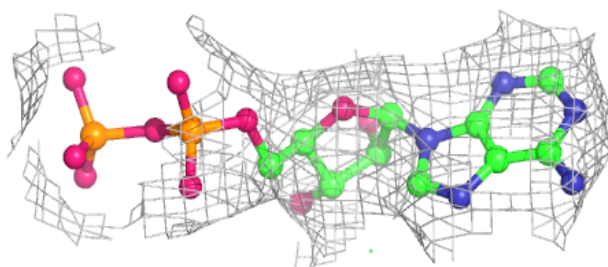
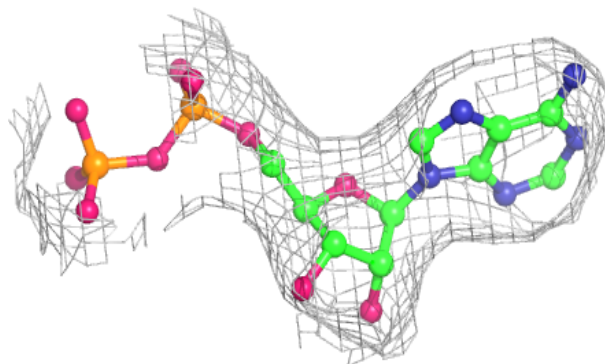
**Electron density around MG B 604:**

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

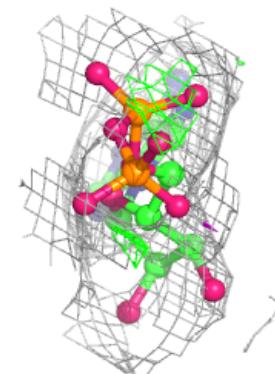
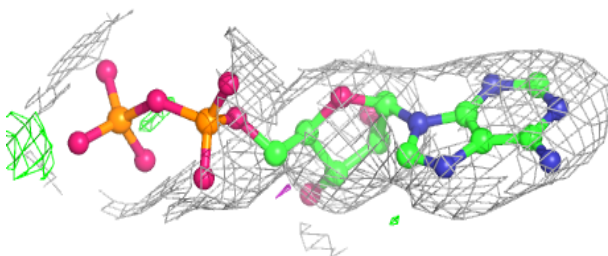
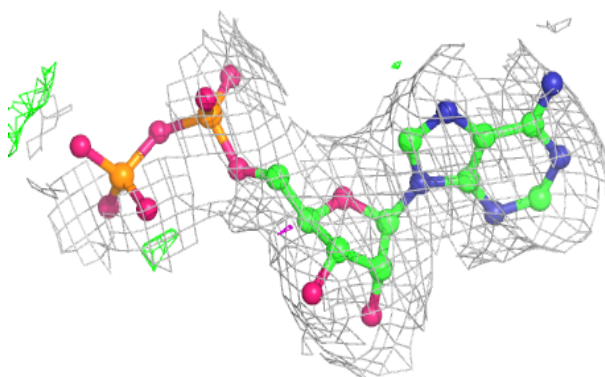


**Electron density around ADP H 601:**

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

**Electron density around ADP I 601:**

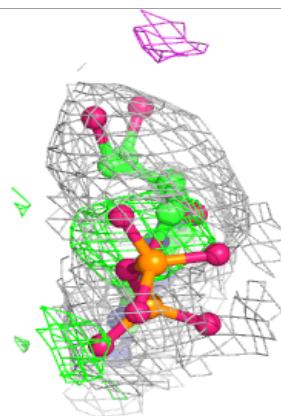
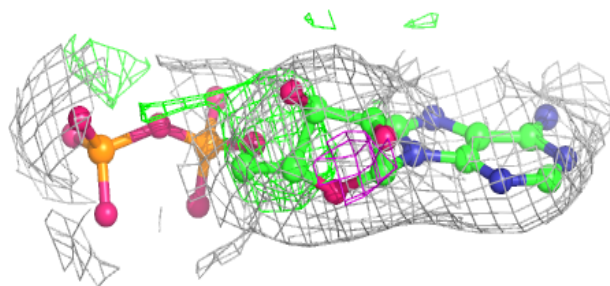
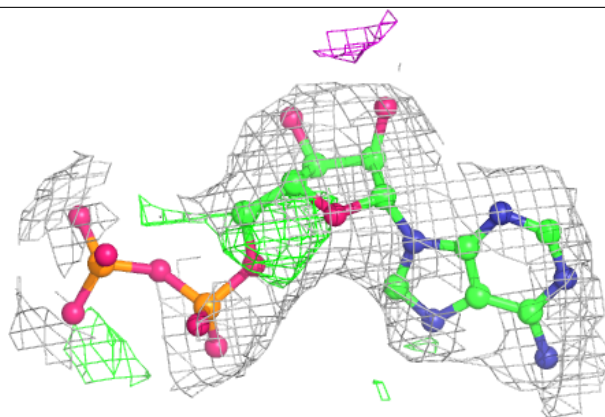
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



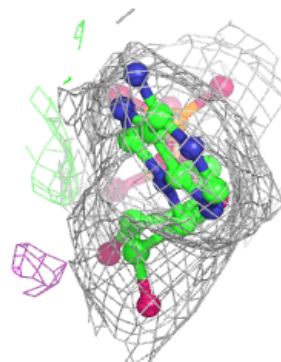
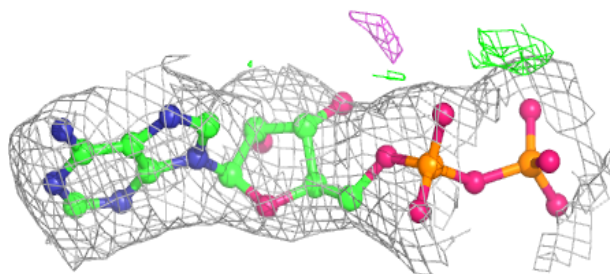
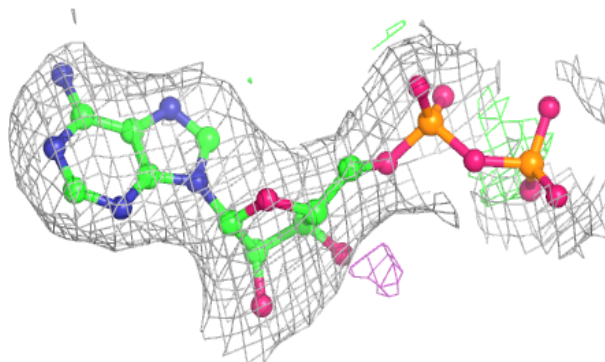


**Electron density around ADP C 601:**

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

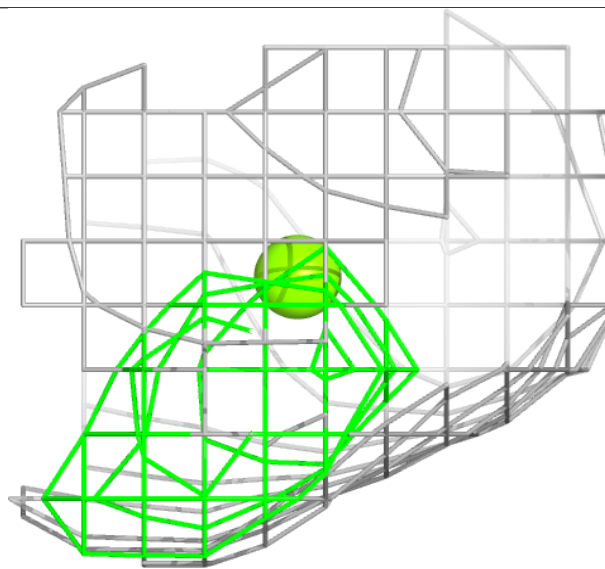
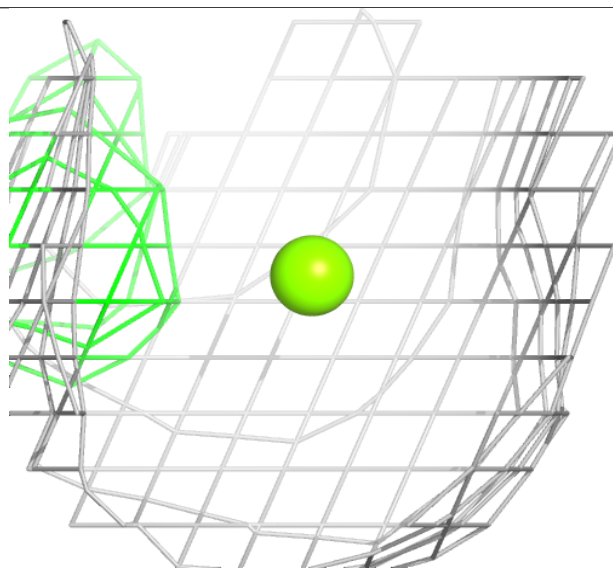
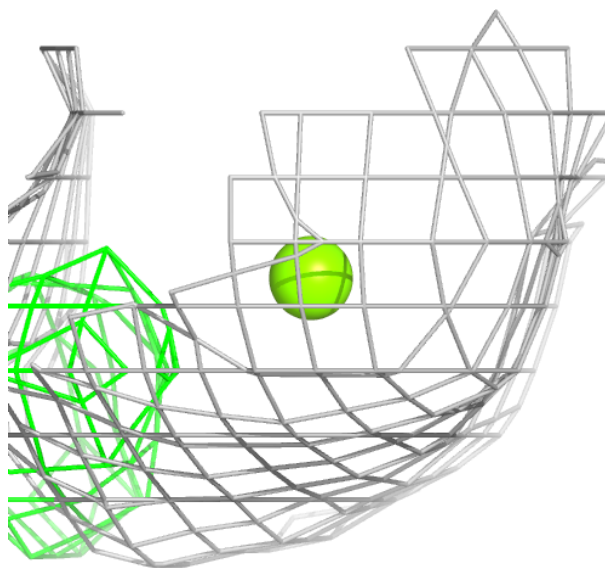
**Electron density around ADP F 602:**

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



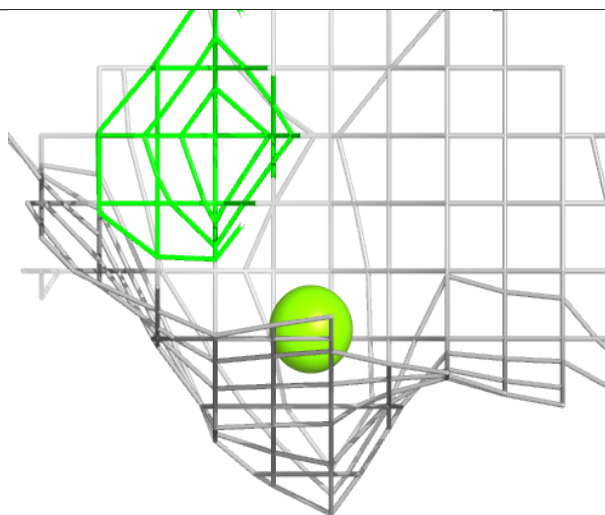
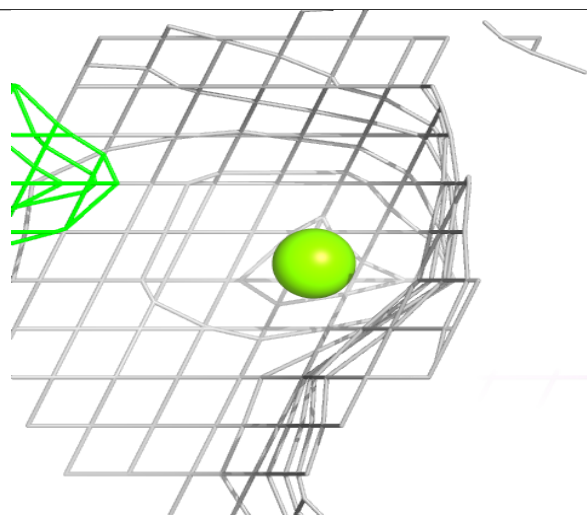
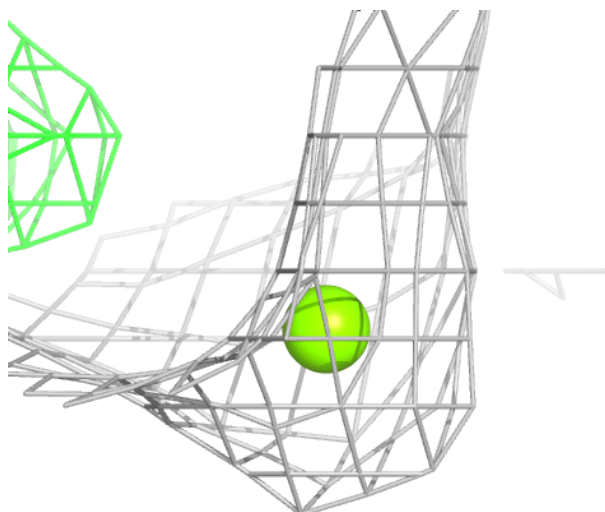
**Electron density around MG I 603:**

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



**Electron density around MG I 604:**

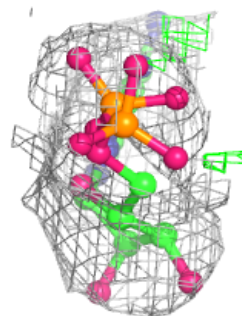
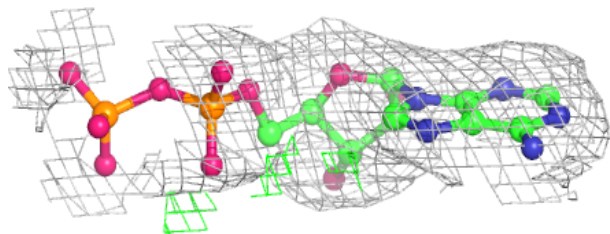
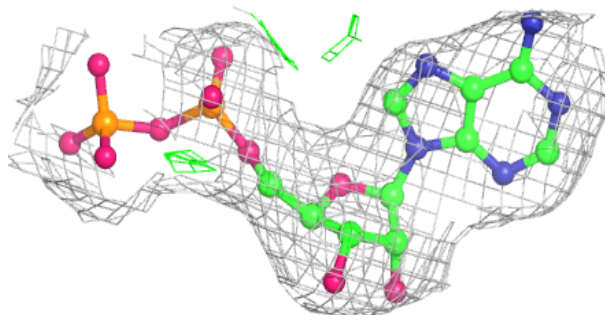
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



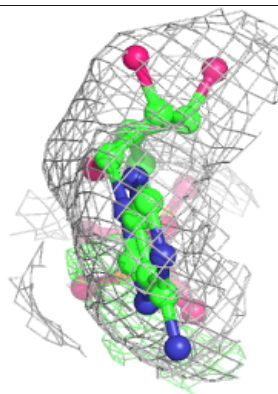
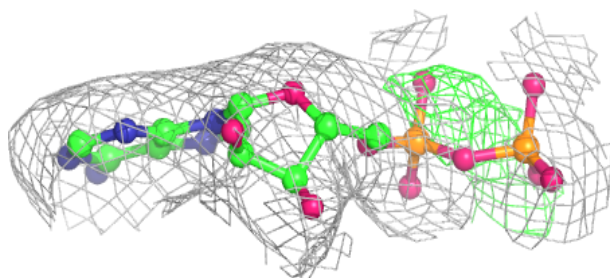
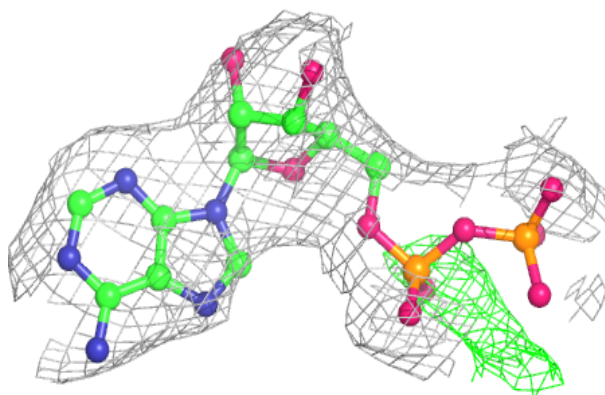


**Electron density around ADP A 601:**

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

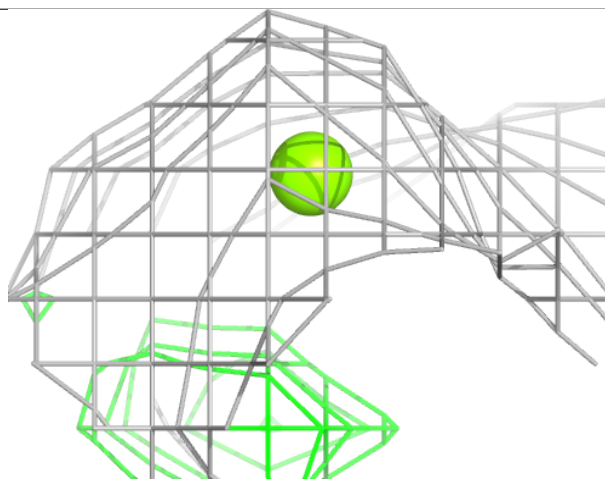
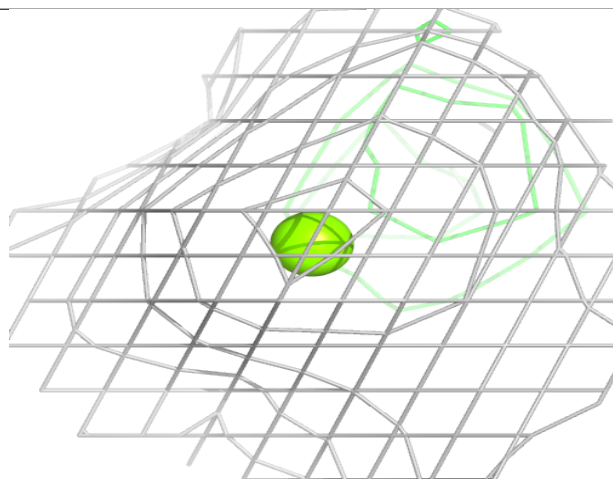
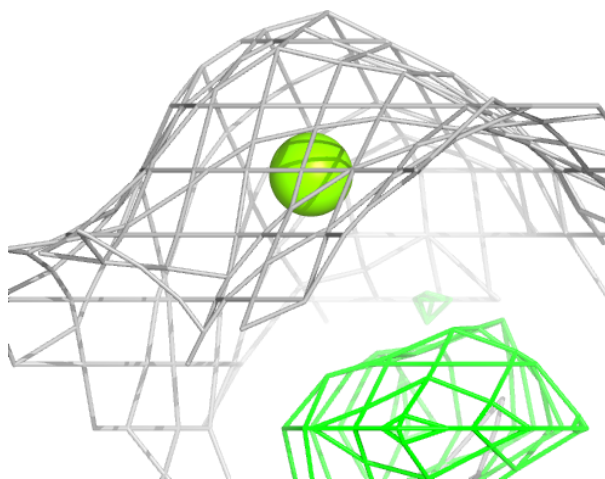
**Electron density around ADP K 602:**

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



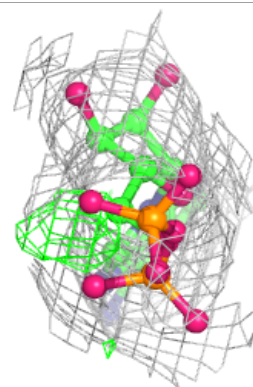
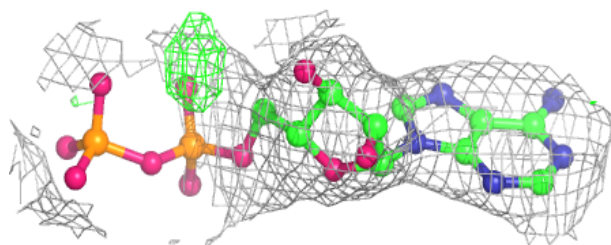
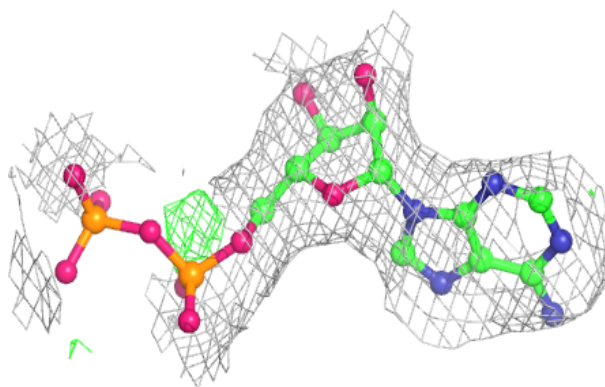
**Electron density around MG C 603:**

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

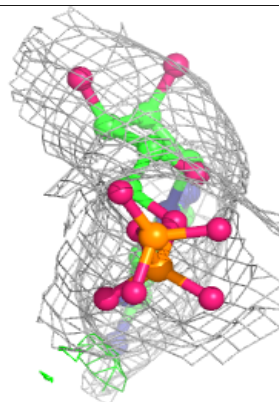
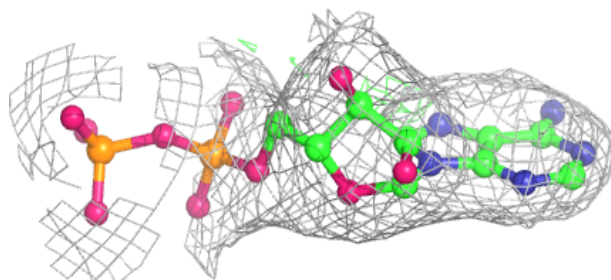
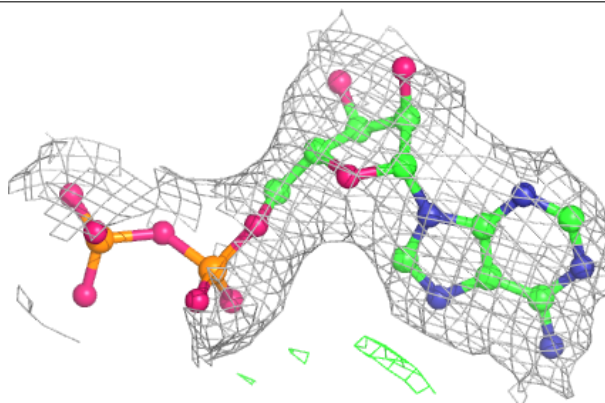


**Electron density around ADP E 602:**

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

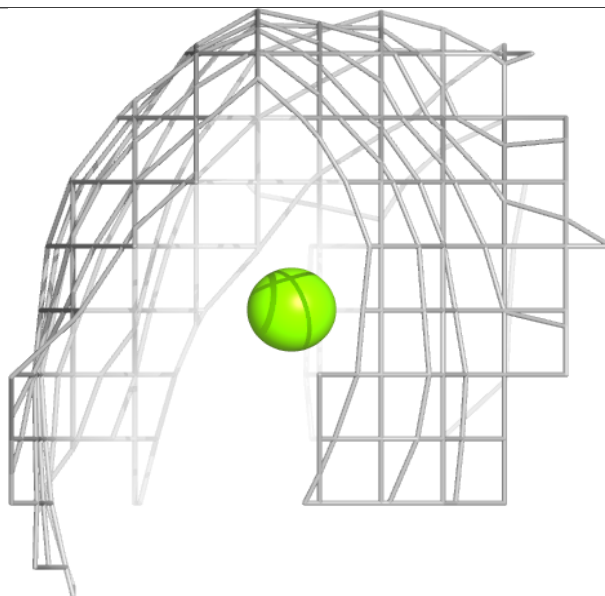
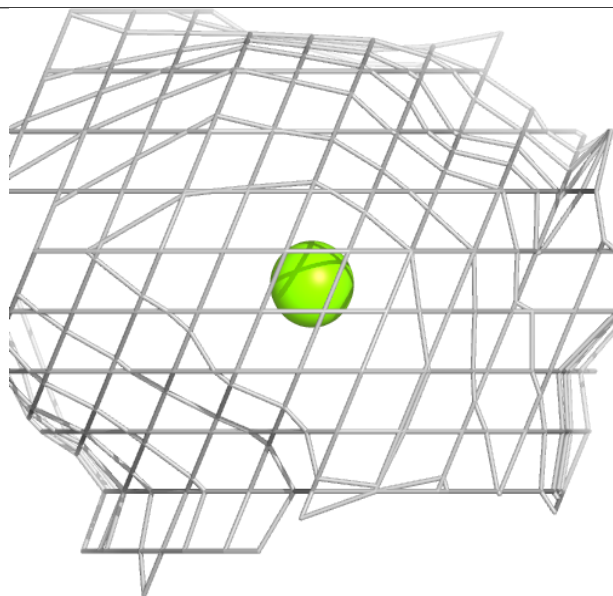
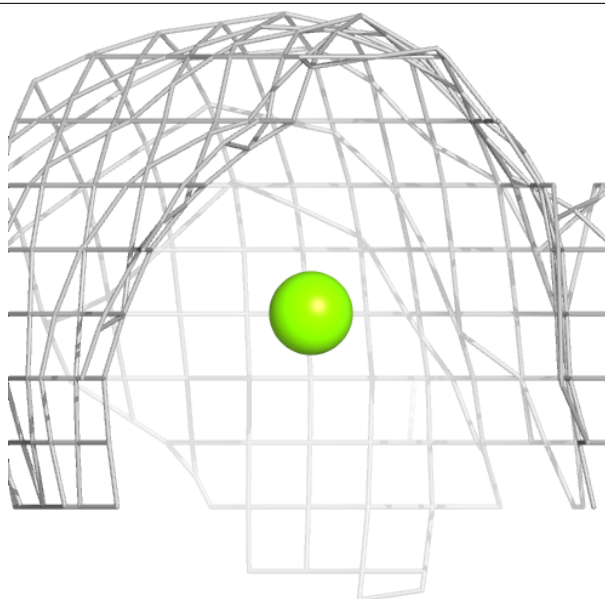
**Electron density around ADP D 601:**

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



**Electron density around MG D 603:**

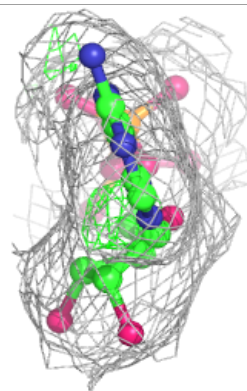
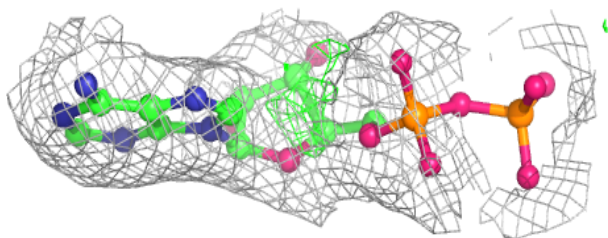
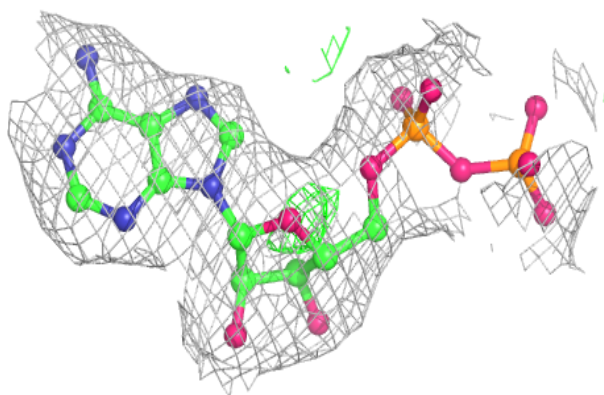
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



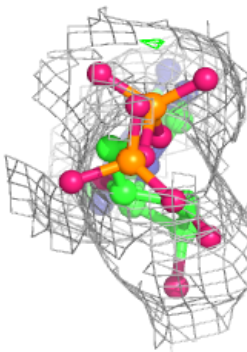
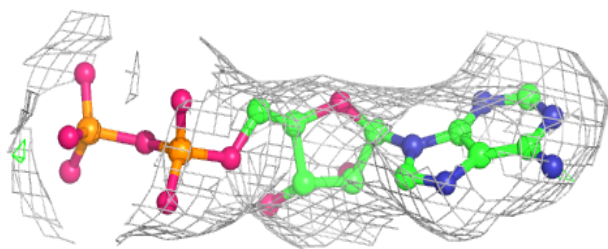
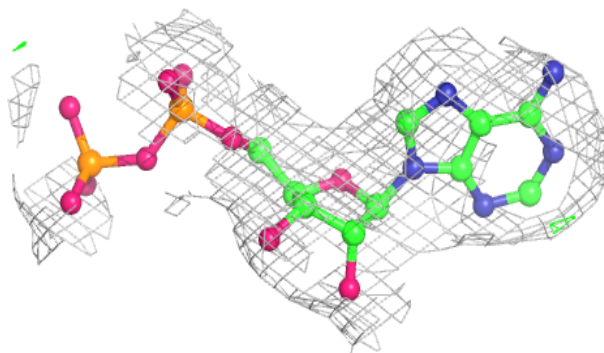


**Electron density around ADP F 601:**

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

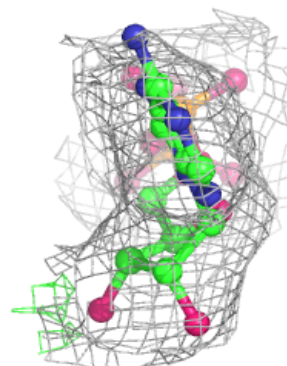
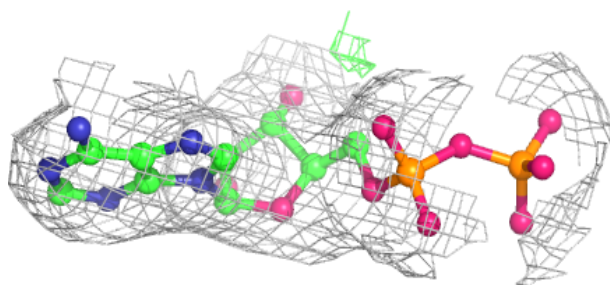
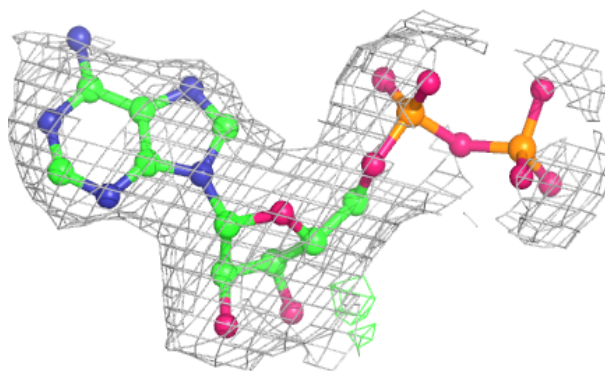
**Electron density around ADP J 601:**

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

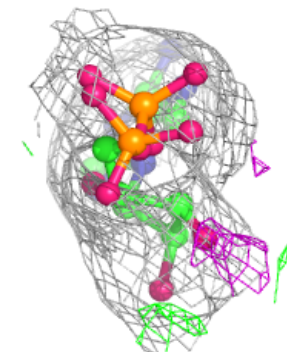
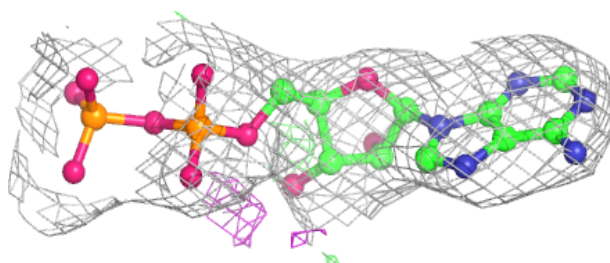


**Electron density around ADP J 602:**

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

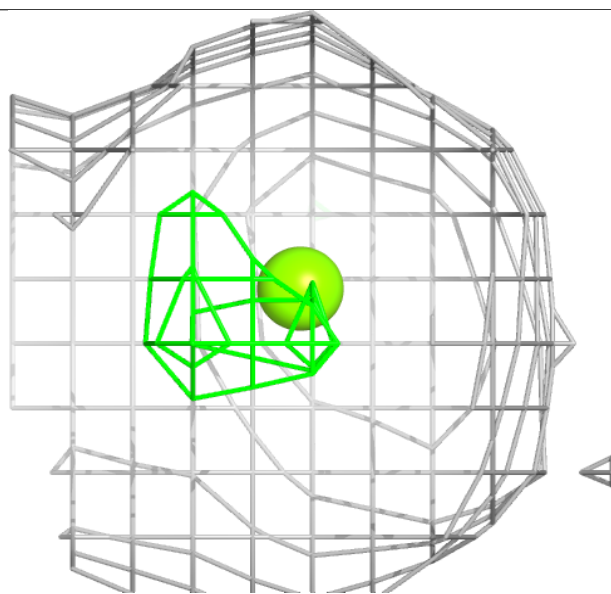
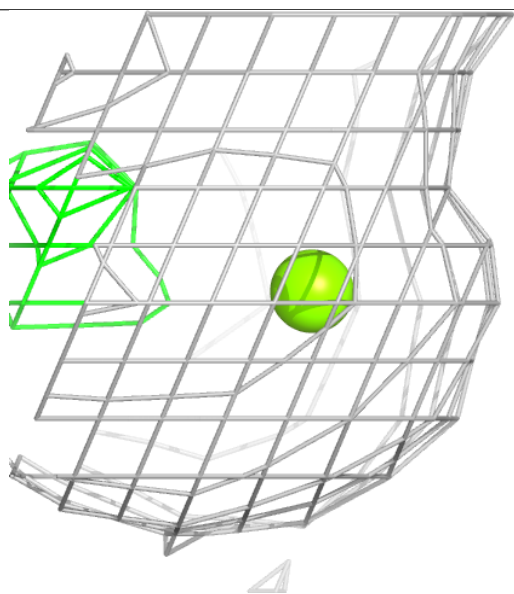
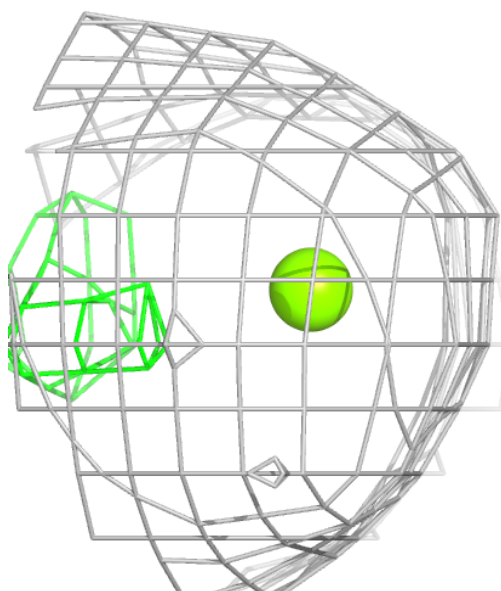
**Electron density around ADP B 602:**

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



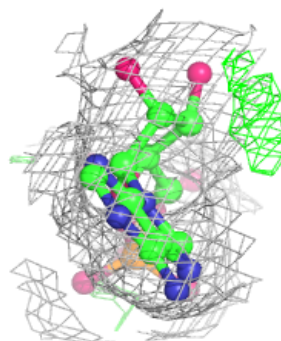
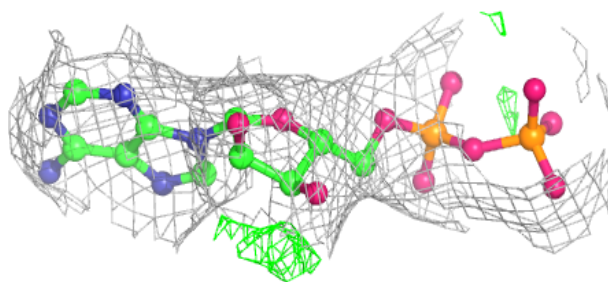
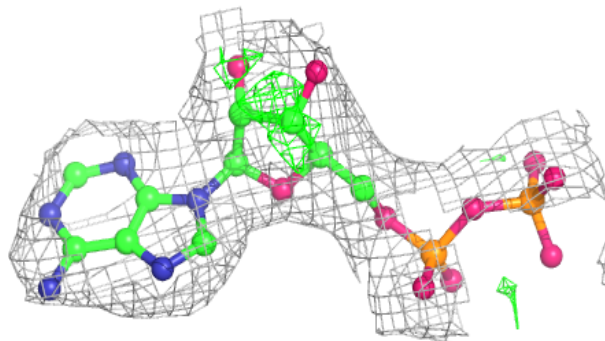
**Electron density around MG E 603:**

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

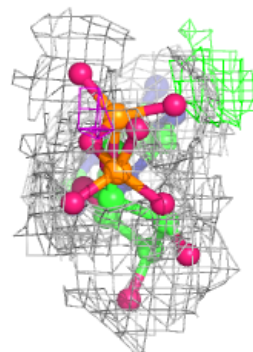
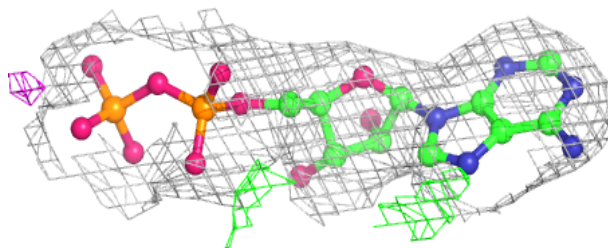
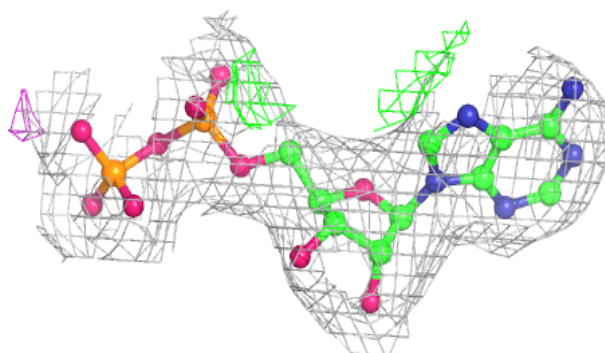


**Electron density around ADP C 602:**

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

**Electron density around ADP A 602:**

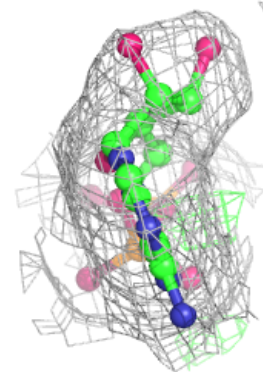
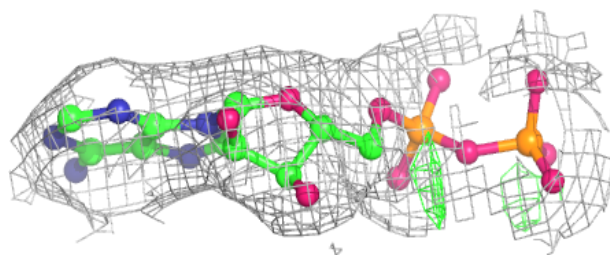
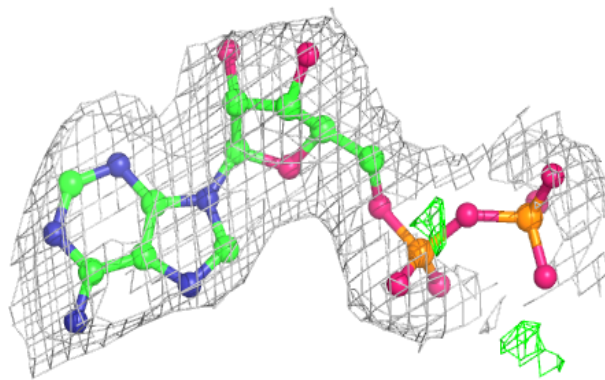
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





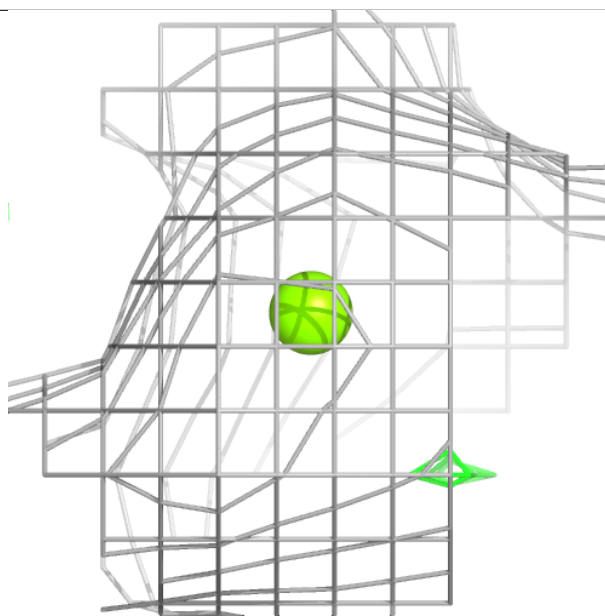
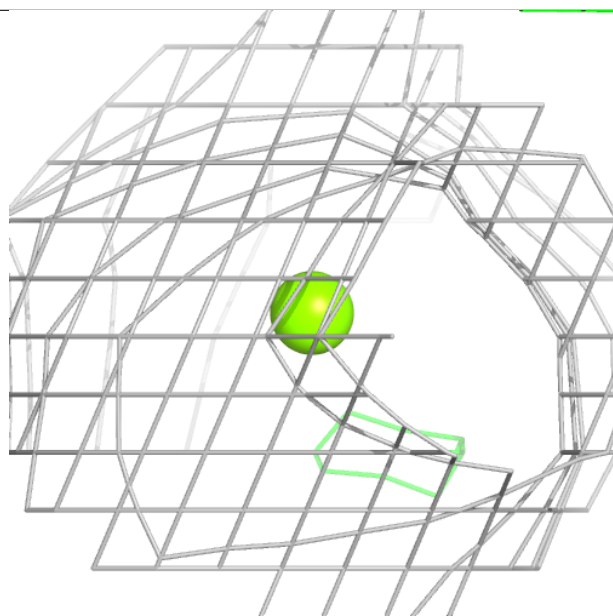
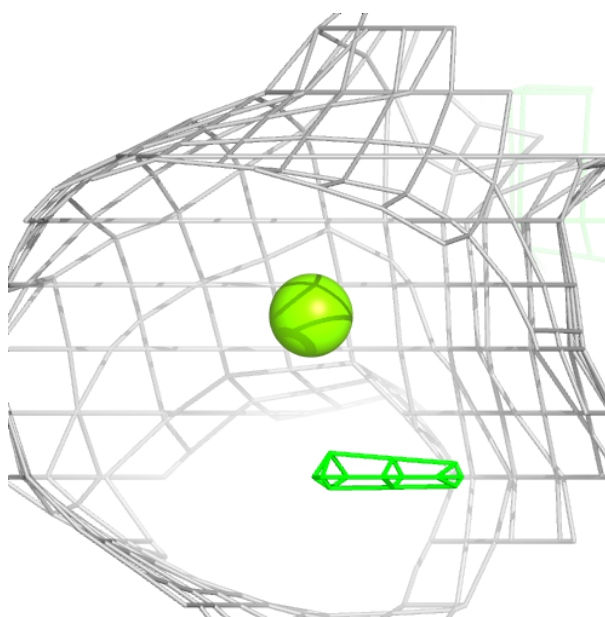
**Electron density around ADP E 601:**

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



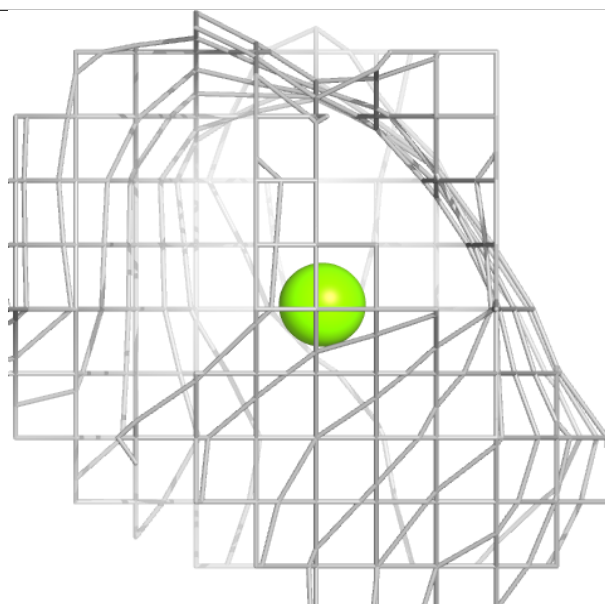
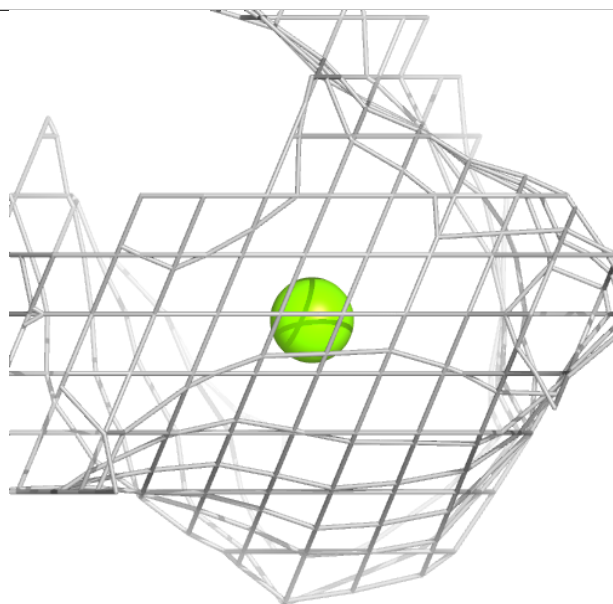
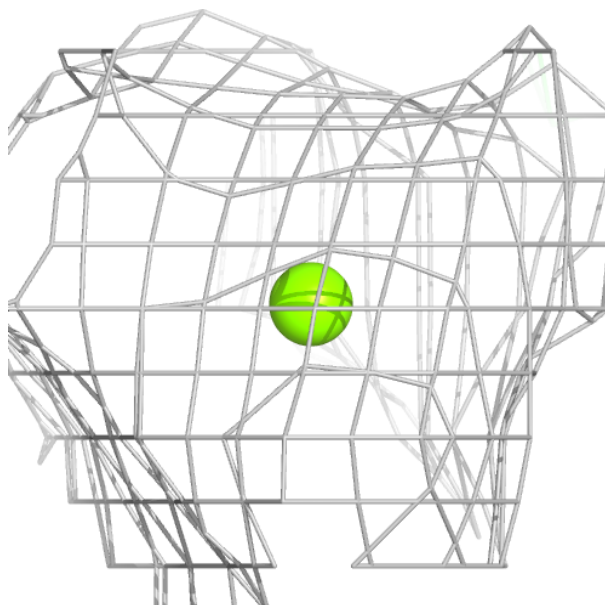
**Electron density around MG E 604:**

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



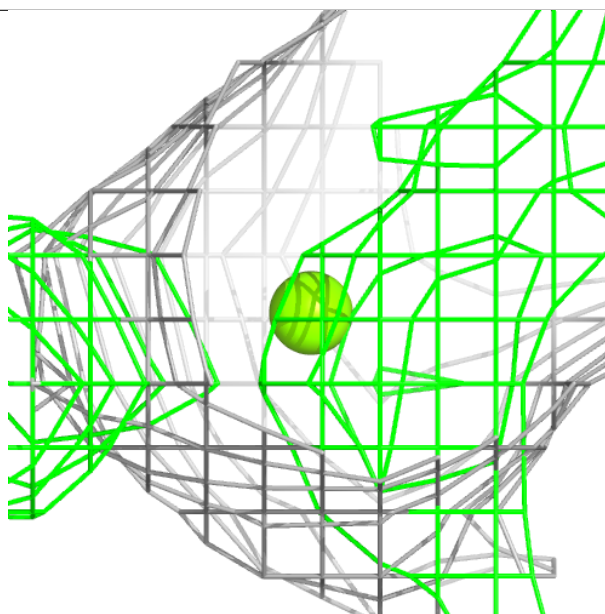
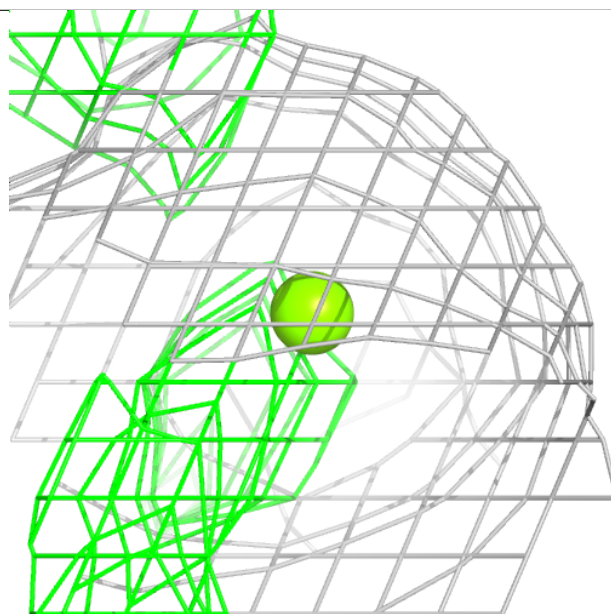
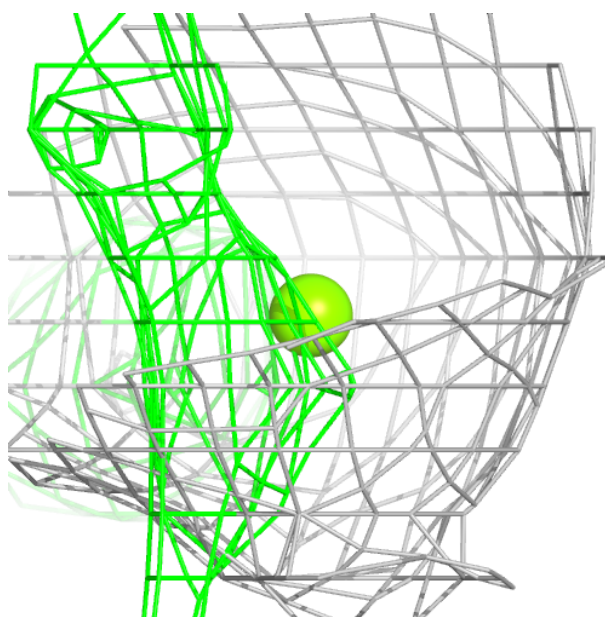
**Electron density around MG A 603:**

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



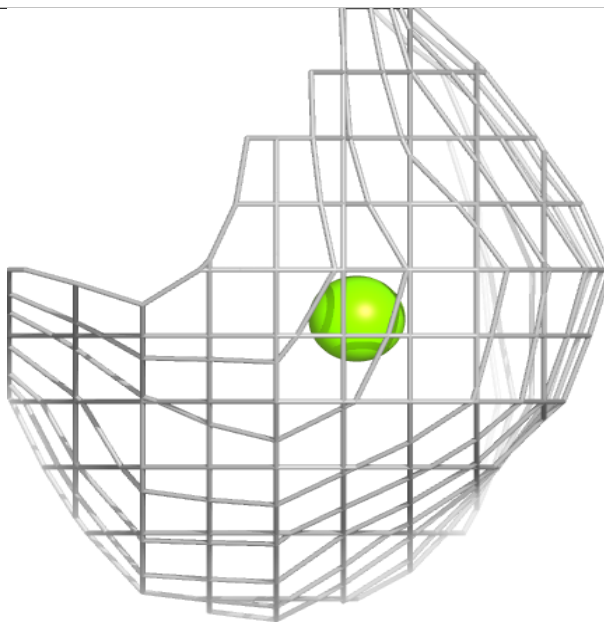
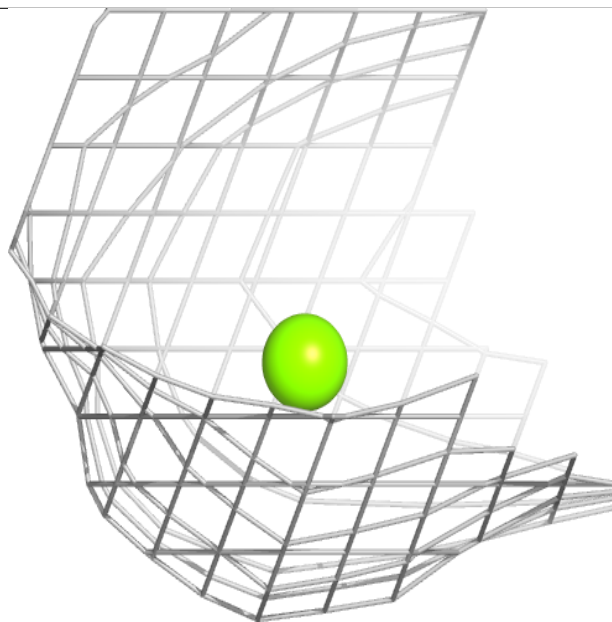
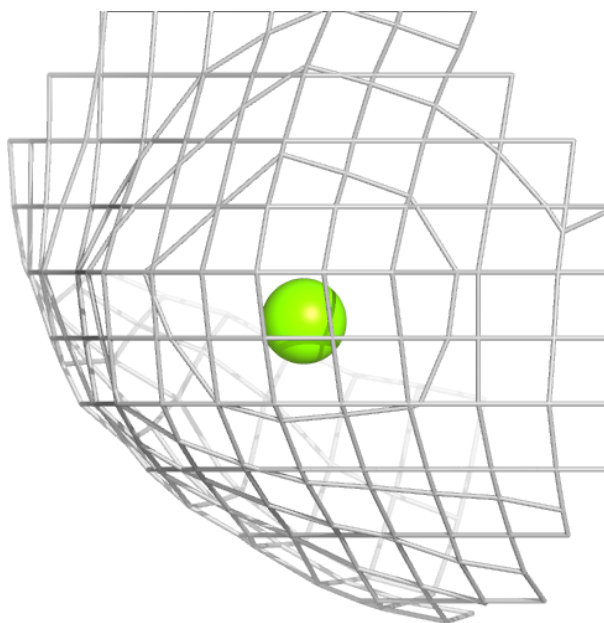
**Electron density around MG K 603:**

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



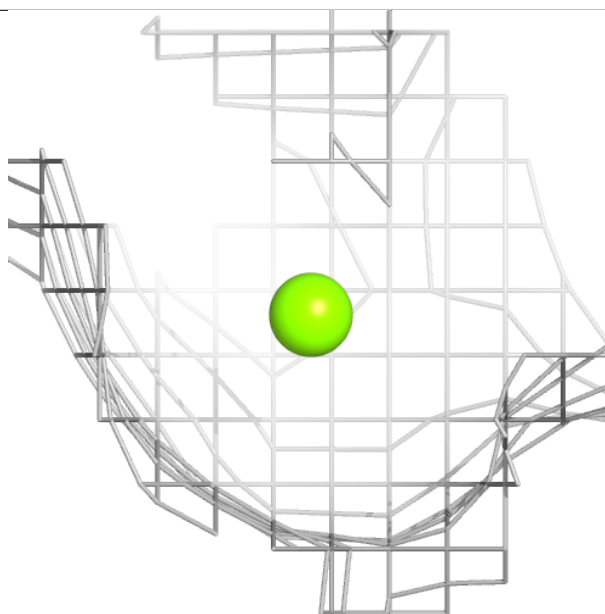
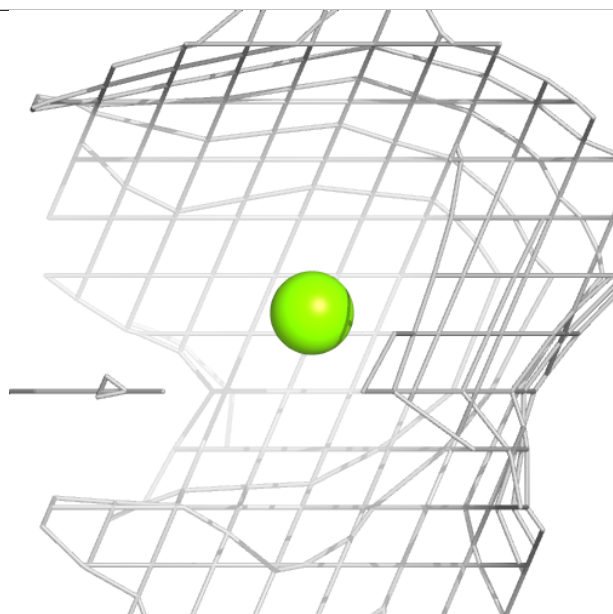
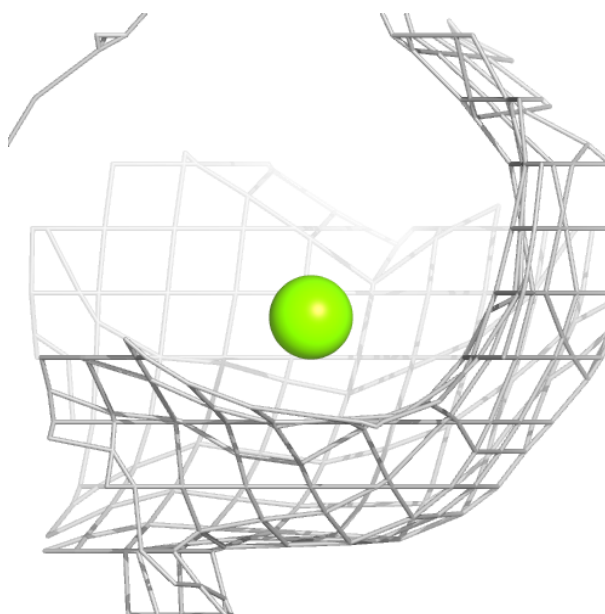
**Electron density around MG K 604:**

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



**Electron density around MG J 603:**

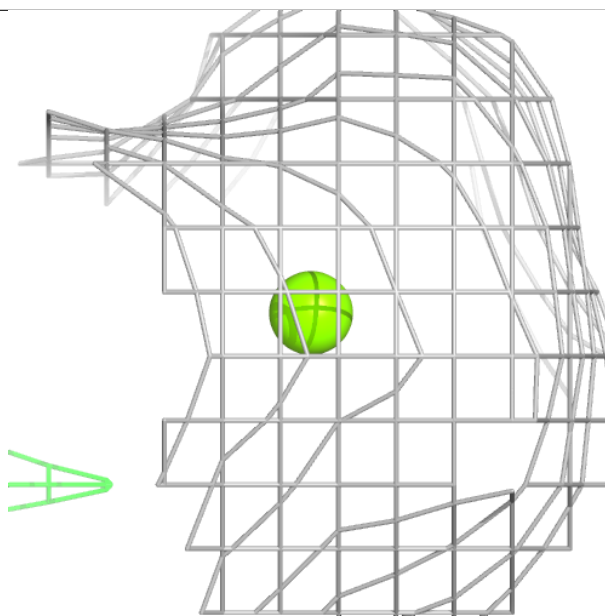
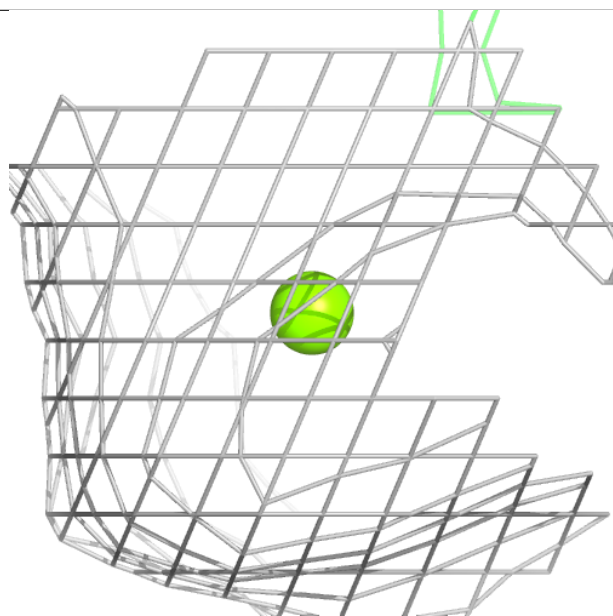
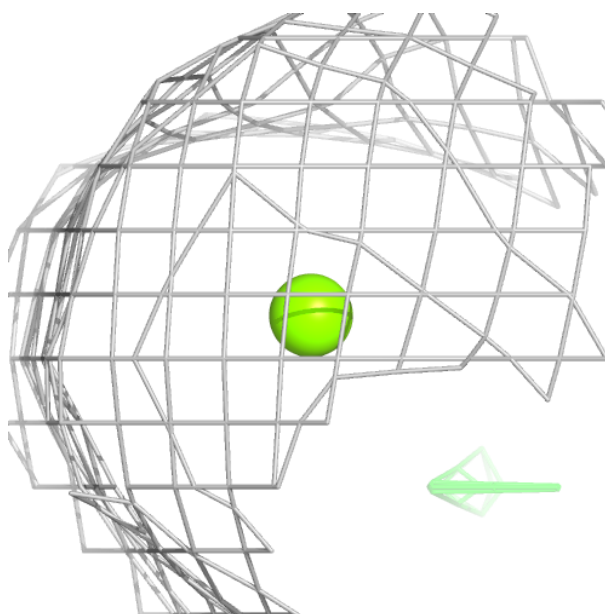
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





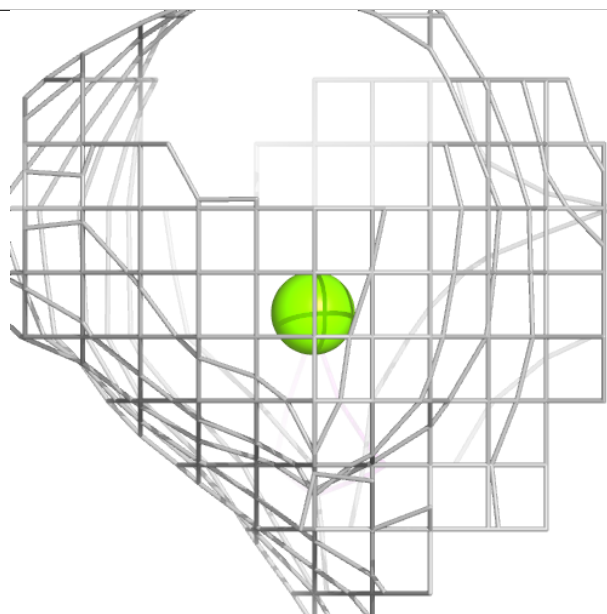
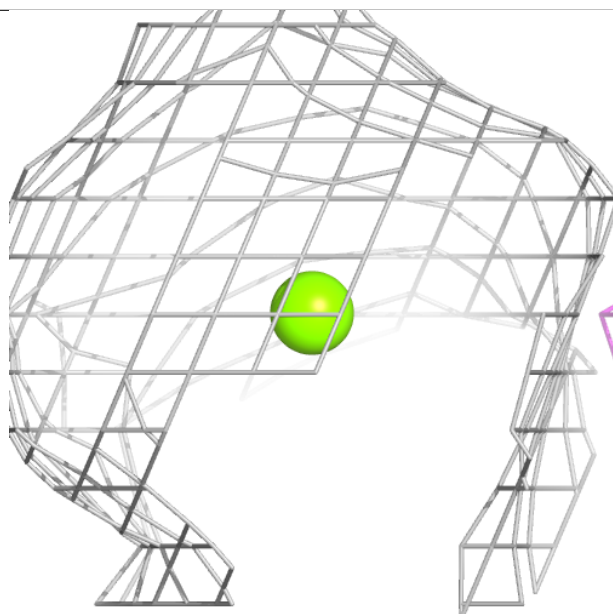
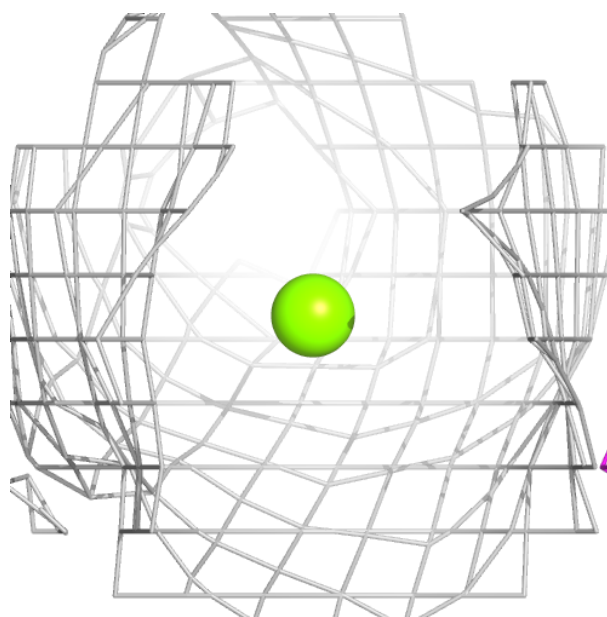
**Electron density around MG C 604:**

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



**Electron density around MG 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.