



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:51 PM UTC

PDB ID : 8000 / pdb_00008000
Title : Glutamine synthetase from Methanothermococcus thermolithotrophicus in complex with 2-oxoglutarate and MgATP at 2.15 Å resolution
Authors : Mueller, M.-C.; Wagner, T.
Deposited on : 2023-04-05
Resolution : 2.15 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

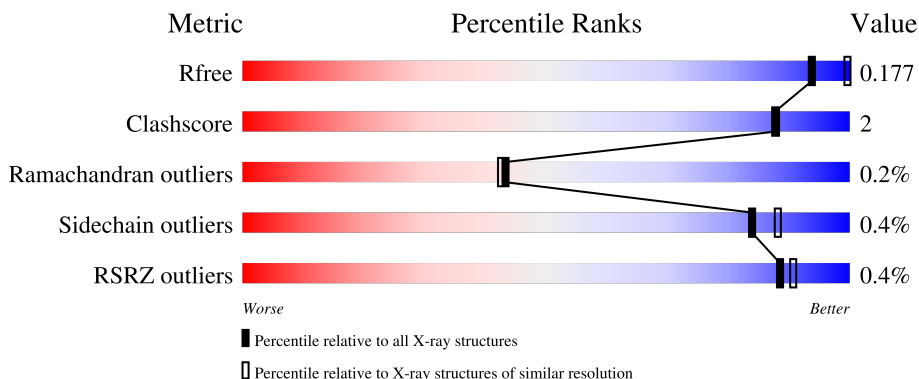
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	94% 5%
1	B	448	95% 5%
1	C	448	95% .
1	D	448	% 93% 6%
1	E	448	95% .

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Mol	Chain	Length	Quality of chain
1	F	448	 95%
1	G	448	 94% 6%
1	H	448	 94% 5%
1	I	448	 94% 5%
1	J	448	 96%
1	K	448	 96%
1	L	448	 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	K	501	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 46159 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 Glutamine synthetase from *Methanothermococcus thermolithotrophicus*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3534	2264	587	667	16	0	0	0
1	B	447	3534	2264	587	667	16	0	0	0
1	C	447	3534	2264	587	667	16	0	0	0
1	D	447	3534	2264	587	667	16	0	0	0
1	E	447	3534	2264	587	667	16	0	0	0
1	F	447	3534	2264	587	667	16	0	0	0
1	G	447	3534	2264	587	667	16	0	0	0
1	H	447	3534	2264	587	667	16	0	0	0
1	I	447	3534	2264	587	667	16	0	0	0
1	J	447	3534	2264	587	667	16	0	0	0
1	K	447	3534	2264	587	667	16	0	0	0
1	L	447	3534	2264	587	667	16	0	0	0

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



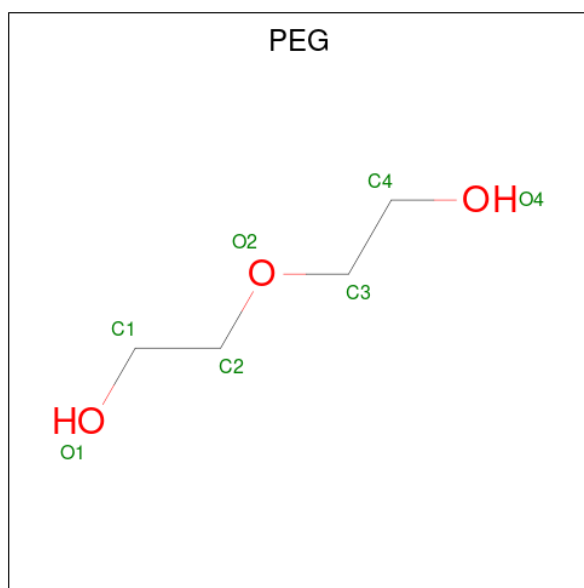
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0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

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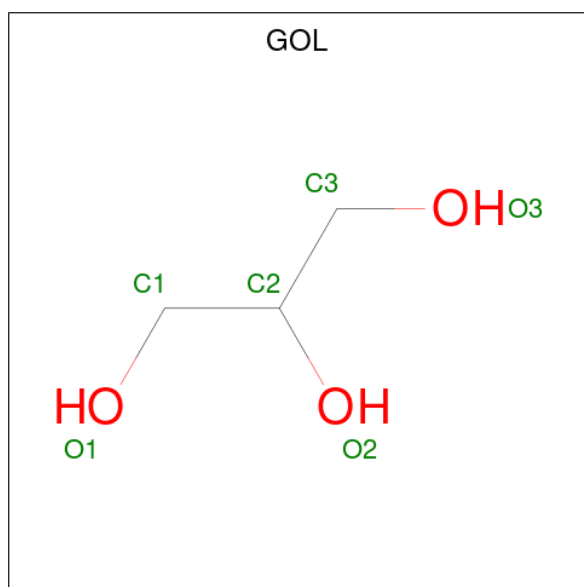
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
3	A	1	7	4	3	0	0
3	D	1	7	4	3	0	0
3	D	1	7	4	3	0	0
3	G	1	7	4	3	0	0
3	G	1	6	4	2	0	0
3	G	1	7	4	3	0	0
3	G	1	7	4	3	0	0
3	J	1	7	4	3	0	0
3	K	1	7	4	3	0	0

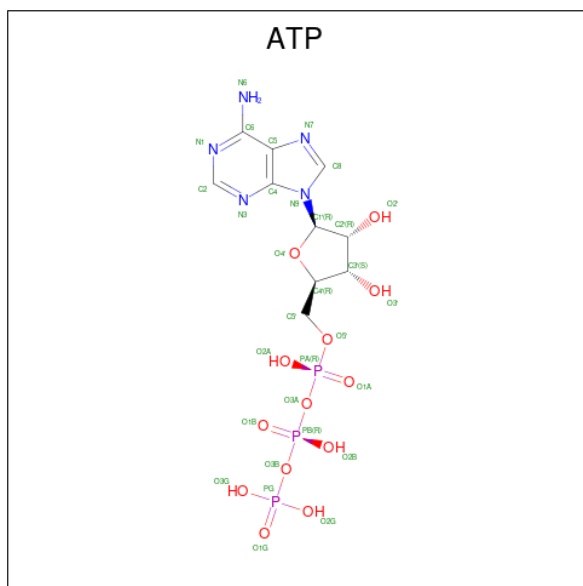
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$)

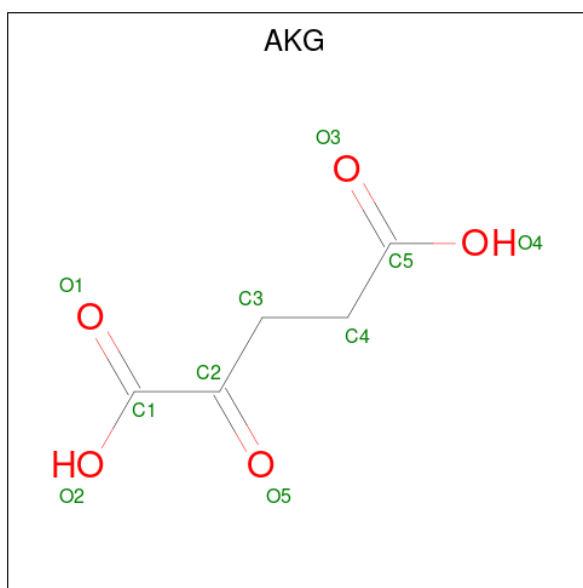
(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

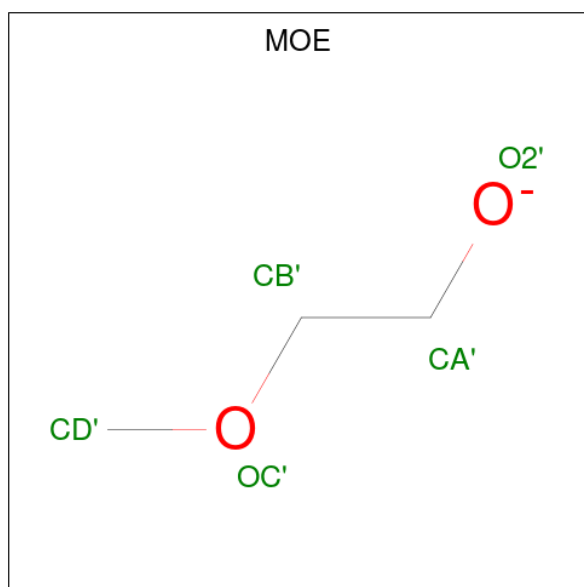
- Molecule 6 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 5 5	0	0
6	B	1	Total C O 10 5 5	0	0
6	C	1	Total C O 10 5 5	0	0
6	D	1	Total C O 10 5 5	0	0
6	E	1	Total C O 10 5 5	0	0
6	F	1	Total C O 10 5 5	0	0
6	G	1	Total C O 10 5 5	0	0
6	H	1	Total C O 10 5 5	0	0
6	I	1	Total C O 10 5 5	0	0
6	J	1	Total C O 10 5 5	0	0
6	K	1	Total C O 10 5 5	0	0
6	L	1	Total C O 10 5 5	0	0

- Molecule 7 is METHOXY-ETHOXYL (CCD ID: MOE) (formula: C₃H₇O₂).

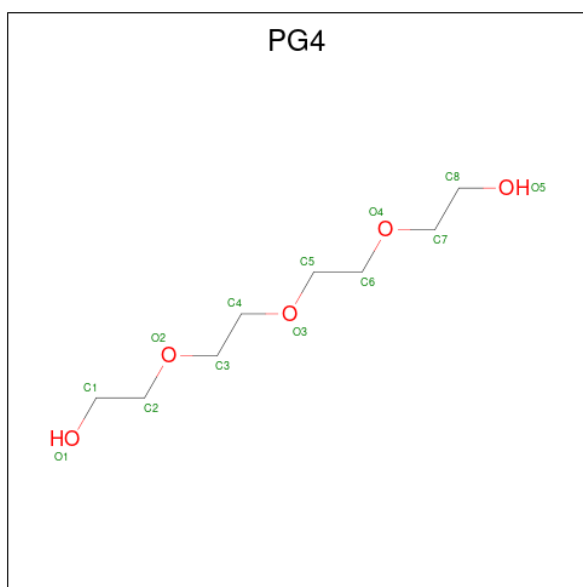


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			5	3	2		
7	F	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		
8	K	1	Total	Mg	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 13 8 5	0	0
9	D	1	Total C O 13 8 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	249	Total O 249 249	0	0
10	B	219	Total O 219 219	0	0
10	C	257	Total O 257 257	0	0
10	D	260	Total O 260 260	0	0
10	E	242	Total O 242 242	0	0
10	F	274	Total O 274 274	0	0
10	G	265	Total O 265 265	0	0
10	H	251	Total O 251 251	0	0
10	I	250	Total O 250 250	0	0
10	J	249	Total O 249 249	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	K	267	Total 267	O 267	0	0
10	L	258	Total 258	O 258	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

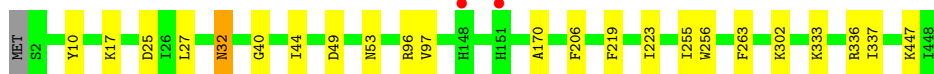
- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain A: 



- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain B: 



- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain C: 



- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain D: 



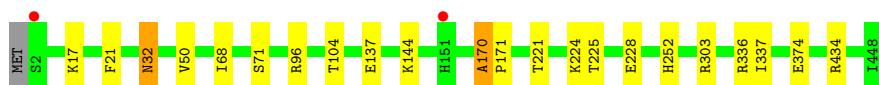
- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain E: 

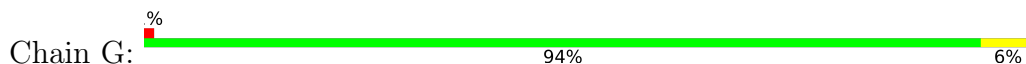




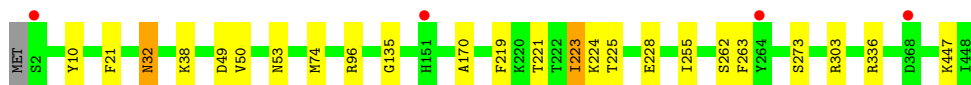
- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain L:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.34Å 131.77Å 131.51Å 60.04° 87.72° 67.34°	Depositor
Resolution (Å)	42.88 – 2.15 42.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	77.0 (42.88-2.15) 72.6 (42.88-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.14Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (21-NOV-2022)	Depositor
R, R_{free}	0.182 , 0.214 (Not available) , 0.177	Depositor DCC
R_{free} test set	12085 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.064 for -h,-k+l,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	46159	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, EDO, ATP, PG4, MOE, PEG, AKG

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	0.77	0/3625	0.95	1/4910 (0.0%)
1	B	0.77	0/3625	0.96	3/4910 (0.1%)
1	C	0.76	0/3625	0.94	3/4910 (0.1%)
1	D	0.77	0/3625	0.95	2/4910 (0.0%)
1	E	0.76	0/3625	0.96	2/4910 (0.0%)
1	F	0.78	0/3625	0.97	3/4910 (0.1%)
1	G	0.77	0/3625	0.95	3/4910 (0.1%)
1	H	0.78	1/3625 (0.0%)	0.94	1/4910 (0.0%)
1	I	0.75	0/3625	0.95	3/4910 (0.1%)
1	J	0.79	0/3625	0.96	3/4910 (0.1%)
1	K	0.77	0/3625	0.97	5/4910 (0.1%)
1	L	0.79	0/3625	0.97	4/4910 (0.1%)
All	All	0.77	1/43500 (0.0%)	0.96	33/58920 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	223	ILE	CG1-CD1	-5.41	1.30	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	32	ASN	CA-CB-CG	8.13	120.73	112.60
1	F	32	ASN	CA-CB-CG	7.81	120.41	112.60
1	C	32	ASN	CA-CB-CG	7.65	120.25	112.60
1	H	32	ASN	CA-CB-CG	7.54	120.14	112.60
1	I	32	ASN	CA-CB-CG	7.52	120.12	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3534	0	3458	14	0
1	B	3534	0	3458	13	0
1	C	3534	0	3458	12	0
1	D	3534	0	3458	22	0
1	E	3534	0	3458	12	0
1	F	3534	0	3458	13	0
1	G	3534	0	3458	15	0
1	H	3534	0	3458	15	0
1	I	3534	0	3458	14	0
1	J	3534	0	3458	11	0
1	K	3534	0	3458	13	0
1	L	3534	0	3458	19	0
2	A	16	0	24	2	0
2	B	12	0	18	0	0
2	C	12	0	18	2	0
2	D	4	0	6	1	0
2	E	4	0	6	0	0
2	F	16	0	24	2	0
2	G	4	0	6	0	0
2	H	4	0	6	1	0
2	I	12	0	18	1	0
2	J	8	0	12	1	0
2	L	12	0	18	0	0
3	A	14	0	20	1	0
3	D	14	0	20	4	0
3	G	27	0	37	6	0
3	J	7	0	10	1	0
3	K	7	0	10	4	0
4	A	6	0	8	1	0
5	A	31	0	12	1	0
5	B	31	0	12	2	0
5	C	31	0	12	2	0
5	D	31	0	12	2	0
5	E	31	0	12	1	0
5	F	31	0	12	1	0
5	G	31	0	12	0	0
5	H	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	31	0	12	3	0
5	J	31	0	12	2	0
5	K	31	0	12	2	0
5	L	31	0	12	2	0
6	A	10	0	4	0	0
6	B	10	0	4	0	0
6	C	10	0	4	0	0
6	D	10	0	4	0	0
6	E	10	0	4	0	0
6	F	10	0	4	0	0
6	G	10	0	4	0	0
6	H	10	0	4	0	0
6	I	10	0	4	0	0
6	J	10	0	4	0	0
6	K	10	0	4	0	0
6	L	10	0	4	0	0
7	B	5	0	7	1	0
7	F	5	0	7	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
8	K	1	0	0	0	0
9	D	26	0	36	8	0
10	A	249	0	0	0	0
10	B	219	0	0	2	0
10	C	257	0	0	0	0
10	D	260	0	0	0	0
10	E	242	0	0	2	0
10	F	274	0	0	0	0
10	G	265	0	0	1	0
10	H	251	0	0	2	0
10	I	250	0	0	1	0
10	J	249	0	0	0	0
10	K	267	0	0	0	0
10	L	258	0	0	2	0
All	All	46159	0	41999	173	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 2.

The worst 5 of 173 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:G:2:SER:HB3	1:G:5:GLU:HB2	1.75	0.67
1:I:336:ARG:HD2	5:I:504:ATP:C5	2.34	0.63
1:D:336:ARG:HD2	5:D:506:ATP:C5	2.36	0.61
1:J:436:SER:HB2	3:J:801:PEG:H12	1.83	0.61
1:L:233:LYS:NZ	10:L:601:HOH:O	2.31	0.60

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	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	B	445/448 (99%)	437 (98%)	7 (2%)	1 (0%)	43	42
1	C	445/448 (99%)	437 (98%)	7 (2%)	1 (0%)	43	42
1	D	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	E	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	43	42
1	F	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	G	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	H	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	43	42
1	I	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	J	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	43	42
1	K	445/448 (99%)	434 (98%)	10 (2%)	1 (0%)	43	42
1	L	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	43	42
All	All	5340/5376 (99%)	5229 (98%)	99 (2%)	12 (0%)	43	42

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ALA

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Mol	Chain	Res	Type
1	E	170	ALA
1	H	170	ALA
1	A	170	ALA
1	C	170	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/383 (100%)	379 (99%)	3 (1%)	73	79
1	B	382/383 (100%)	380 (100%)	2 (0%)	81	86
1	C	382/383 (100%)	381 (100%)	1 (0%)	86	90
1	D	382/383 (100%)	380 (100%)	2 (0%)	81	86
1	E	382/383 (100%)	380 (100%)	2 (0%)	81	86
1	F	382/383 (100%)	380 (100%)	2 (0%)	81	86
1	G	382/383 (100%)	381 (100%)	1 (0%)	86	90
1	H	382/383 (100%)	381 (100%)	1 (0%)	86	90
1	I	382/383 (100%)	381 (100%)	1 (0%)	86	90
1	J	382/383 (100%)	381 (100%)	1 (0%)	86	90
1	K	382/383 (100%)	380 (100%)	2 (0%)	81	86
1	L	382/383 (100%)	381 (100%)	1 (0%)	86	90
All	All	4584/4596 (100%)	4565 (100%)	19 (0%)	84	88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	32	ASN
1	K	223	ILE
1	L	32	ASN
1	K	32	ASN
1	E	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	406	ASN
1	K	406	ASN
1	F	406	ASN
1	L	313	ASN
1	J	295	ASN

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 68 ligands modelled in this entry, 3 are monoatomic - leaving 65 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	$\# Z > 2$
6	AKG	K	503	-	9,9,9	1.81	1 (11%)	11,11,11	1.66	3 (27%)
6	AKG	D	507	-	9,9,9	1.75	1 (11%)	11,11,11	1.59	3 (27%)
2	EDO	C	601	-	3,3,3	0.17	0	2,2,2	0.16	0
3	PEG	G	602	-	5,5,6	0.20	0	4,4,5	0.10	0
5	ATP	J	805	-	32,33,33	1.34	5 (15%)	48,52,52	1.74	11 (22%)
2	EDO	L	503	-	3,3,3	0.16	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	L	501	-	3,3,3	0.17	0	2,2,2	0.23	0
5	ATP	E	604	8	32,33,33	1.30	5 (15%)	48,52,52	1.75	10 (20%)
3	PEG	D	503	-	6,6,6	0.11	0	5,5,5	0.09	0
3	PEG	G	603	-	6,6,6	0.12	0	5,5,5	0.07	0
3	PEG	D	504	-	6,6,6	0.11	0	5,5,5	0.07	0
2	EDO	B	502	-	3,3,3	0.20	0	2,2,2	0.22	0
3	PEG	G	601	-	6,6,6	0.12	0	5,5,5	0.09	0
5	ATP	C	604	-	32,33,33	1.26	4 (12%)	48,52,52	1.70	9 (18%)
2	EDO	L	502	-	3,3,3	0.14	0	2,2,2	0.24	0
6	AKG	F	505	-	9,9,9	1.89	2 (22%)	11,11,11	1.12	0
5	ATP	F	506	-	32,33,33	1.31	5 (15%)	48,52,52	1.73	10 (20%)
2	EDO	F	504	-	3,3,3	0.16	0	2,2,2	0.23	0
5	ATP	L	505	-	32,33,33	1.34	5 (15%)	48,52,52	1.70	11 (22%)
6	AKG	C	605	-	9,9,9	2.22	2 (22%)	11,11,11	1.29	2 (18%)
6	AKG	G	606	-	9,9,9	1.69	1 (11%)	11,11,11	1.73	3 (27%)
6	AKG	E	603	-	9,9,9	2.29	2 (22%)	11,11,11	1.37	1 (9%)
2	EDO	I	502	-	3,3,3	0.14	0	2,2,2	0.22	0
2	EDO	C	603	-	3,3,3	0.16	0	2,2,2	0.23	0
2	EDO	B	501	-	3,3,3	0.37	0	2,2,2	0.38	0
2	EDO	B	504	-	3,3,3	0.16	0	2,2,2	0.23	0
2	EDO	A	506	-	3,3,3	0.16	0	2,2,2	0.18	0
2	EDO	F	502	-	3,3,3	0.66	0	2,2,2	0.31	0
2	EDO	I	505	-	3,3,3	0.72	0	2,2,2	0.28	0
7	MOE	B	503	-	4,4,4	0.21	0	3,3,3	0.18	0
2	EDO	J	803	-	3,3,3	0.16	0	2,2,2	0.23	0
3	PEG	J	801	-	6,6,6	0.13	0	5,5,5	0.25	0
9	PG4	D	501	-	12,12,12	0.15	0	11,11,11	0.16	0
5	ATP	B	506	-	32,33,33	1.32	5 (15%)	48,52,52	1.69	9 (18%)
6	AKG	J	804	-	9,9,9	1.81	1 (11%)	11,11,11	1.45	1 (9%)
2	EDO	J	802	-	3,3,3	0.16	0	2,2,2	0.23	0
3	PEG	A	502	-	6,6,6	0.08	0	5,5,5	0.06	0
2	EDO	D	502	-	3,3,3	0.16	0	2,2,2	0.23	0
2	EDO	G	605	-	3,3,3	0.17	0	2,2,2	0.36	0
2	EDO	C	602	-	3,3,3	0.17	0	2,2,2	0.32	0
5	ATP	K	504	8	32,33,33	1.31	5 (15%)	48,52,52	1.71	9 (18%)
6	AKG	H	602	-	9,9,9	1.86	2 (22%)	11,11,11	1.61	3 (27%)
2	EDO	F	503	-	3,3,3	0.15	0	2,2,2	0.24	0
2	EDO	F	501	-	3,3,3	0.63	0	2,2,2	0.13	0
5	ATP	I	504	-	32,33,33	1.33	5 (15%)	48,52,52	1.69	9 (18%)
5	ATP	D	506	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	K	501	-	6,6,6	0.11	0	5,5,5	0.08	0
2	EDO	A	501	-	3,3,3	0.33	0	2,2,2	0.10	0
2	EDO	I	501	-	3,3,3	0.15	0	2,2,2	0.21	0
2	EDO	A	505	-	3,3,3	0.13	0	2,2,2	0.22	0
3	PEG	G	604	-	6,6,6	0.14	0	5,5,5	0.12	0
2	EDO	H	601	-	3,3,3	0.16	0	2,2,2	0.23	0
4	GOL	A	507	-	5,5,5	0.08	0	5,5,5	0.33	0
2	EDO	A	503	-	3,3,3	0.15	0	2,2,2	0.22	0
5	ATP	G	607	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	10 (20%)
2	EDO	E	601	-	3,3,3	0.14	0	2,2,2	0.23	0
6	AKG	A	509	-	9,9,9	1.93	1 (11%)	11,11,11	1.95	2 (18%)
7	MOE	F	507	-	4,4,4	0.20	0	3,3,3	0.21	0
6	AKG	I	503	-	9,9,9	1.73	1 (11%)	11,11,11	1.13	1 (9%)
6	AKG	B	507	-	9,9,9	1.57	1 (11%)	11,11,11	1.51	2 (18%)
9	PG4	D	505	-	12,12,12	0.15	0	11,11,11	0.17	0
6	AKG	L	504	-	9,9,9	1.64	1 (11%)	11,11,11	1.52	1 (9%)
5	ATP	H	603	-	32,33,33	1.33	5 (15%)	48,52,52	1.70	10 (20%)
5	ATP	A	508	-	32,33,33	1.34	5 (15%)	48,52,52	1.74	10 (20%)
3	PEG	A	504	-	6,6,6	0.11	0	5,5,5	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AKG	K	503	-	-	1/9/9/9	-
6	AKG	D	507	-	-	4/9/9/9	-
2	EDO	C	601	-	-	1/1/1/1	-
3	PEG	G	602	-	-	1/3/3/4	-
5	ATP	J	805	-	-	3/22/38/38	0/3/3/3
2	EDO	L	503	-	-	1/1/1/1	-
2	EDO	L	501	-	-	1/1/1/1	-
5	ATP	E	604	8	-	3/22/38/38	0/3/3/3
3	PEG	D	503	-	-	2/4/4/4	-
3	PEG	G	603	-	-	4/4/4/4	-
3	PEG	D	504	-	-	4/4/4/4	-
2	EDO	B	502	-	-	1/1/1/1	-
3	PEG	G	601	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	C	604	-	-	6/22/38/38	0/3/3/3
2	EDO	L	502	-	-	0/1/1/1	-
6	AKG	F	505	-	-	3/9/9/9	-
5	ATP	F	506	-	-	6/22/38/38	0/3/3/3
2	EDO	F	504	-	-	0/1/1/1	-
5	ATP	L	505	-	-	3/22/38/38	0/3/3/3
6	AKG	C	605	-	-	4/9/9/9	-
6	AKG	G	606	-	-	4/9/9/9	-
6	AKG	E	603	-	-	4/9/9/9	-
2	EDO	I	502	-	-	1/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	A	506	-	-	1/1/1/1	-
2	EDO	F	502	-	-	1/1/1/1	-
2	EDO	I	505	-	-	1/1/1/1	-
7	MOE	B	503	-	-	2/2/2/2	-
2	EDO	J	803	-	-	0/1/1/1	-
3	PEG	J	801	-	-	2/4/4/4	-
9	PG4	D	501	-	-	5/10/10/10	-
5	ATP	B	506	-	-	2/22/38/38	0/3/3/3
6	AKG	J	804	-	-	1/9/9/9	-
2	EDO	J	802	-	-	1/1/1/1	-
3	PEG	A	502	-	-	2/4/4/4	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	G	605	-	-	0/1/1/1	-
2	EDO	C	602	-	-	0/1/1/1	-
5	ATP	K	504	8	-	5/22/38/38	0/3/3/3
6	AKG	H	602	-	-	4/9/9/9	-
2	EDO	F	503	-	-	0/1/1/1	-
2	EDO	F	501	-	-	0/1/1/1	-
5	ATP	I	504	-	-	4/22/38/38	0/3/3/3
5	ATP	D	506	-	-	7/22/38/38	0/3/3/3
3	PEG	K	501	-	-	3/4/4/4	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	I	501	-	-	1/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
3	PEG	G	604	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	H	601	-	-	0/1/1/1	-
4	GOL	A	507	-	-	1/4/4/4	-
2	EDO	A	503	-	-	1/1/1/1	-
5	ATP	G	607	-	-	10/22/38/38	0/3/3/3
2	EDO	E	601	-	-	1/1/1/1	-
6	AKG	A	509	-	-	3/9/9/9	-
7	MOE	F	507	-	-	2/2/2/2	-
6	AKG	I	503	-	-	4/9/9/9	-
6	AKG	B	507	-	-	1/9/9/9	-
9	PG4	D	505	-	-	8/10/10/10	-
6	AKG	L	504	-	-	2/9/9/9	-
5	ATP	H	603	-	-	6/22/38/38	0/3/3/3
5	ATP	A	508	-	-	2/22/38/38	0/3/3/3
3	PEG	A	504	-	-	2/4/4/4	-

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	603	AKG	C2-C1	-6.00	1.44	1.53
6	C	605	AKG	C2-C1	-5.73	1.44	1.53
6	K	503	AKG	C2-C1	-4.70	1.46	1.53
6	A	509	AKG	C2-C1	-4.62	1.46	1.53
6	F	505	AKG	C2-C1	-4.56	1.46	1.53

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	508	ATP	C5-C4-N3	-5.70	118.87	126.72
5	F	506	ATP	C5-C4-N3	-5.69	118.88	126.72
5	C	604	ATP	C5-C4-N3	-5.67	118.91	126.72
5	H	603	ATP	C5-C4-N3	-5.62	118.97	126.72
5	G	607	ATP	C5-C4-N3	-5.55	119.08	126.72

There are no chirality outliers.

5 of 152 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	506	ATP	C5'-O5'-PA-O1A
5	G	607	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	H	603	ATP	C5'-O5'-PA-O1A
6	A	509	AKG	O2-C1-C2-C3
6	B	507	AKG	O2-C1-C2-C3

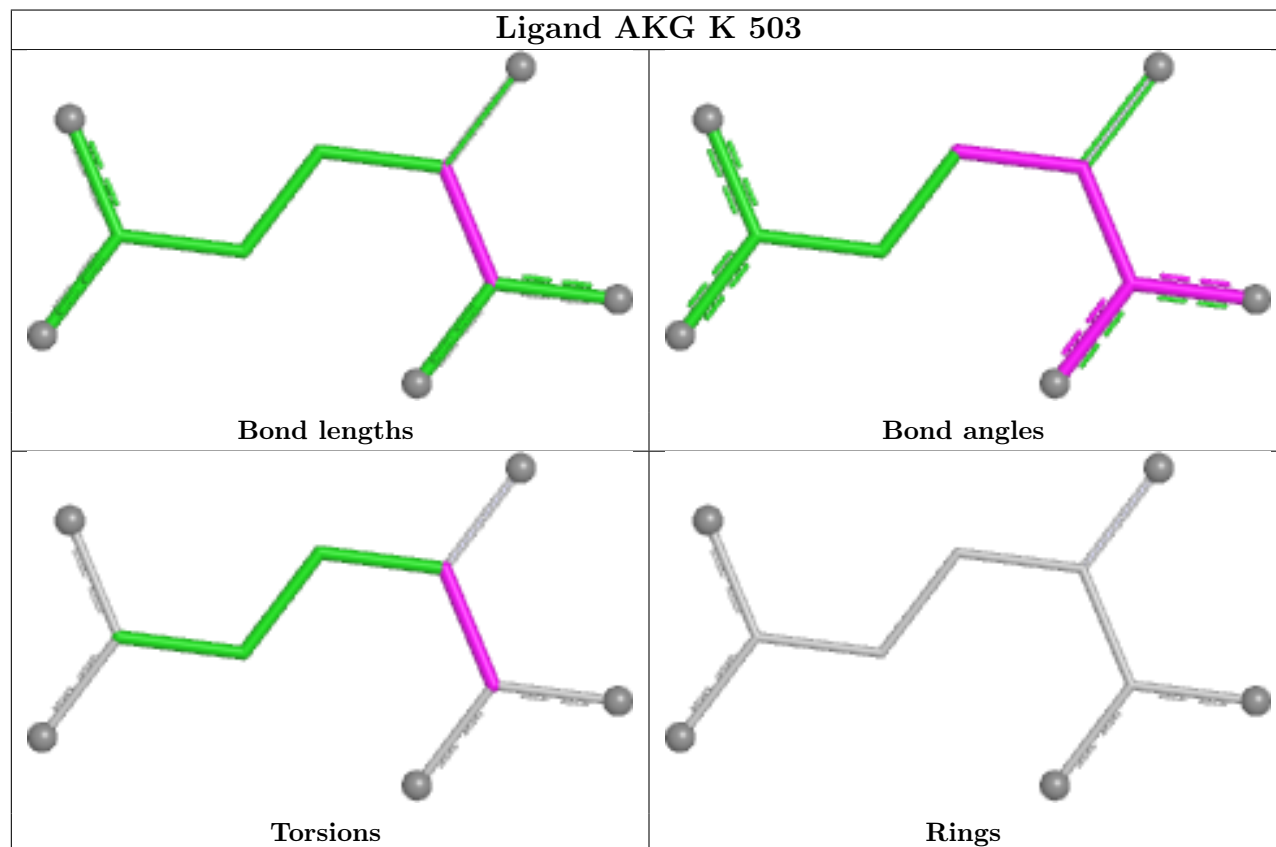
There are no ring outliers.

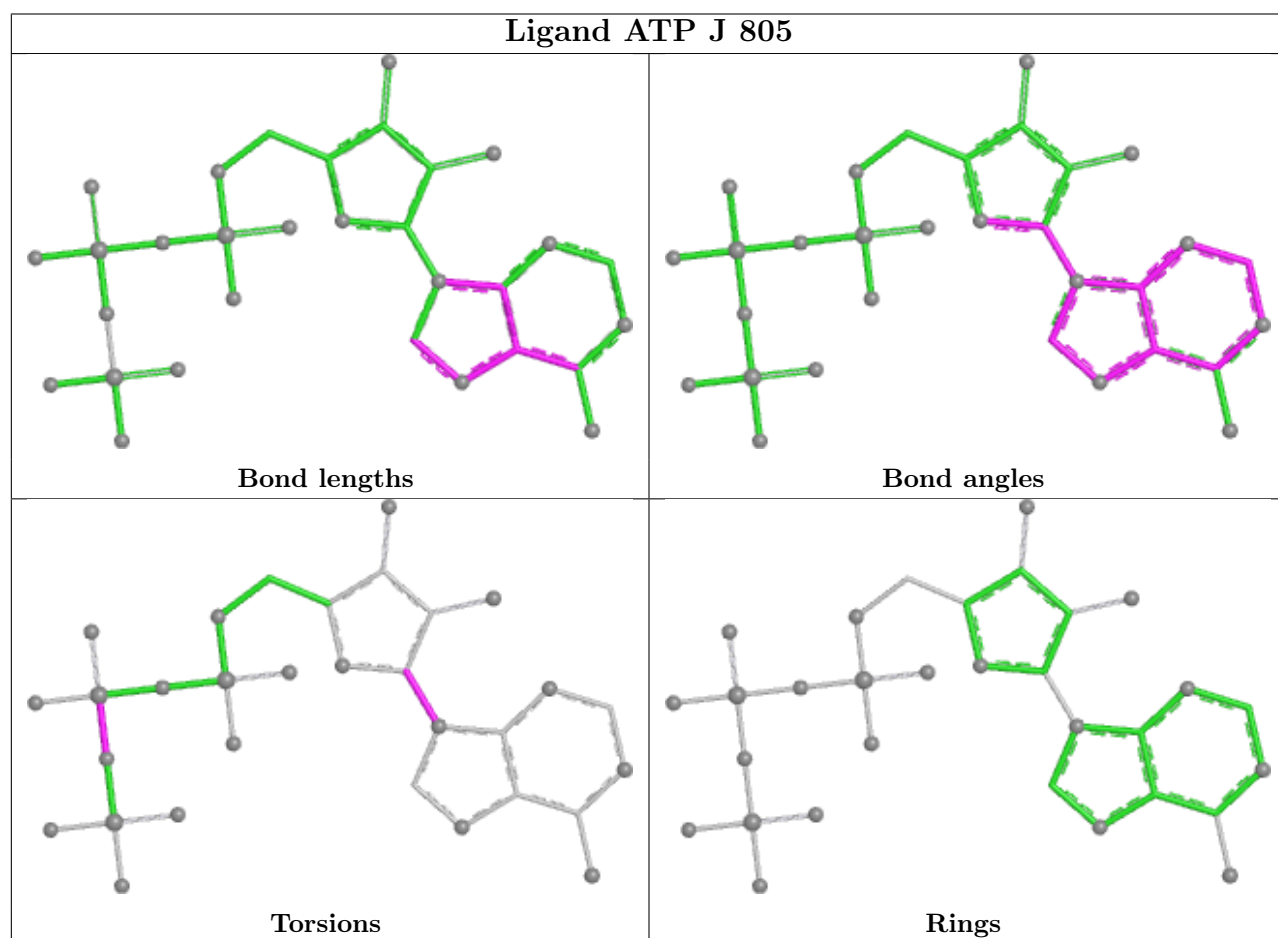
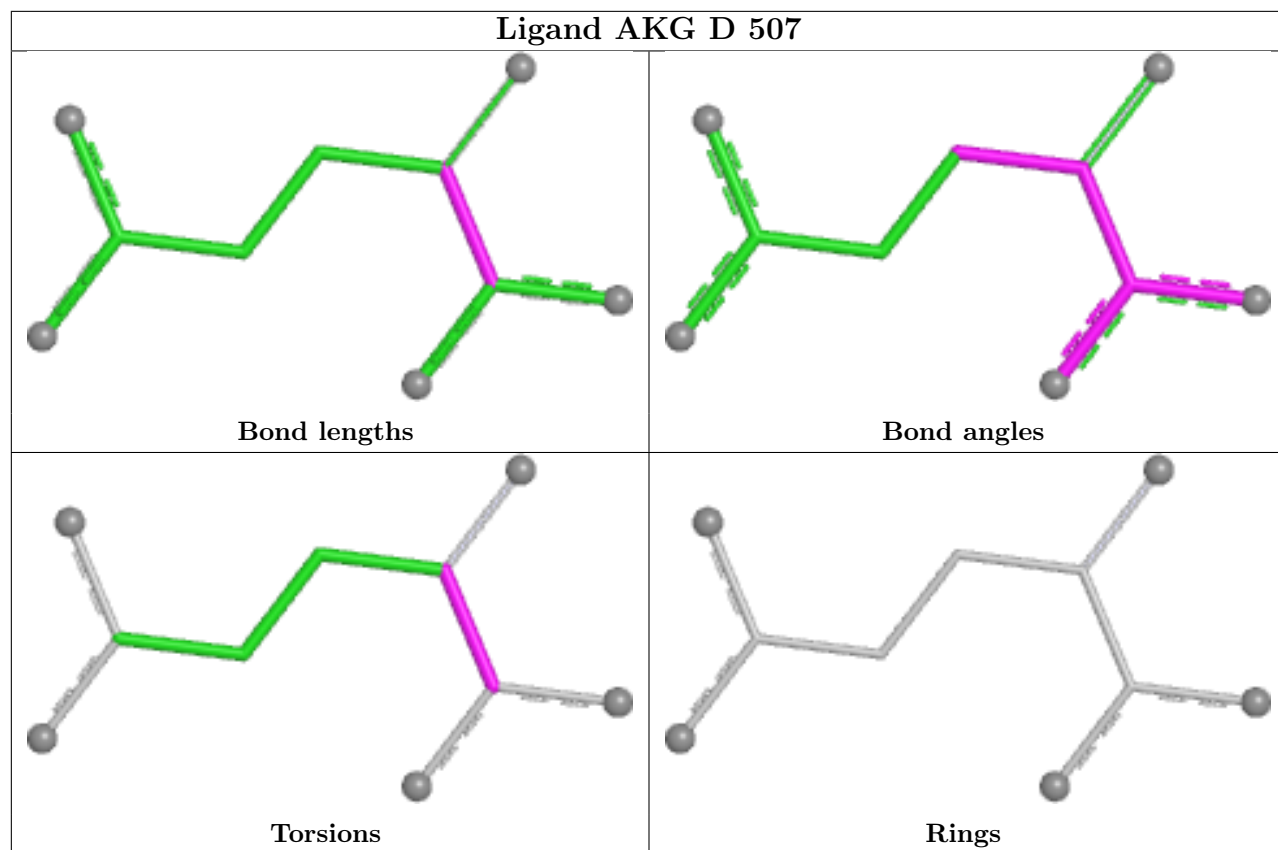
31 monomers are involved in 56 short contacts:

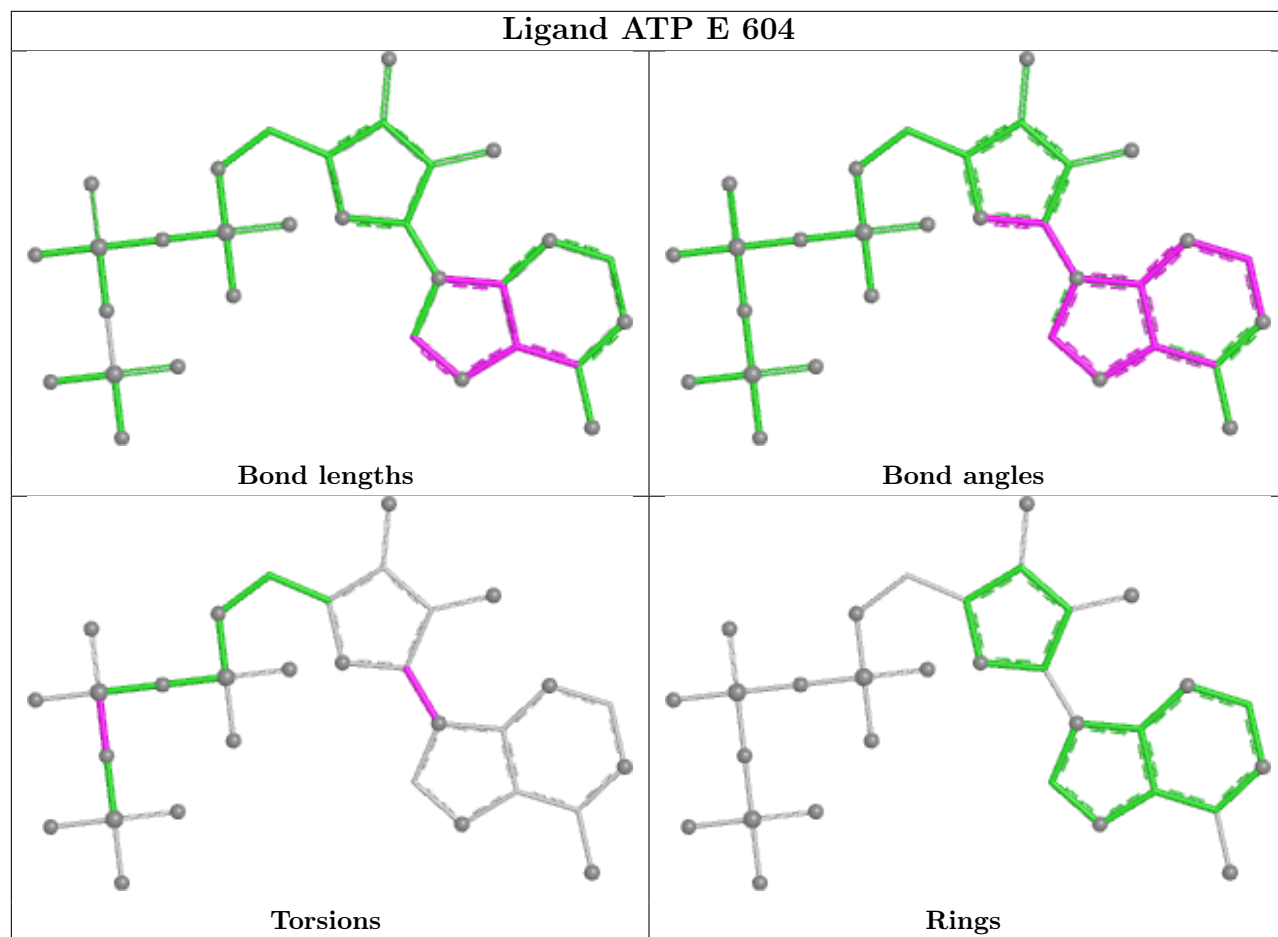
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	PEG	1	0
5	J	805	ATP	2	0
5	E	604	ATP	1	0
3	D	503	PEG	1	0
3	G	603	PEG	2	0
3	D	504	PEG	3	0
3	G	601	PEG	2	0
5	C	604	ATP	2	0
5	F	506	ATP	1	0
5	L	505	ATP	2	0
2	C	603	EDO	2	0
7	B	503	MOE	1	0
2	J	803	EDO	1	0
3	J	801	PEG	1	0
9	D	501	PG4	6	0
5	B	506	ATP	2	0
2	D	502	EDO	1	0
5	K	504	ATP	2	0
2	F	503	EDO	2	0
5	I	504	ATP	3	0
5	D	506	ATP	2	0
3	K	501	PEG	4	0
2	A	501	EDO	2	0
2	I	501	EDO	1	0
3	G	604	PEG	1	0
2	H	601	EDO	1	0
4	A	507	GOL	1	0
9	D	505	PG4	2	0
5	H	603	ATP	2	0
5	A	508	ATP	1	0
3	A	504	PEG	1	0

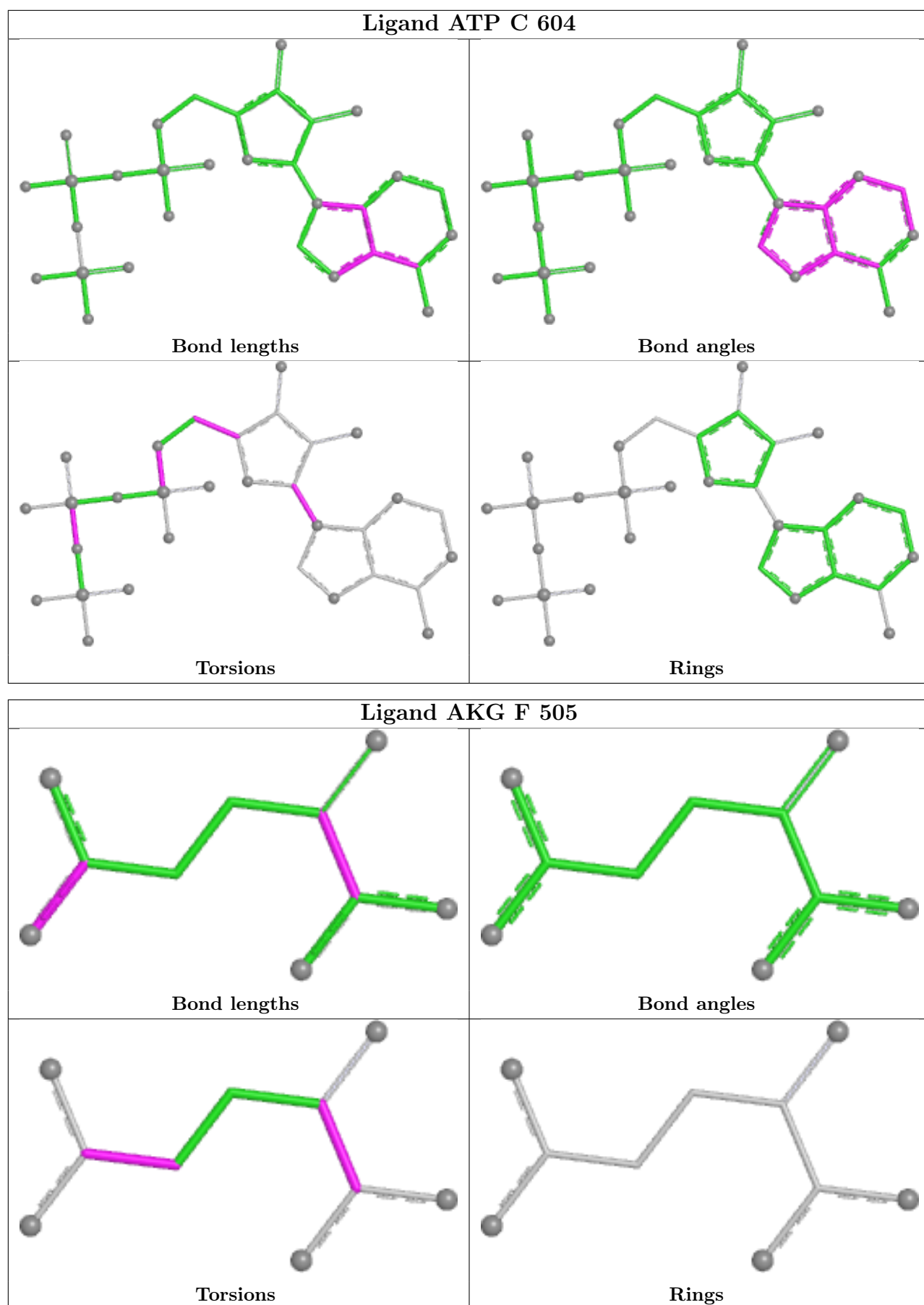
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

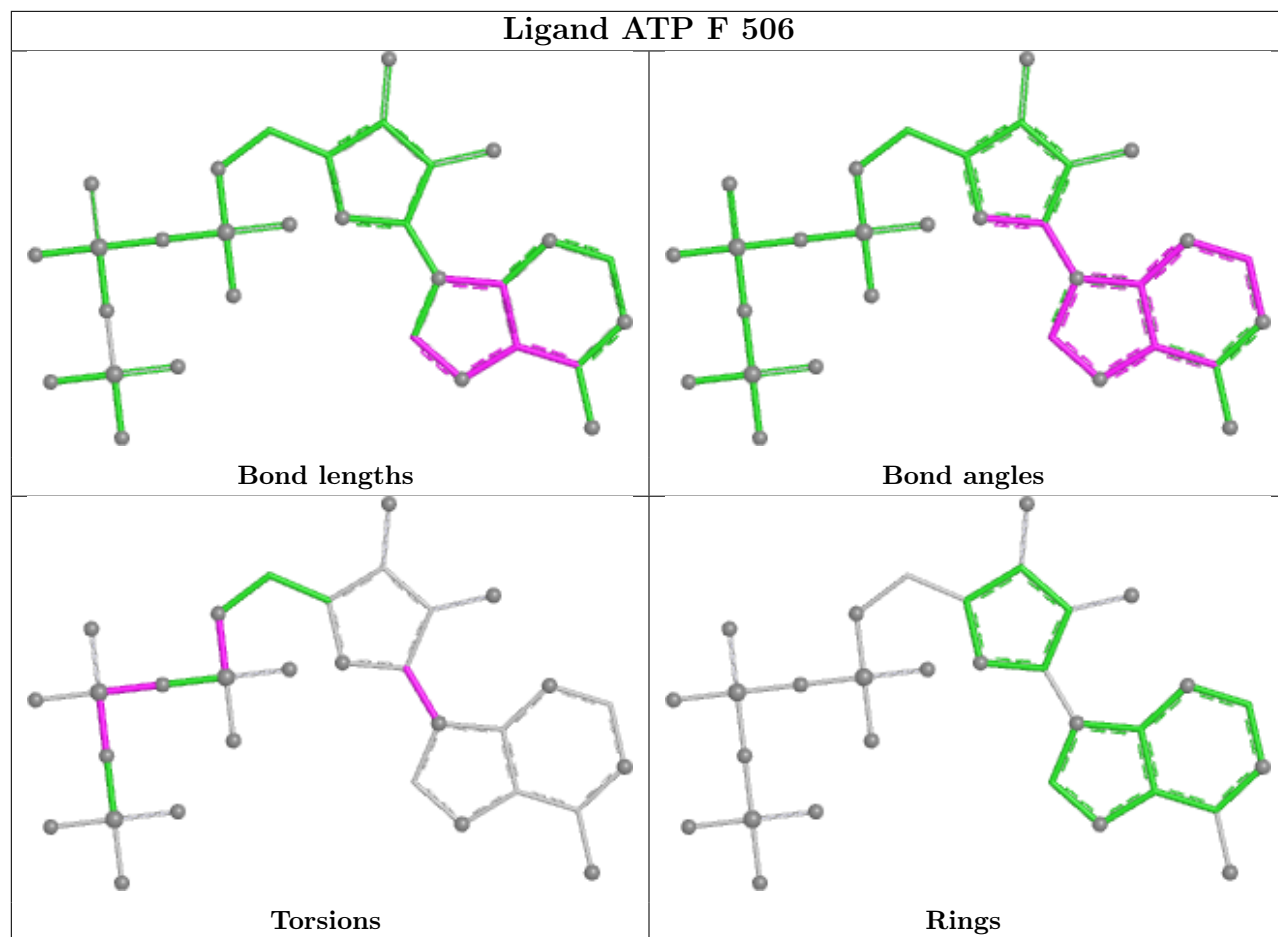
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

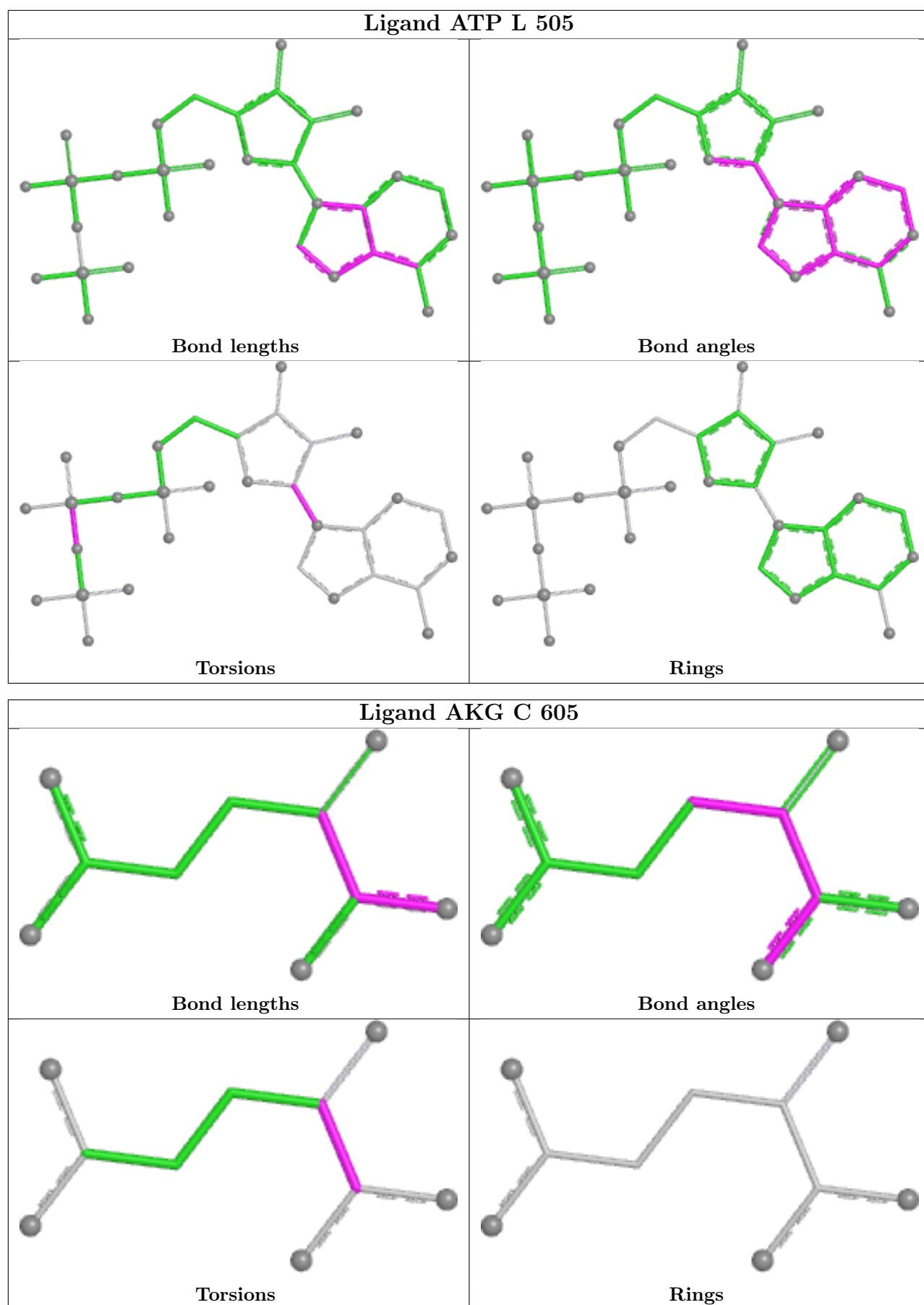


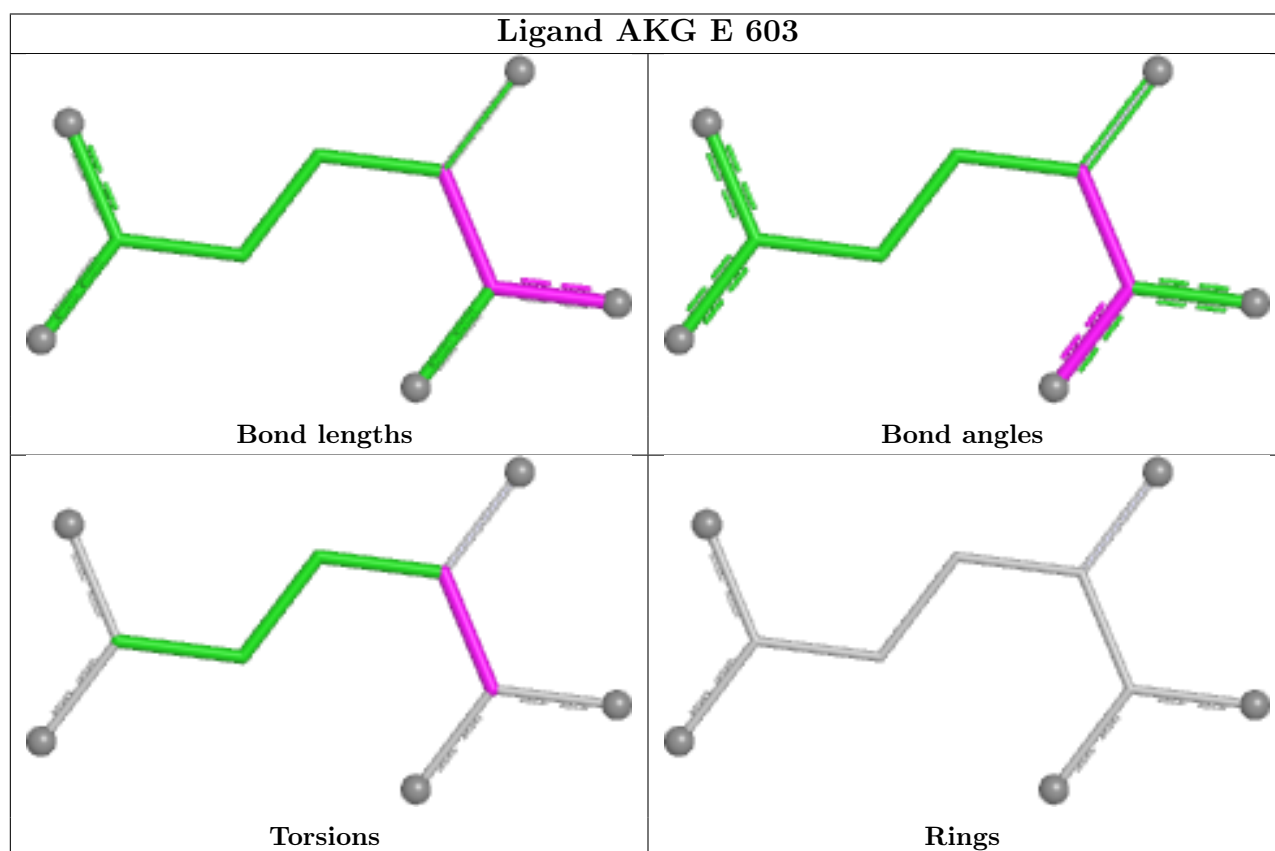
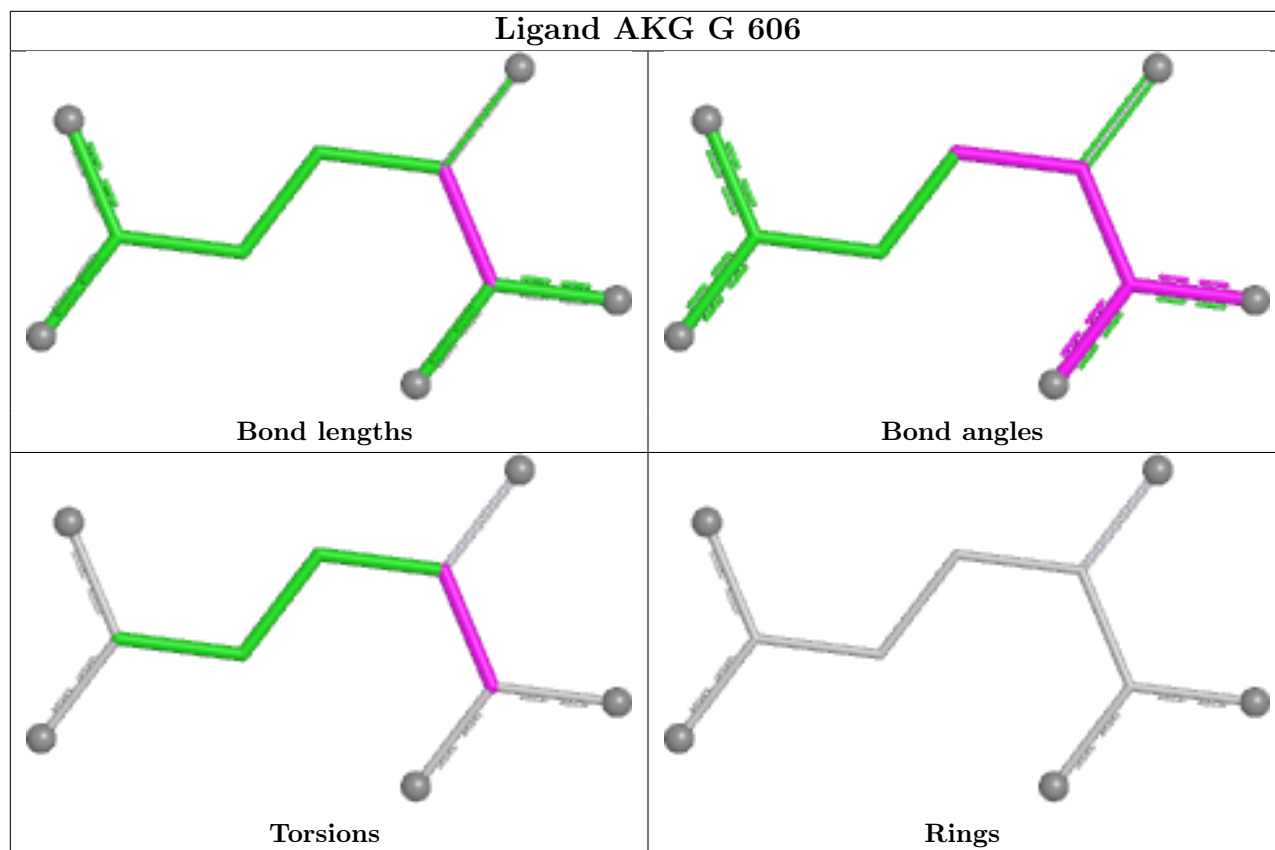


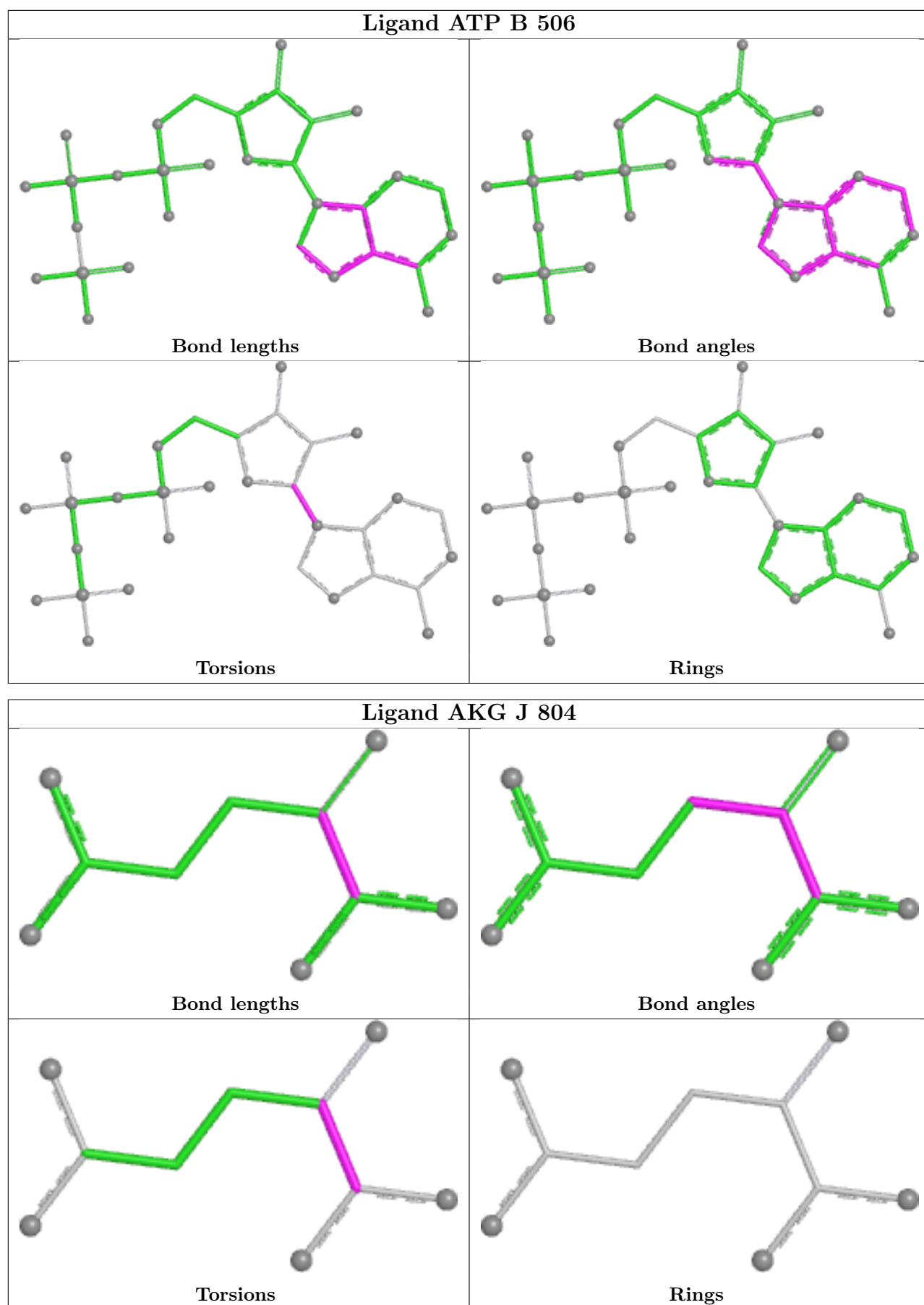


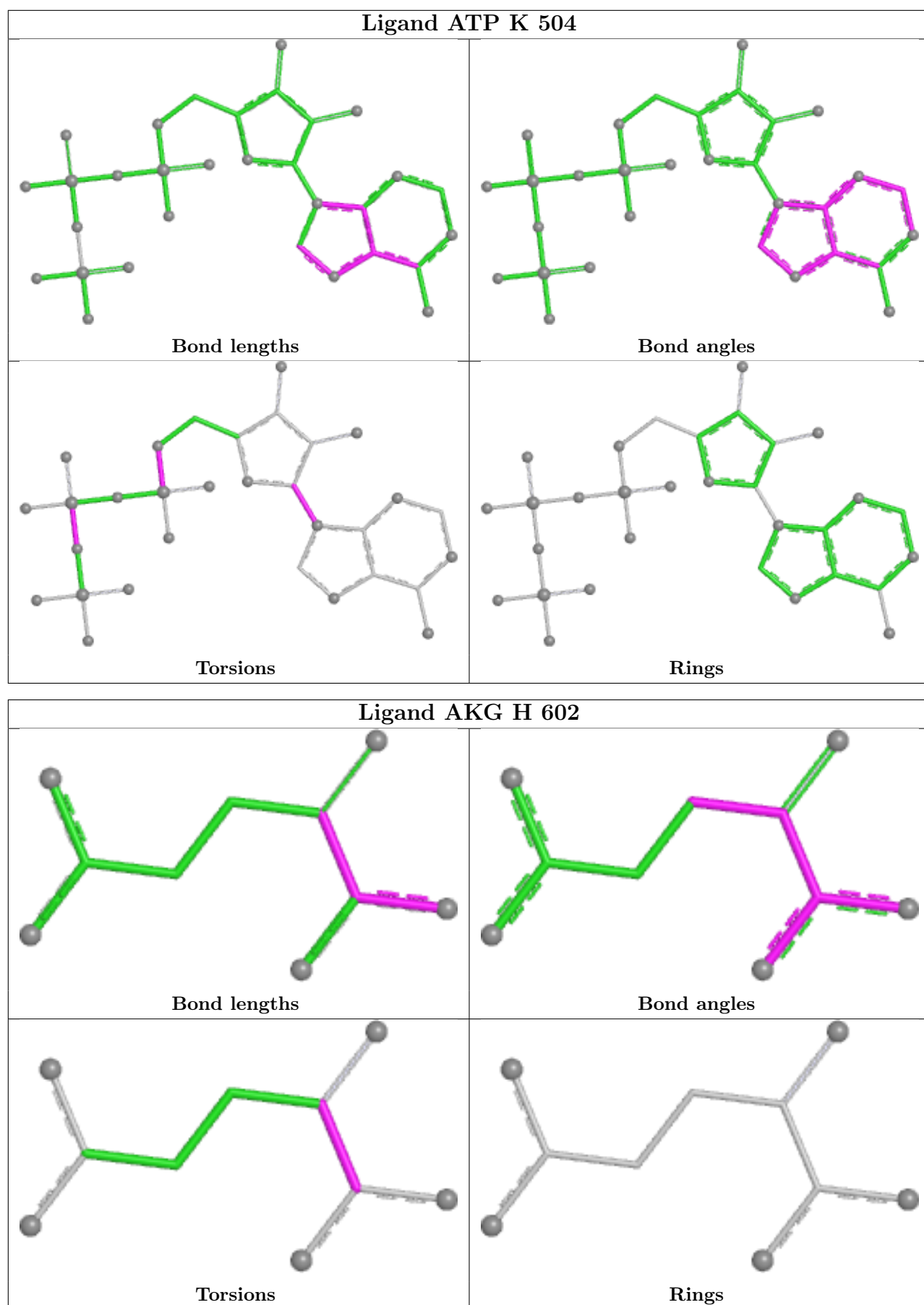


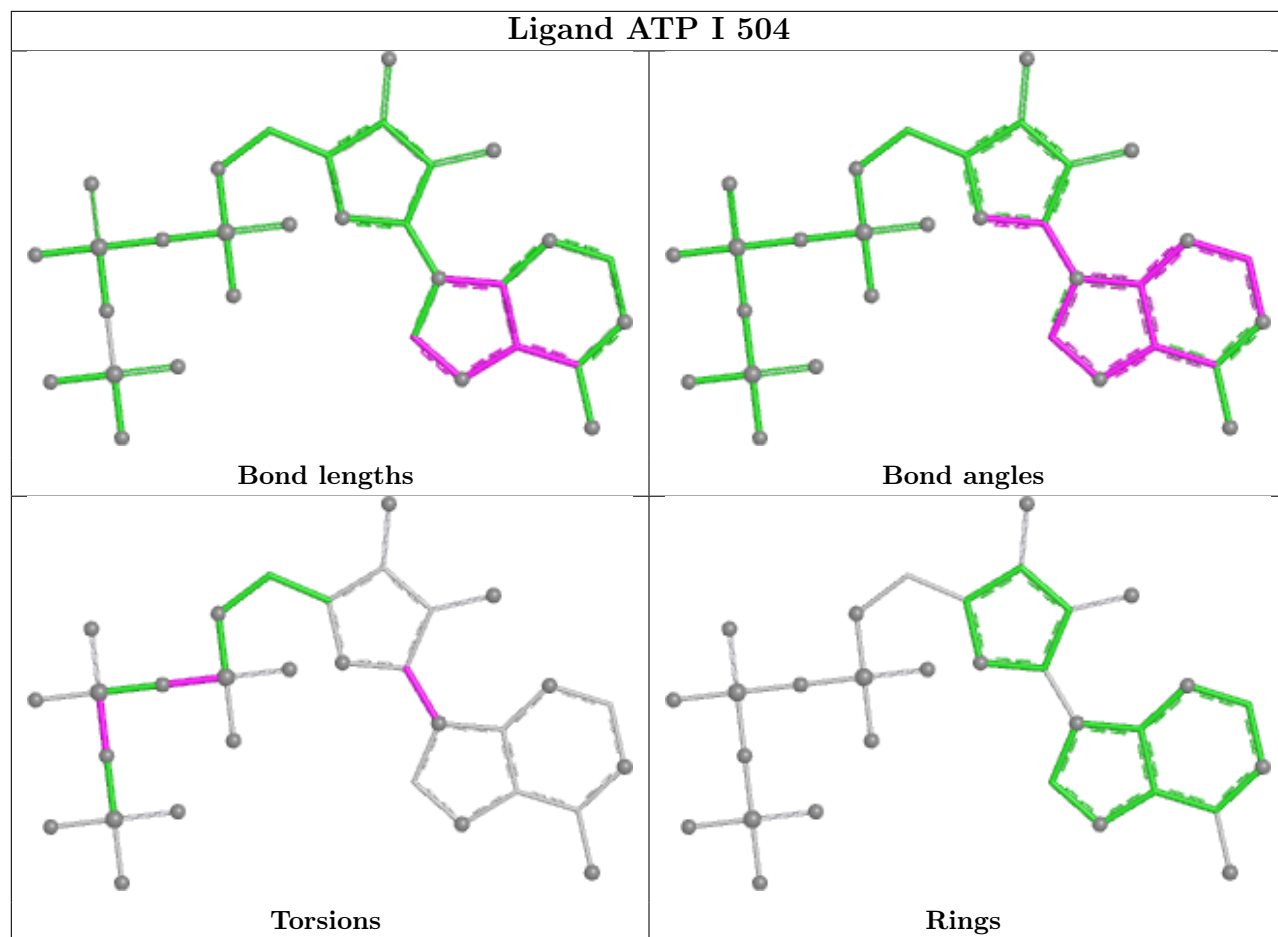


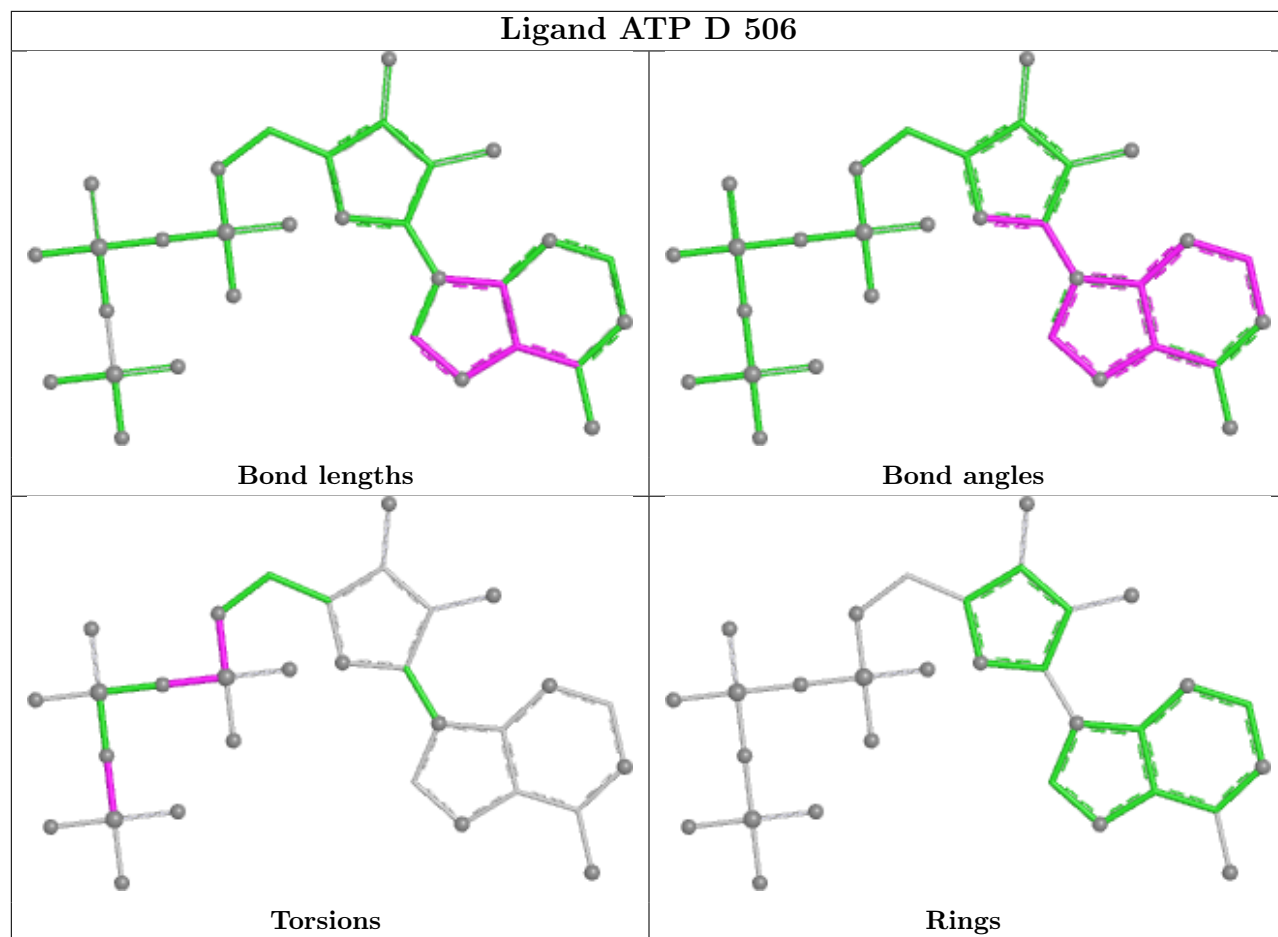


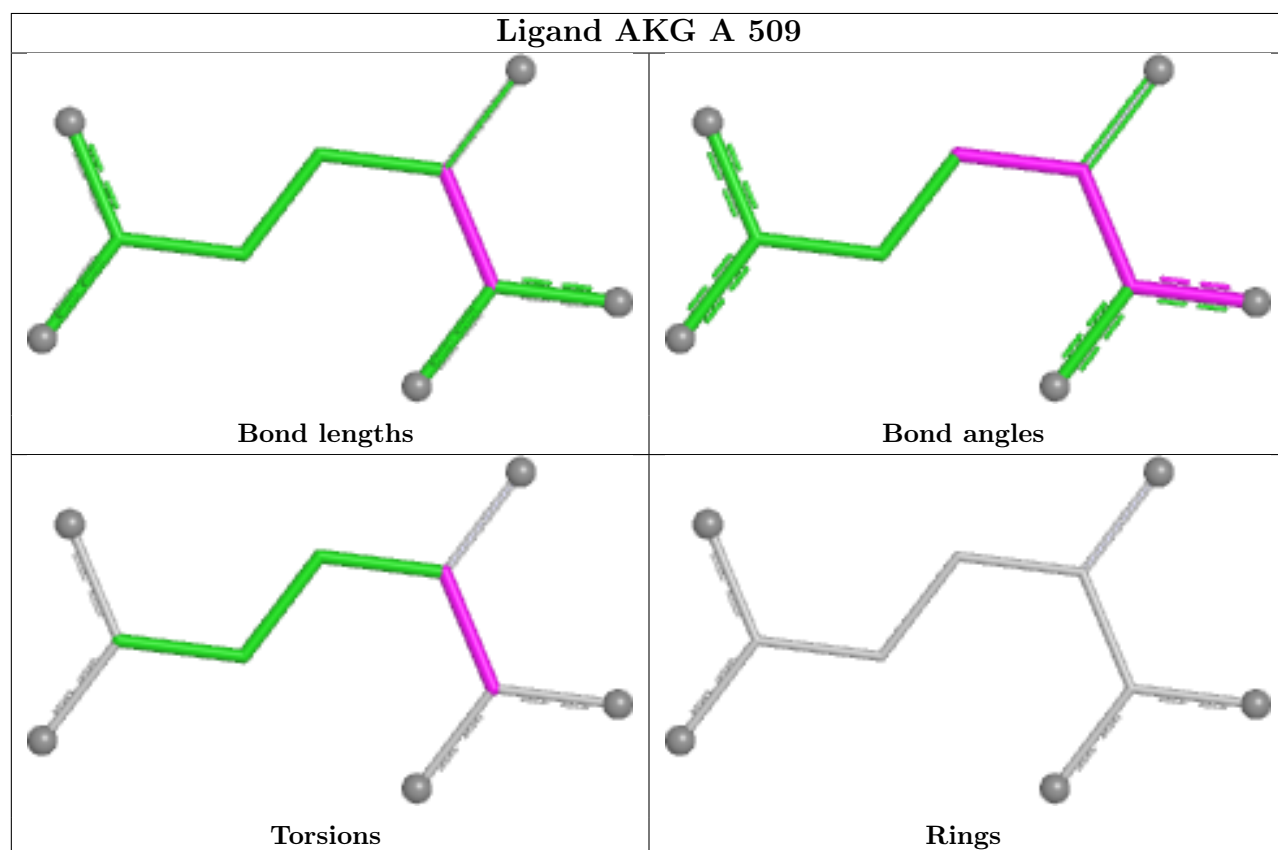
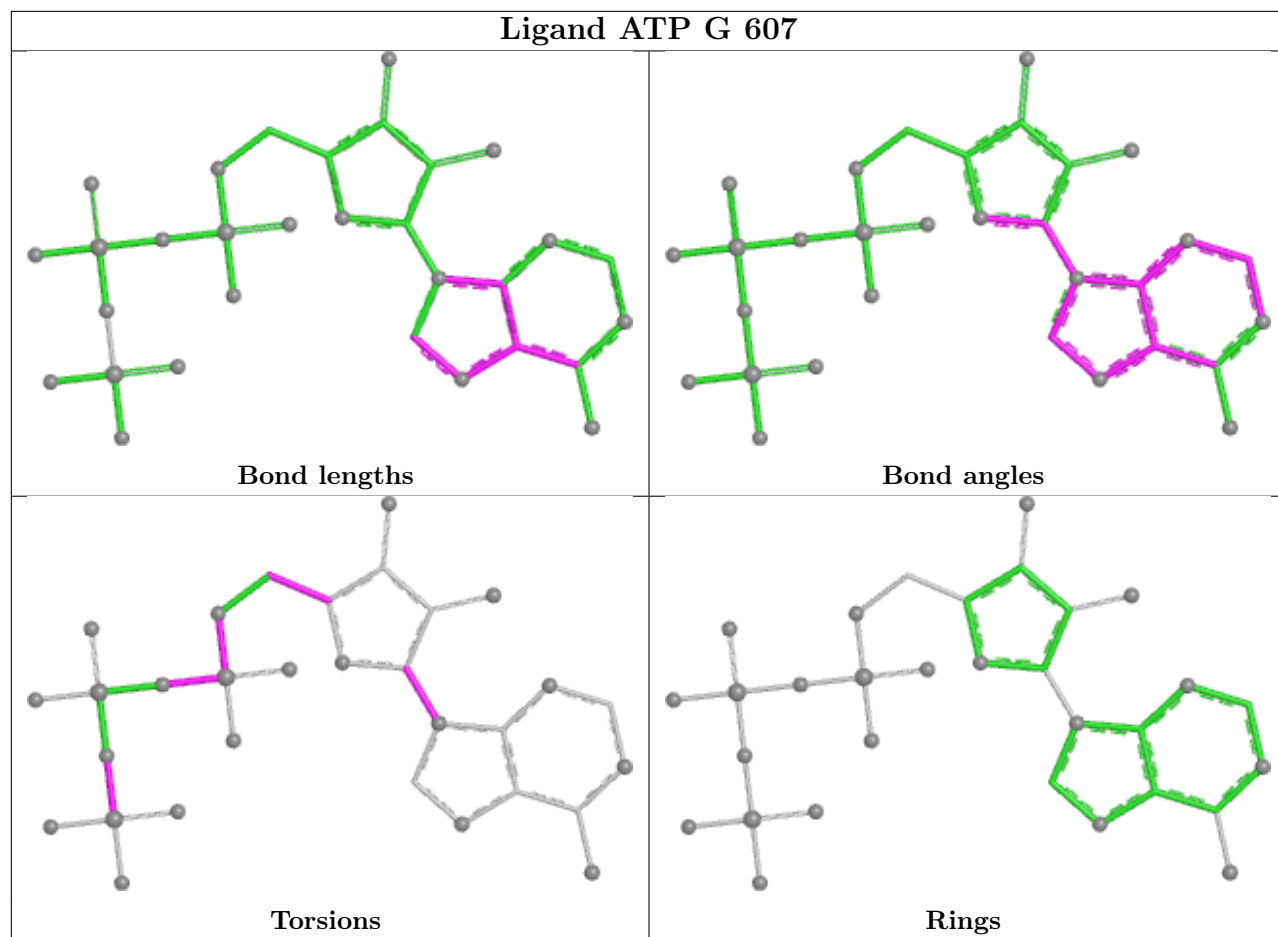


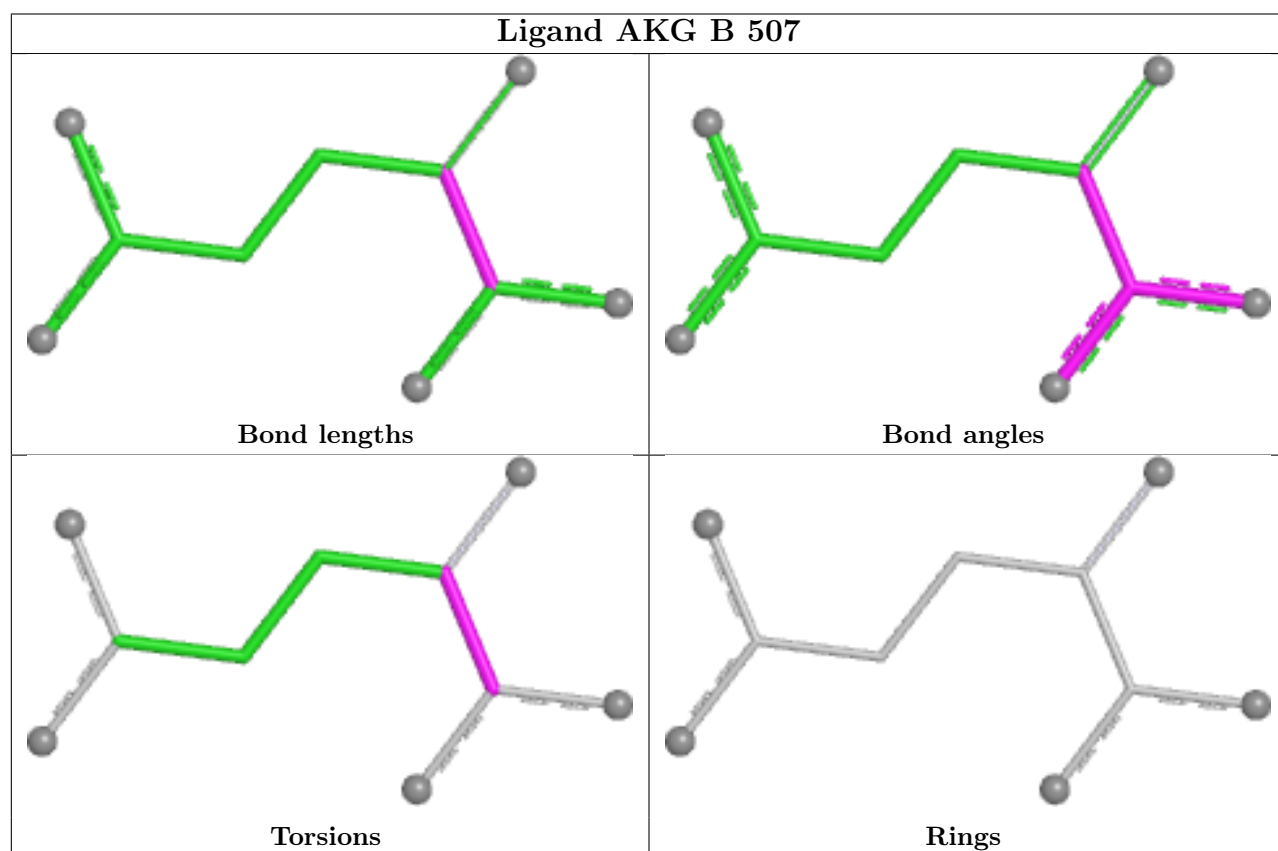
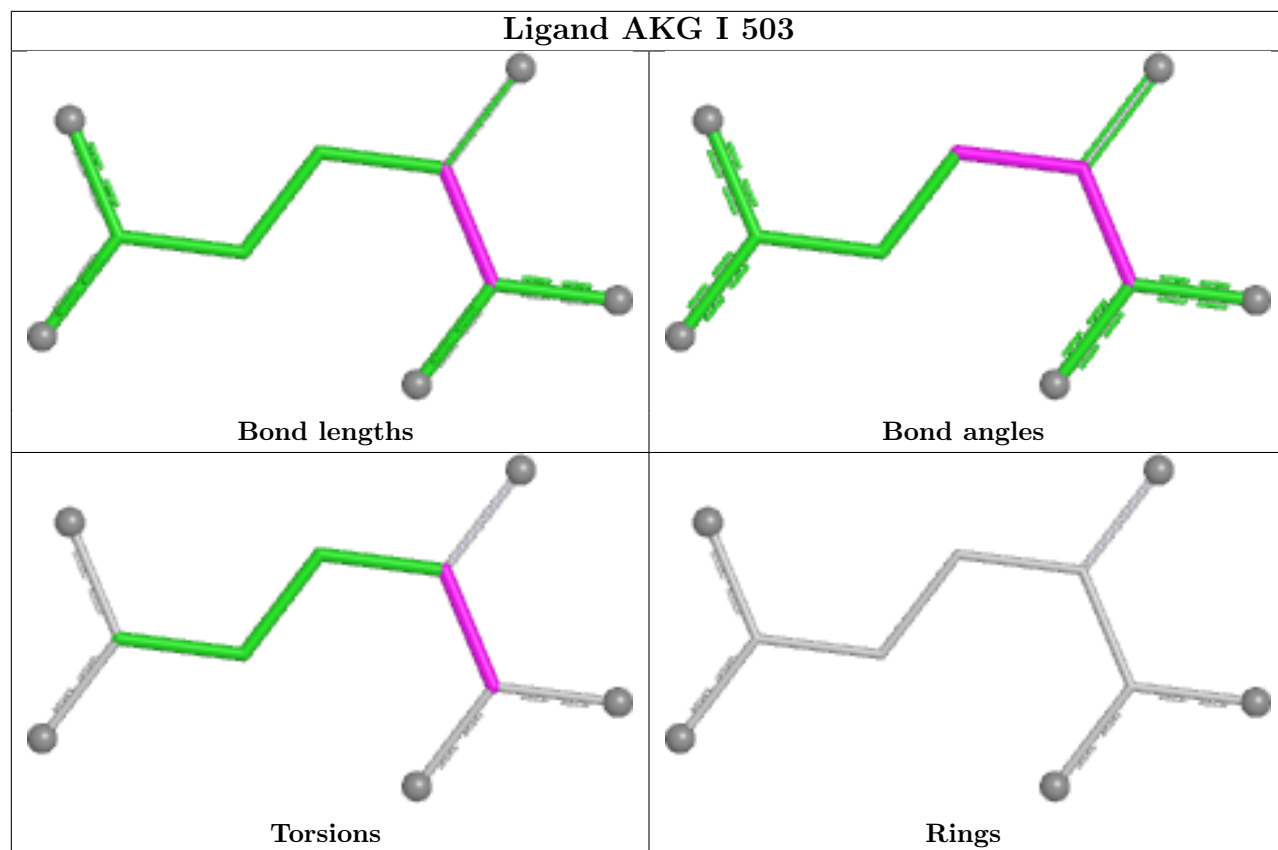


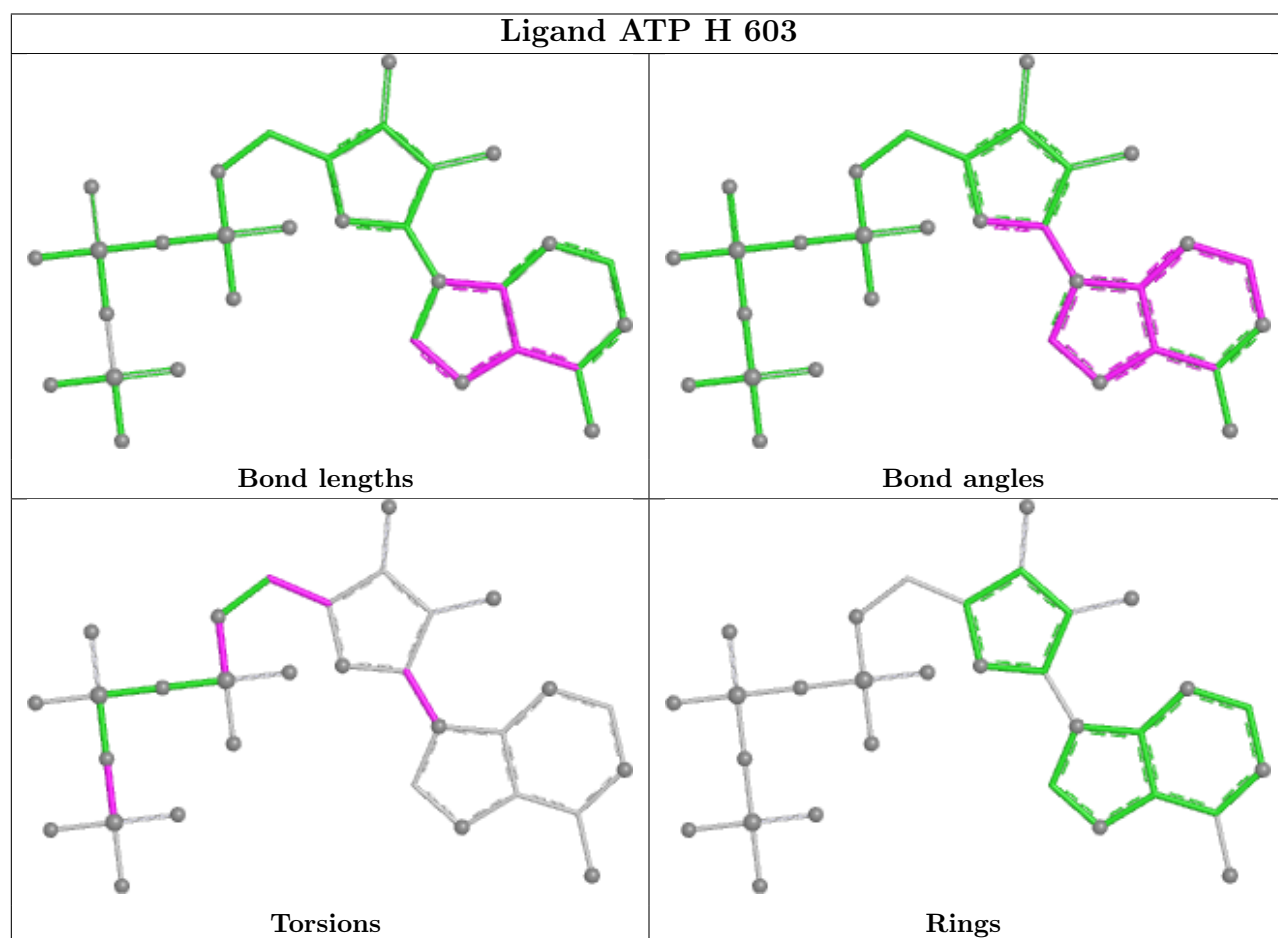
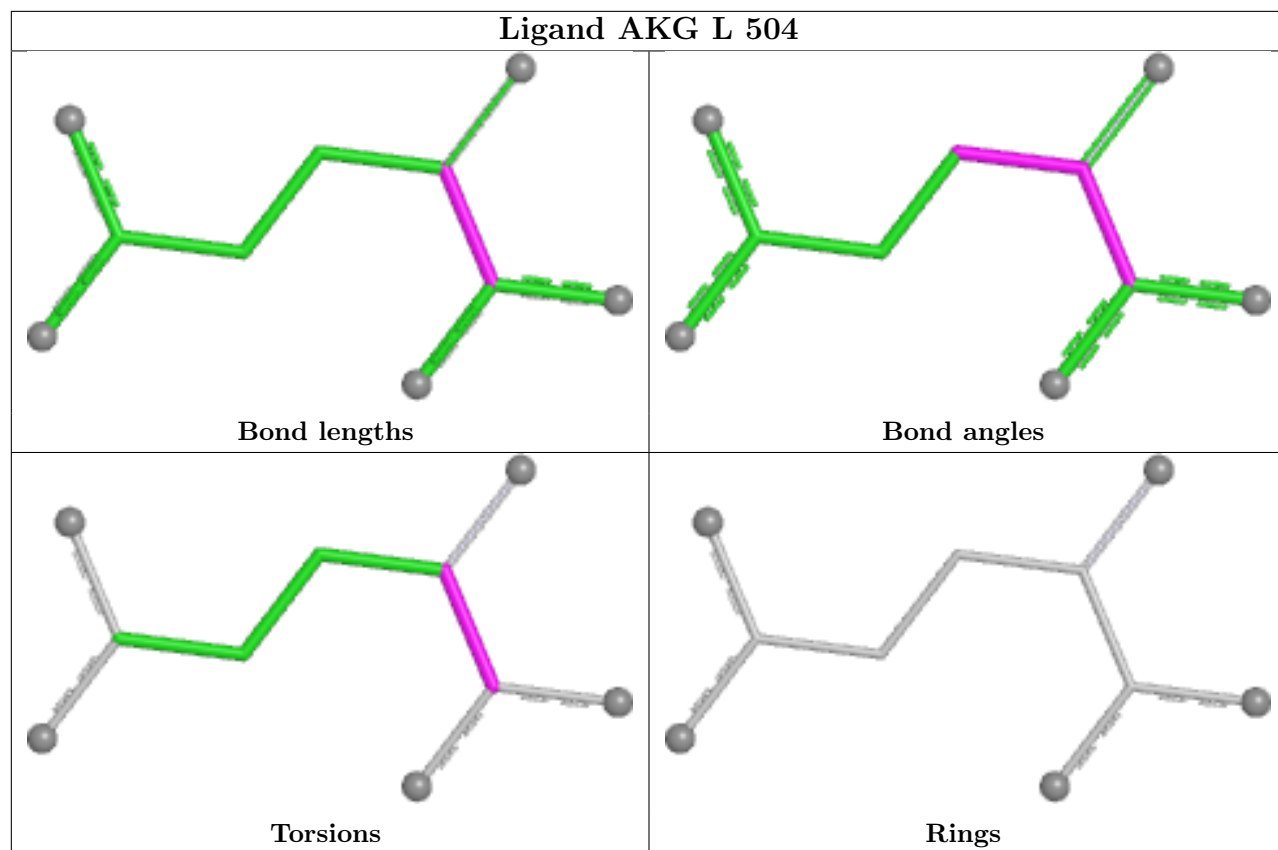


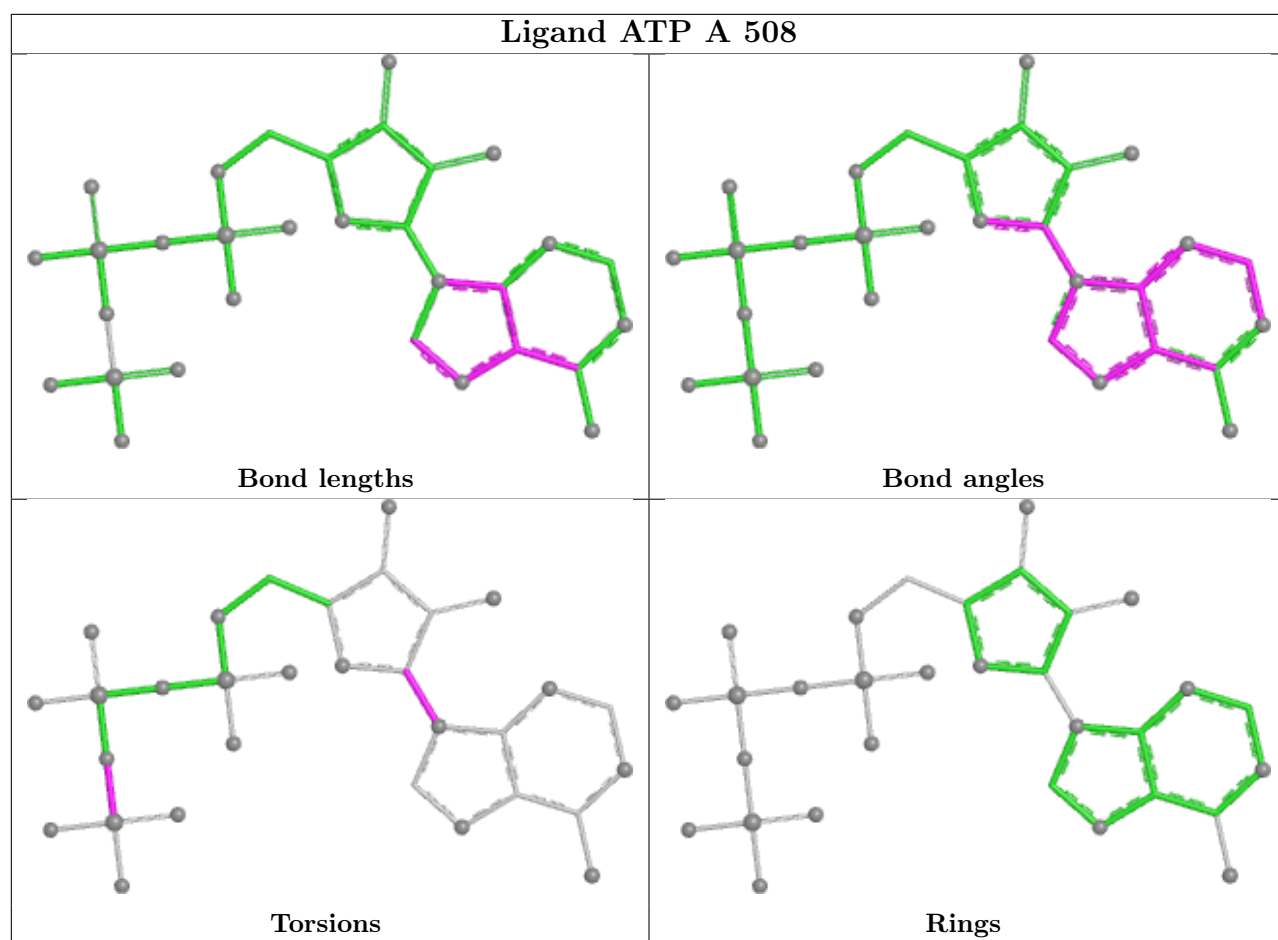












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/448 (99%)	-0.39	0 100 100	22, 33, 58, 81	0
1	B	447/448 (99%)	-0.41	2 (0%) 88 91	21, 34, 58, 78	0
1	C	447/448 (99%)	-0.31	1 (0%) 91 93	22, 35, 62, 78	0
1	D	447/448 (99%)	-0.35	3 (0%) 84 86	20, 32, 58, 76	1 (0%)
1	E	447/448 (99%)	-0.37	2 (0%) 88 91	21, 33, 59, 78	0
1	F	447/448 (99%)	-0.40	2 (0%) 88 91	22, 34, 57, 79	1 (0%)
1	G	447/448 (99%)	-0.32	3 (0%) 84 86	22, 36, 63, 83	0
1	H	447/448 (99%)	-0.25	4 (0%) 81 84	23, 35, 68, 89	0
1	I	447/448 (99%)	-0.30	2 (0%) 88 91	24, 36, 62, 81	0
1	J	447/448 (99%)	-0.39	0 100 100	21, 32, 58, 79	0
1	K	447/448 (99%)	-0.33	2 (0%) 88 91	23, 34, 58, 75	0
1	L	447/448 (99%)	-0.38	1 (0%) 91 93	23, 35, 60, 80	0
All	All	5364/5376 (99%)	-0.35	22 (0%) 88 91	20, 34, 61, 89	2 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	6.3
1	F	2	SER	5.8
1	H	2	SER	3.1
1	L	2	SER	3.1
1	I	148	HIS	2.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MOE	B	503	5/5	0.56	0.23	47,48,49,50	0
2	EDO	G	605	4/4	0.59	0.29	62,62,62,62	4
8	MG	E	602	1/1	0.61	0.36	50,50,50,50	1
3	PEG	D	504	7/7	0.62	0.24	52,54,57,58	7
3	PEG	G	604	7/7	0.66	0.21	41,42,42,42	7
2	EDO	I	502	4/4	0.68	0.20	52,52,53,54	4
9	PG4	D	505	13/13	0.72	0.17	27,31,34,34	13
2	EDO	H	601	4/4	0.73	0.21	59,59,60,60	0
3	PEG	K	501	7/7	0.75	0.17	32,35,37,37	7
3	PEG	G	602	6/7	0.76	0.22	54,56,56,56	6
8	MG	K	502	1/1	0.76	0.26	31,31,31,31	1
2	EDO	J	803	4/4	0.76	0.18	59,59,59,60	0
9	PG4	D	501	13/13	0.77	0.17	40,43,48,49	13
2	EDO	B	501	4/4	0.77	0.11	32,34,35,37	0
2	EDO	L	501	4/4	0.78	0.15	42,42,42,42	4
2	EDO	F	501	4/4	0.79	0.14	42,44,44,44	0
3	PEG	G	601	7/7	0.79	0.19	54,55,56,56	7
4	GOL	A	507	6/6	0.80	0.12	74,75,75,75	0
2	EDO	L	503	4/4	0.80	0.15	51,51,51,52	4
2	EDO	D	502	4/4	0.82	0.20	63,64,64,64	0
7	MOE	F	507	5/5	0.82	0.16	57,58,59,59	0
2	EDO	C	603	4/4	0.82	0.17	43,44,45,46	0
3	PEG	J	801	7/7	0.82	0.19	51,54,55,55	7
2	EDO	F	502	4/4	0.82	0.12	34,35,35,35	0
2	EDO	F	504	4/4	0.82	0.13	56,56,57,57	0
2	EDO	E	601	4/4	0.83	0.18	75,75,75,75	0
3	PEG	A	504	7/7	0.83	0.16	58,61,62,62	7
3	PEG	D	503	7/7	0.83	0.19	56,57,58,58	7
2	EDO	L	502	4/4	0.83	0.25	55,56,56,57	4
2	EDO	B	502	4/4	0.84	0.20	42,42,42,43	4
2	EDO	J	802	4/4	0.85	0.13	56,56,57,57	0
2	EDO	I	501	4/4	0.85	0.18	48,49,50,50	4

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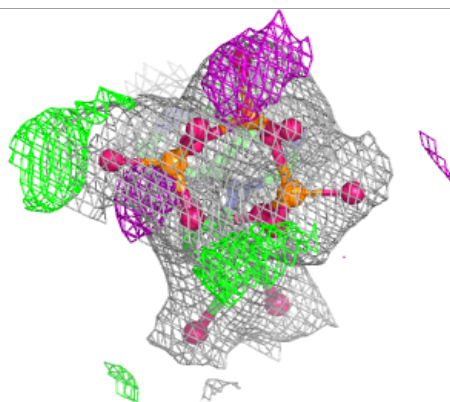
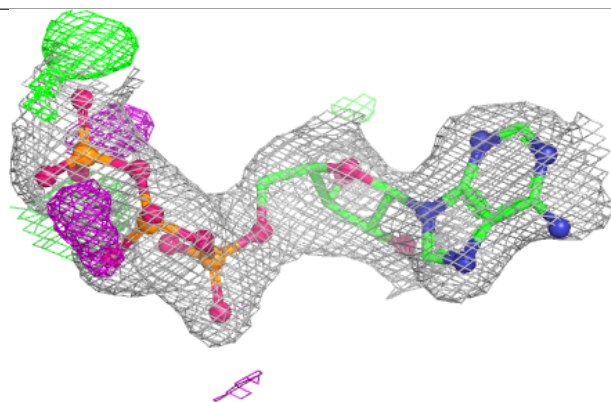
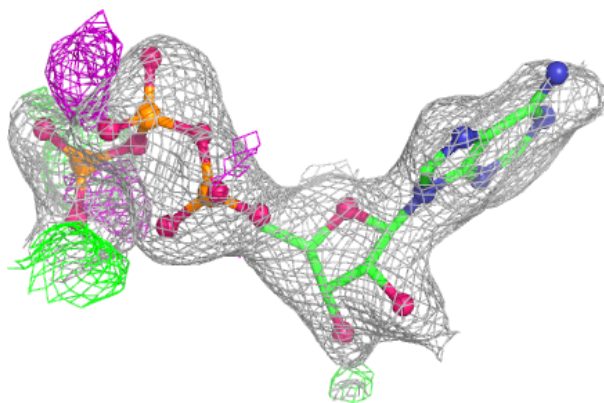
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	502	7/7	0.86	0.16	49,49,50,50	7
2	EDO	A	506	4/4	0.86	0.13	37,40,41,41	0
2	EDO	C	602	4/4	0.87	0.10	23,24,25,26	4
2	EDO	A	505	4/4	0.87	0.10	36,38,40,42	0
2	EDO	B	504	4/4	0.88	0.11	57,57,58,59	0
3	PEG	G	603	7/7	0.89	0.14	53,54,55,55	7
5	ATP	B	506	31/31	0.90	0.08	41,45,63,64	0
5	ATP	H	603	31/31	0.90	0.08	45,56,76,76	0
2	EDO	C	601	4/4	0.91	0.13	53,53,54,55	0
5	ATP	L	505	31/31	0.91	0.07	37,42,61,61	0
5	ATP	D	506	31/31	0.91	0.08	35,40,62,63	0
5	ATP	E	604	31/31	0.91	0.07	42,46,66,66	0
5	ATP	A	508	31/31	0.92	0.07	39,41,61,61	0
5	ATP	I	504	31/31	0.92	0.07	40,44,62,63	0
5	ATP	J	805	31/31	0.92	0.08	39,46,65,66	0
2	EDO	A	503	4/4	0.92	0.17	54,55,55,55	4
5	ATP	G	607	31/31	0.92	0.08	43,50,67,68	0
2	EDO	I	505	4/4	0.93	0.10	47,48,48,48	0
5	ATP	C	604	31/31	0.93	0.07	45,48,65,65	0
2	EDO	F	503	4/4	0.93	0.09	53,53,54,54	0
2	EDO	A	501	4/4	0.93	0.09	45,46,48,49	0
5	ATP	K	504	31/31	0.93	0.08	39,44,65,67	0
5	ATP	F	506	31/31	0.93	0.07	40,45,66,68	0
8	MG	B	505	1/1	0.94	0.49	49,49,49,49	1
6	AKG	H	602	10/10	0.95	0.07	33,34,36,37	0
6	AKG	F	505	10/10	0.96	0.06	32,33,34,36	0
6	AKG	I	503	10/10	0.96	0.06	28,33,38,39	0
6	AKG	G	606	10/10	0.96	0.06	29,31,34,35	0
6	AKG	E	603	10/10	0.97	0.06	27,31,35,36	0
6	AKG	A	509	10/10	0.97	0.05	31,32,33,34	0
6	AKG	B	507	10/10	0.97	0.06	28,30,34,34	0
6	AKG	C	605	10/10	0.97	0.06	30,30,32,32	0
6	AKG	D	507	10/10	0.97	0.05	32,34,36,37	0
6	AKG	J	804	10/10	0.97	0.06	27,29,30,31	0
6	AKG	K	503	10/10	0.97	0.06	31,34,37,38	0
6	AKG	L	504	10/10	0.98	0.05	31,32,32,33	0

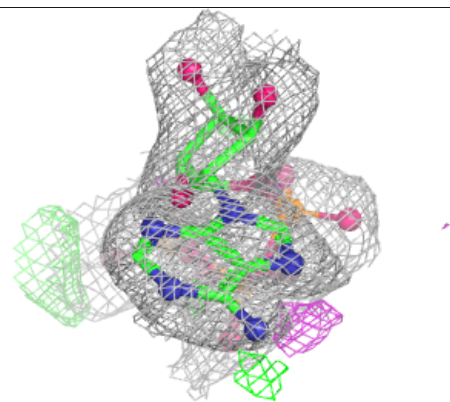
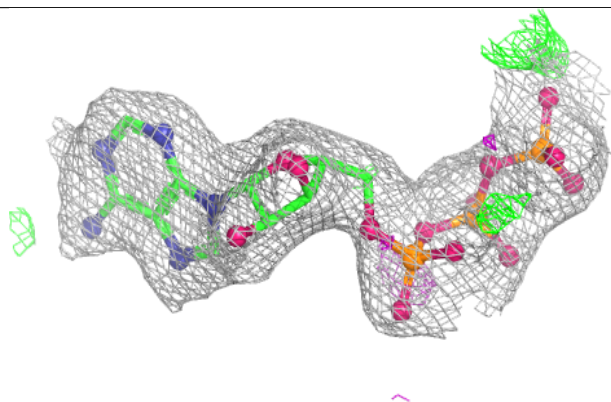
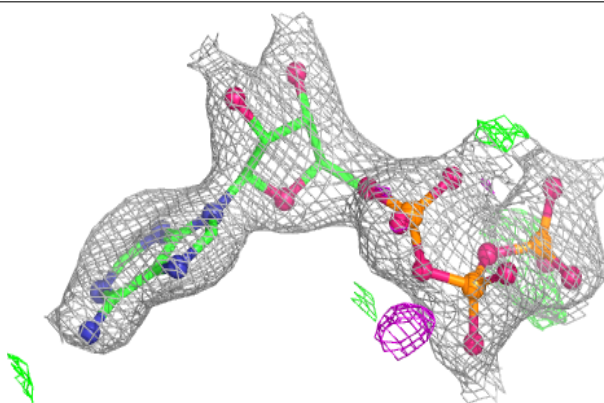
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 506:

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

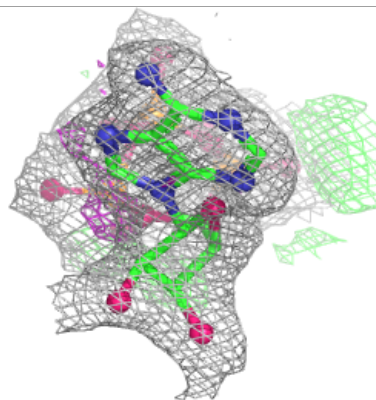
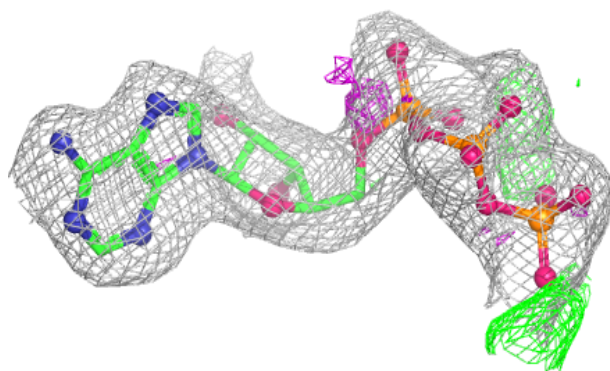
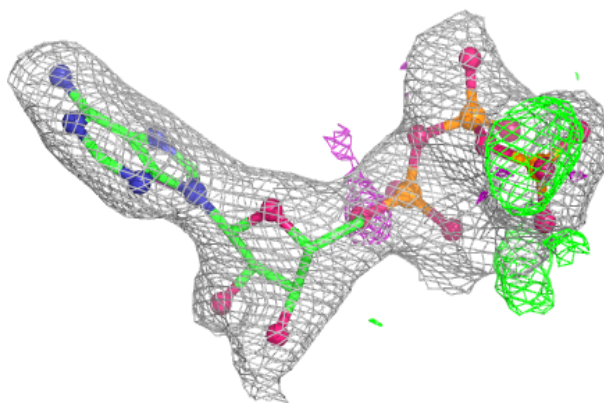
**Electron density around ATP H 603:**

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

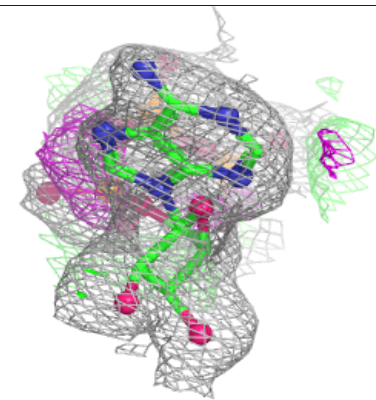
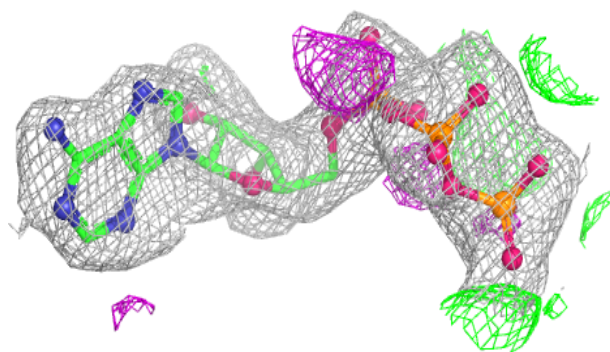
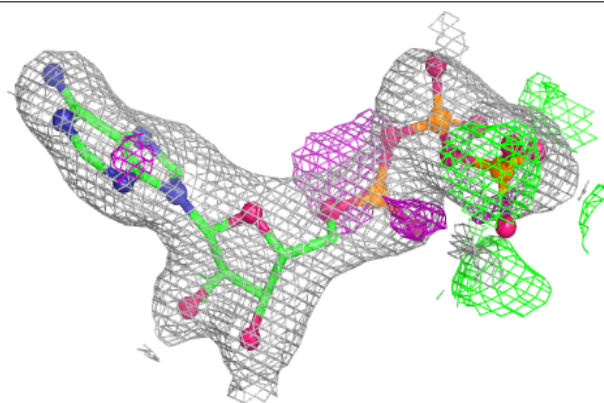


Electron density around ATP L 505:

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

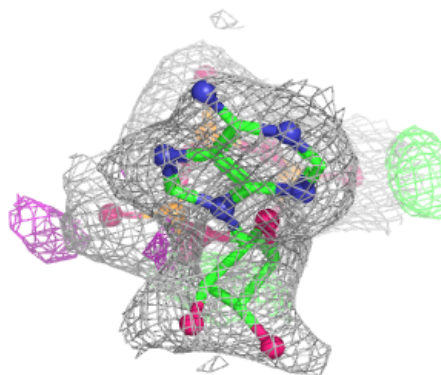
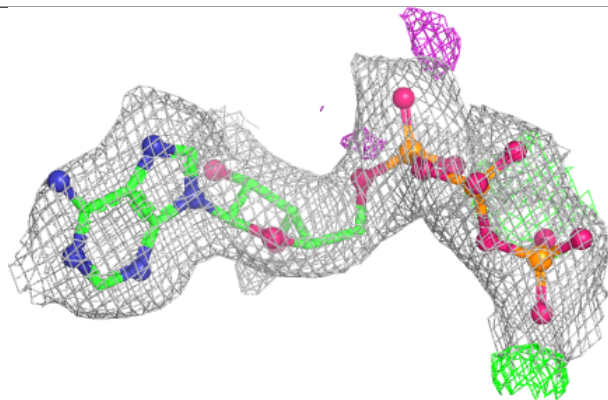
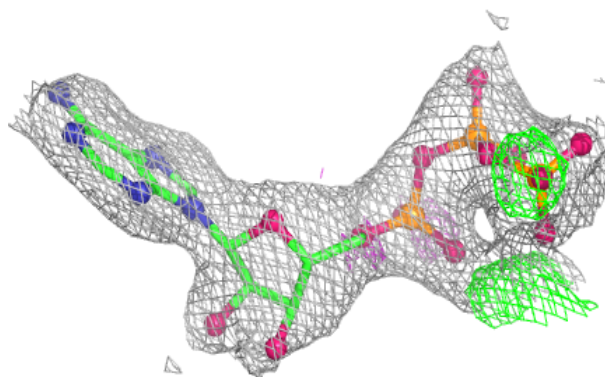
**Electron density around ATP D 506:**

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

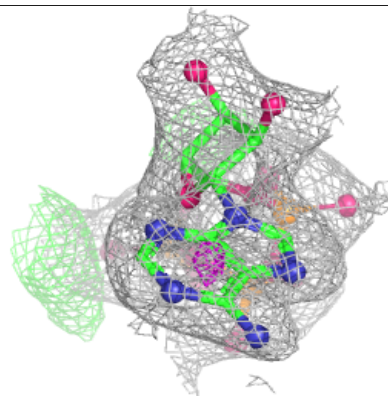
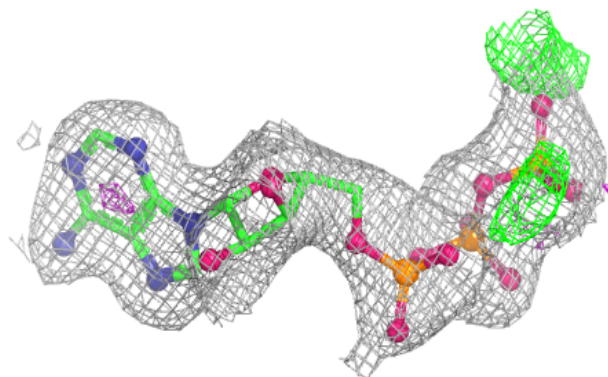
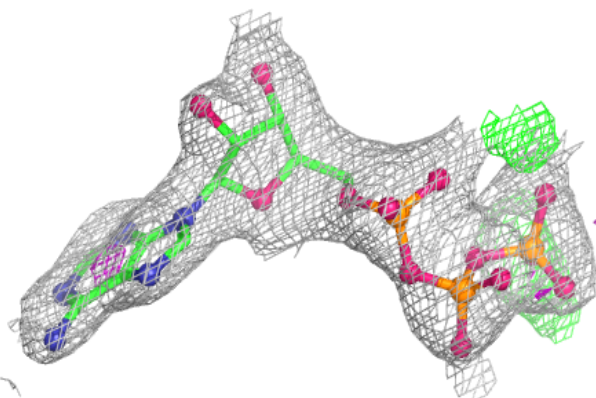


Electron density around ATP E 604:

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

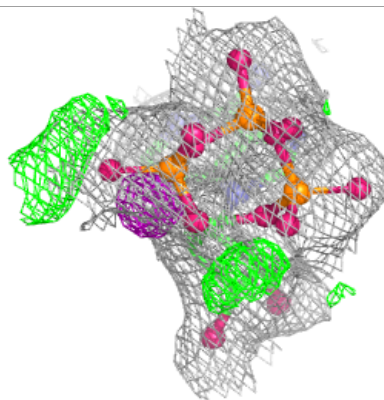
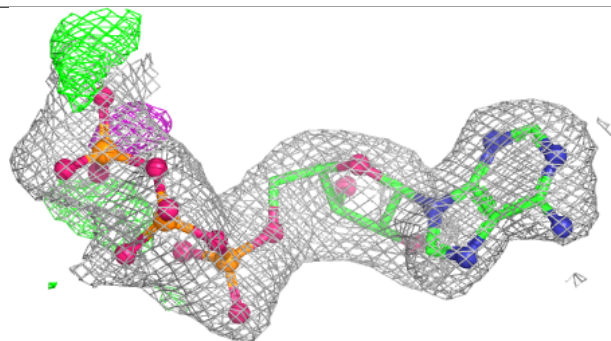
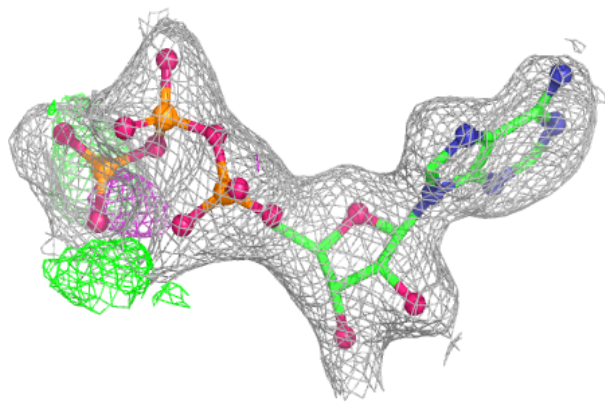
**Electron density around ATP A 508:**

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

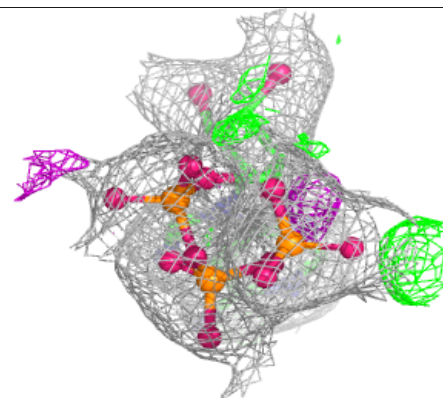
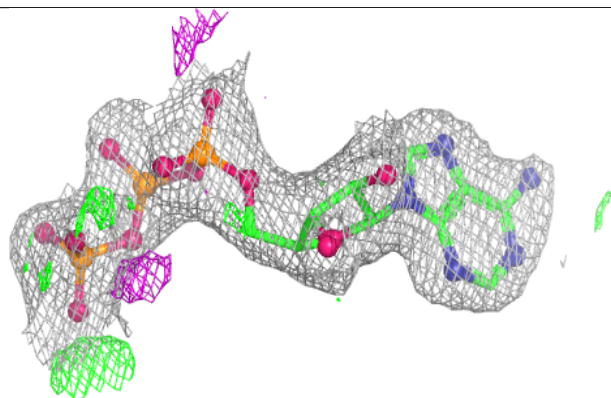
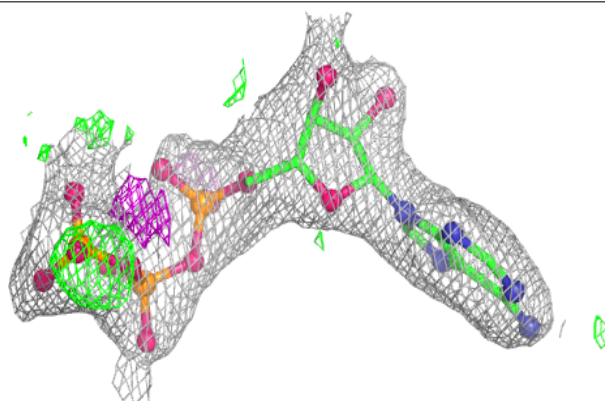


Electron density around ATP I 504:

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and green (positive)

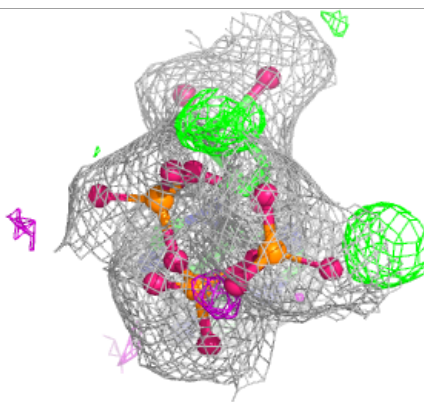
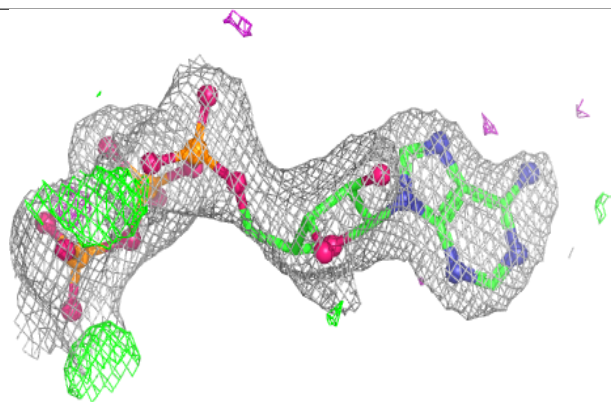
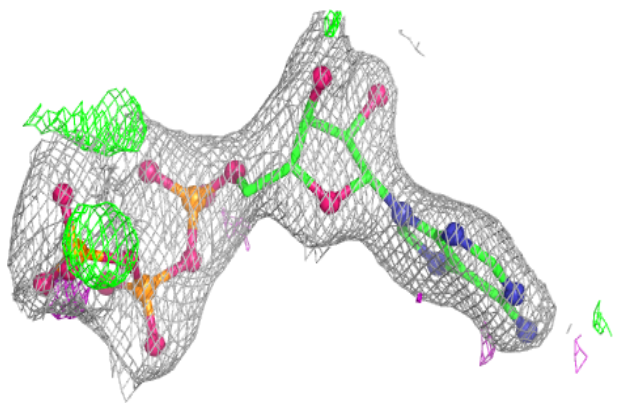
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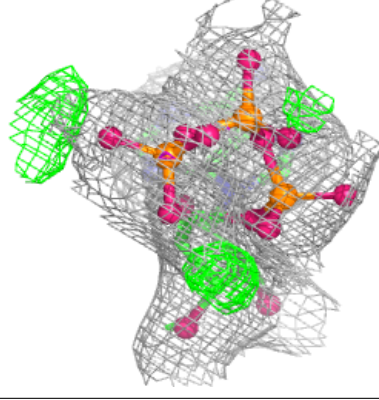
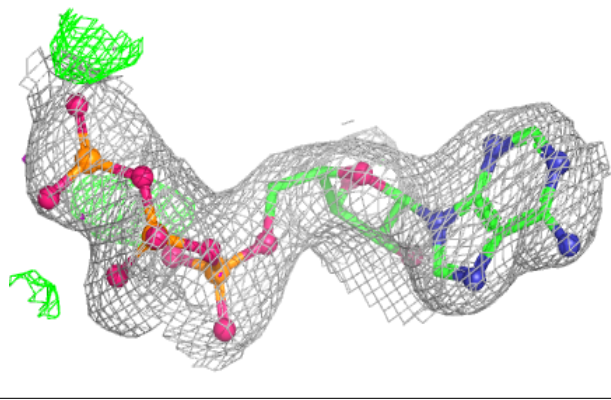
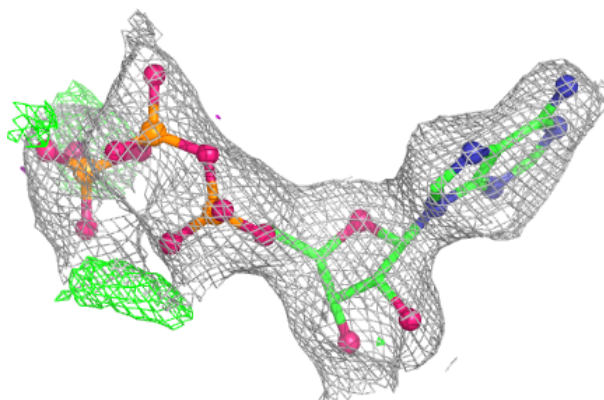


Electron density around ATP G 607:

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

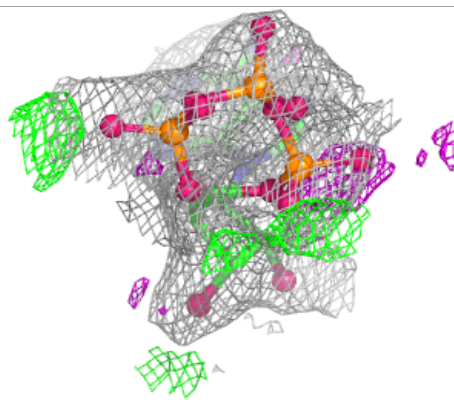
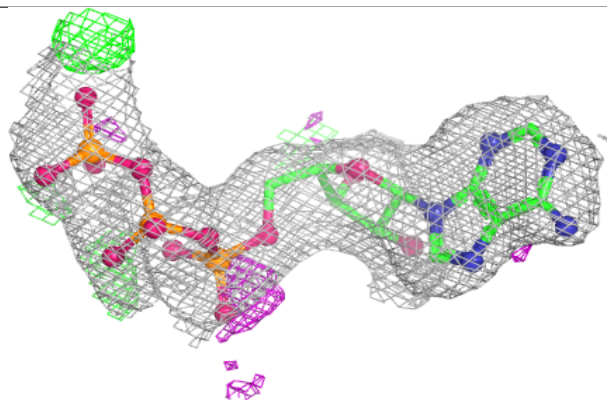
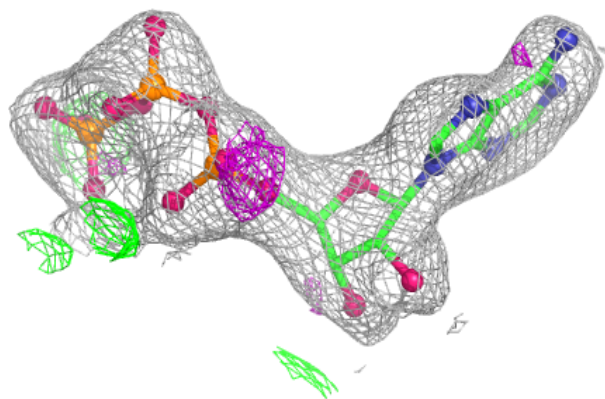
**Electron density around ATP C 604:**

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

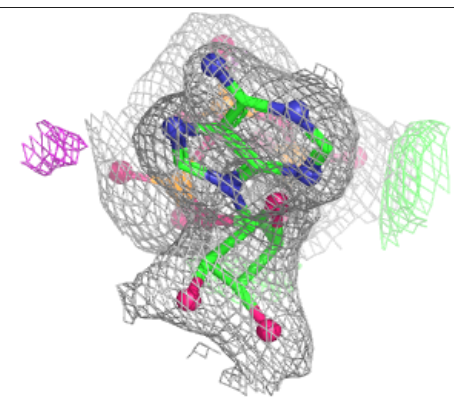
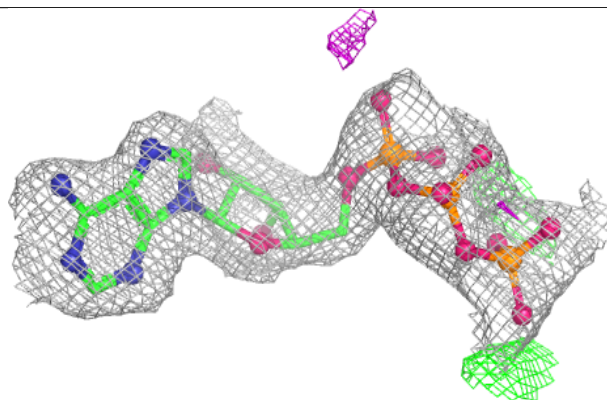
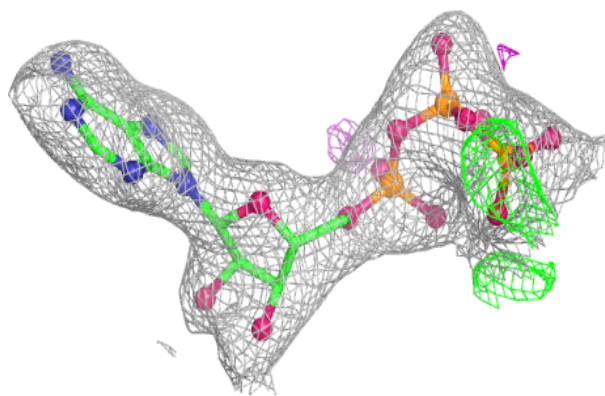


Electron density around ATP K 504:

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and green (positive)

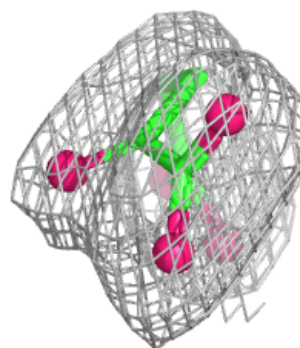
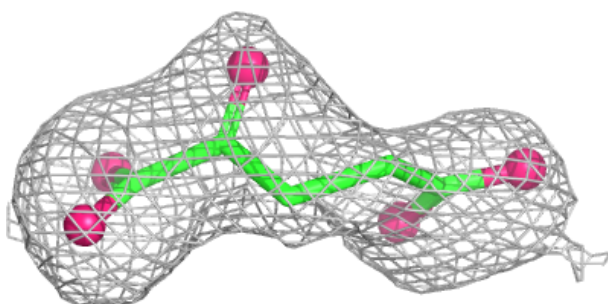
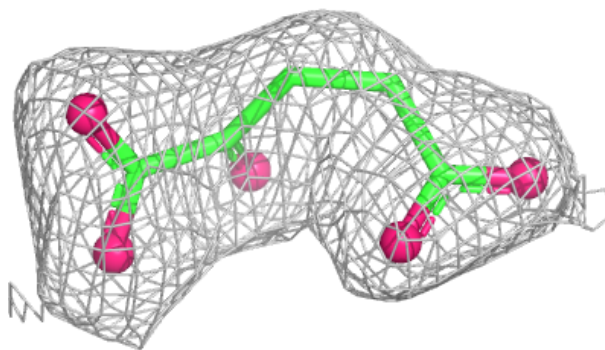
**Electron density around ATP F 506:**

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

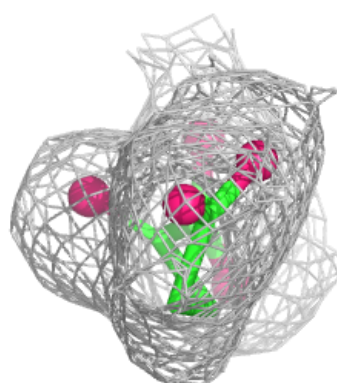
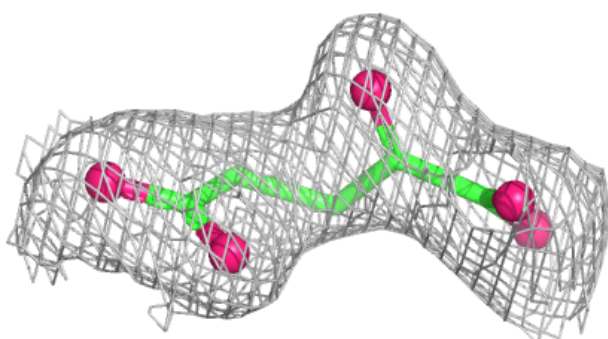
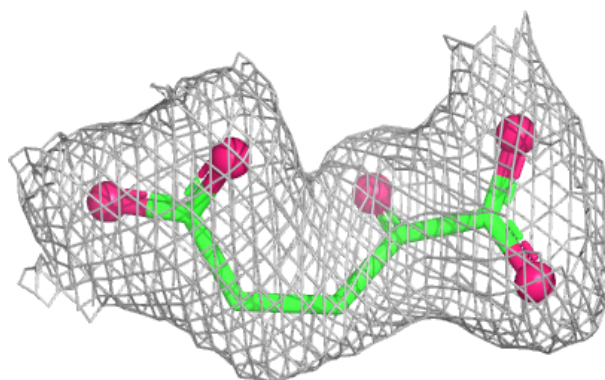


Electron density around AKG H 602:

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

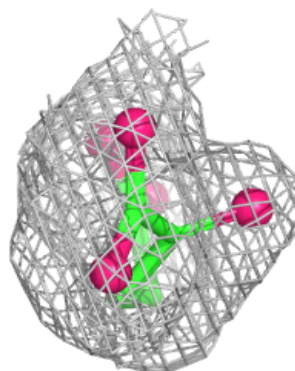
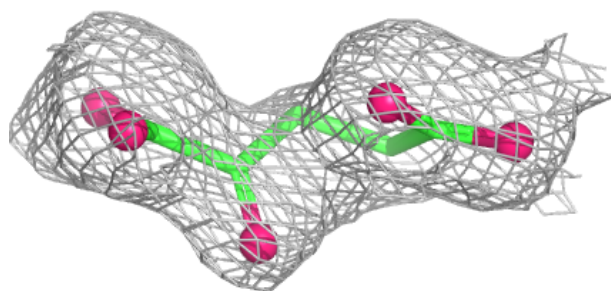
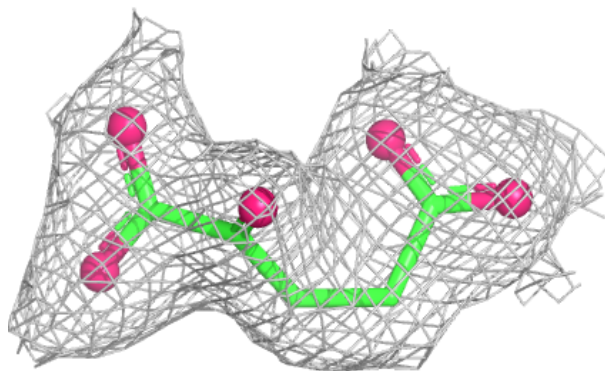
**Electron density around AKG F 505:**

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

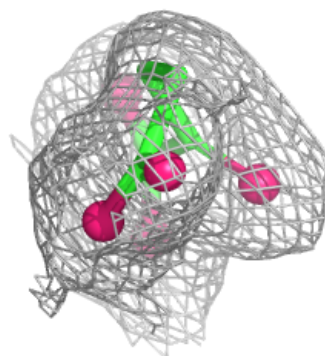
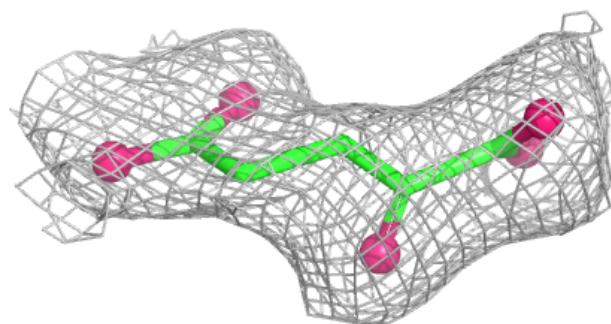
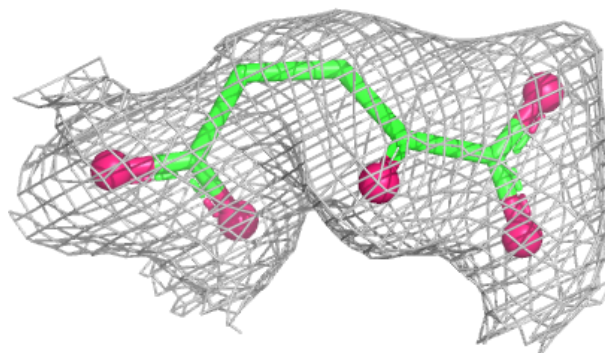


Electron density around AKG I 503:

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

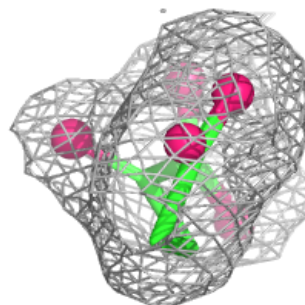
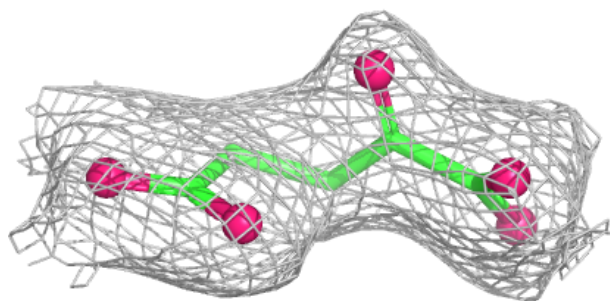
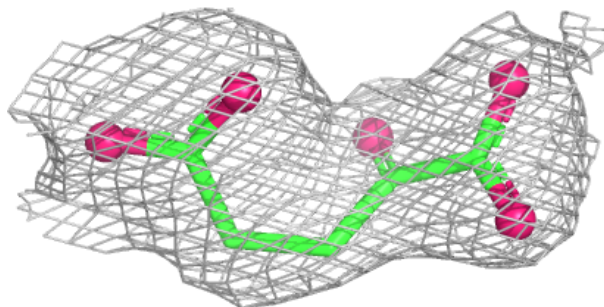
**Electron density around AKG G 606:**

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

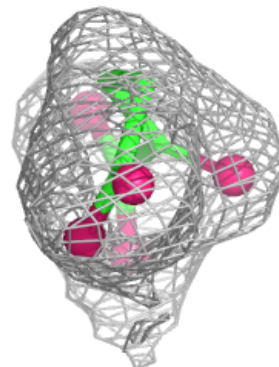
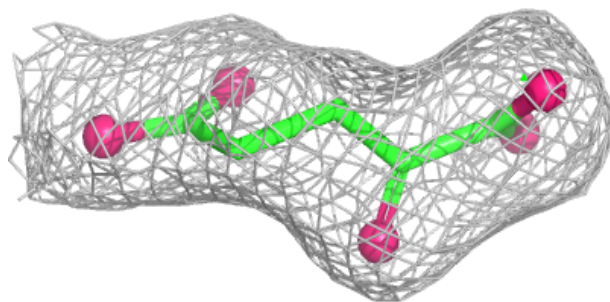
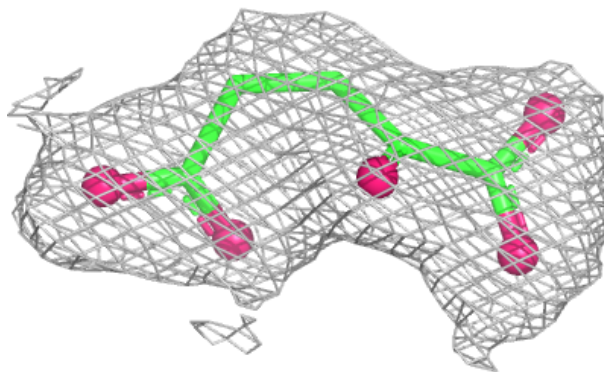


Electron density around AKG E 603:

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

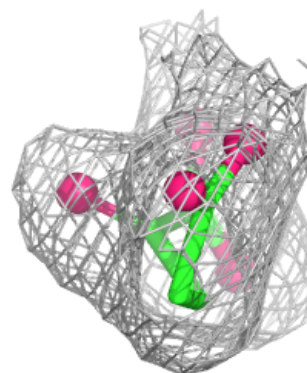
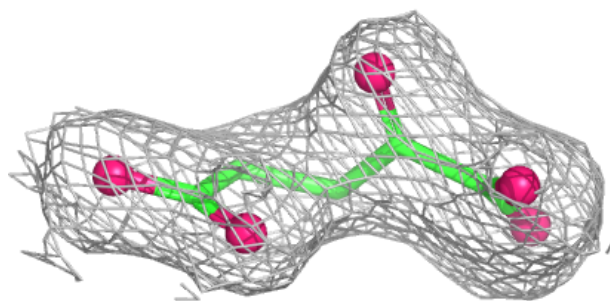
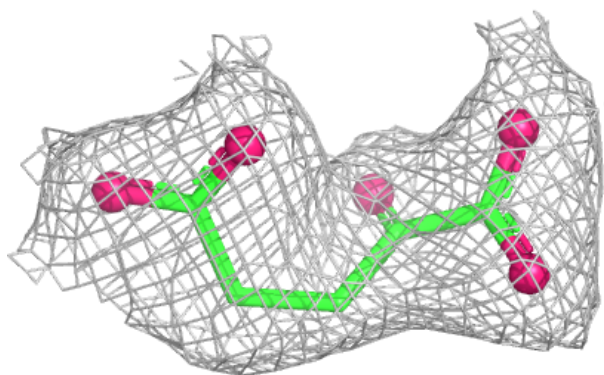
**Electron density around AKG A 509:**

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

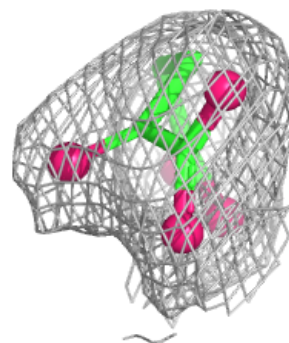
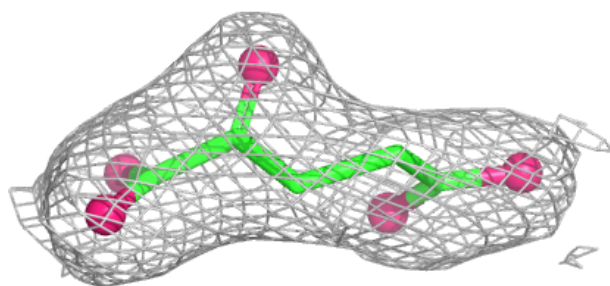
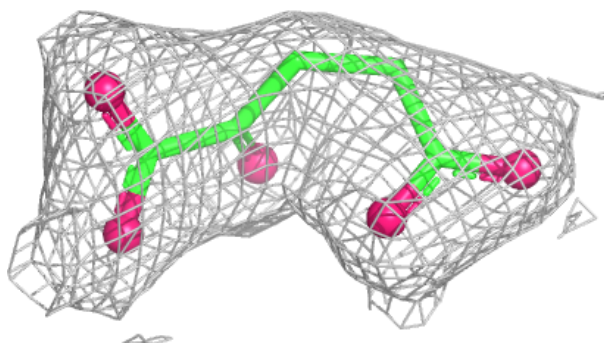


Electron density around AKG B 507:

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

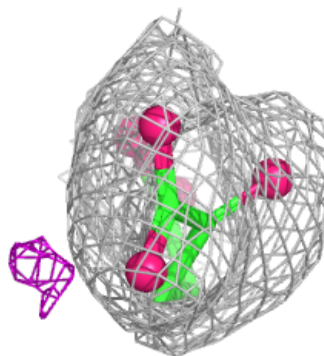
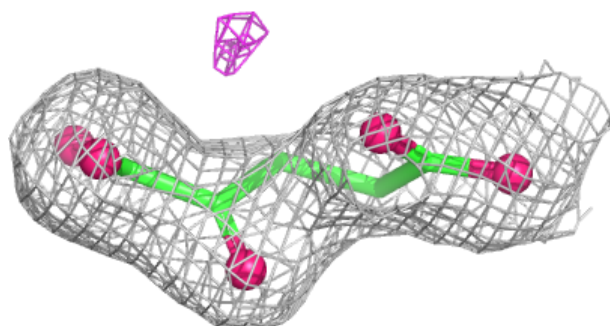
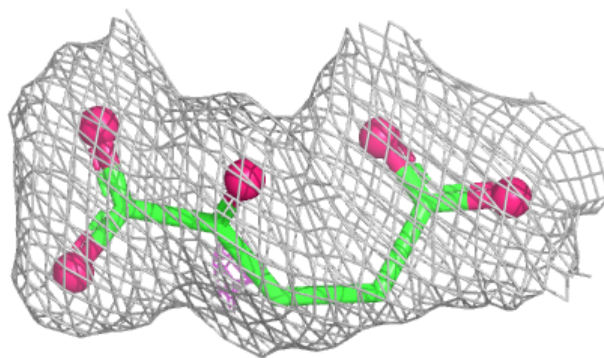
**Electron density around AKG C 605:**

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

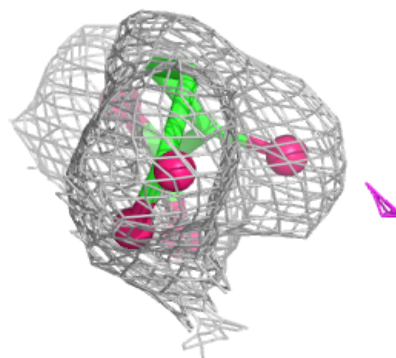
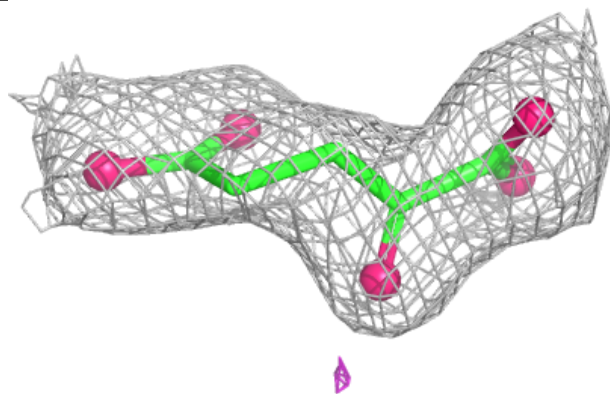
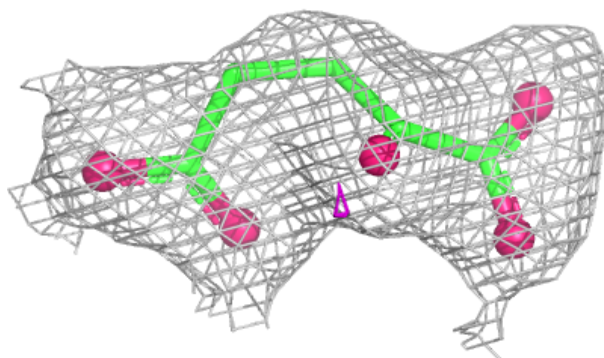


Electron density around AKG D 507:

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

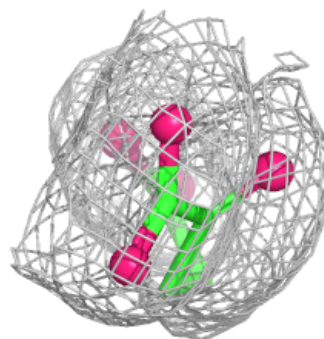
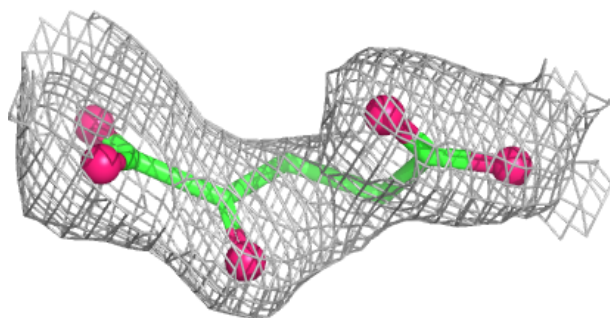
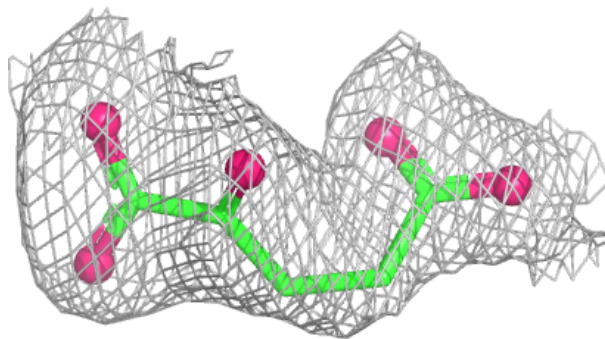
**Electron density around AKG J 804:**

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

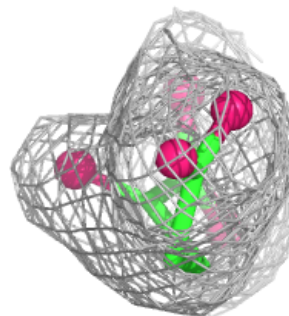
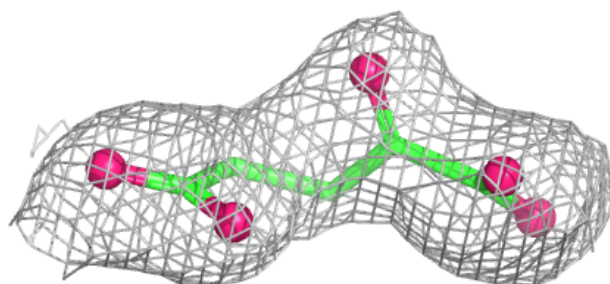
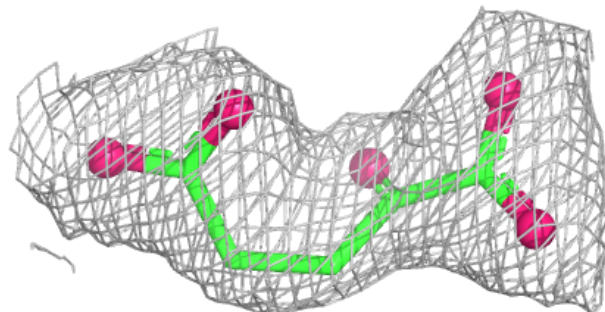


Electron density around AKG K 503:

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

**Electron density around AKG L 504:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.