



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 4V7N / pdb_00004v7n
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp., with transition state analog Mg(II)-ADP-NO₃-glycocyamine.
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.
Deposited on : 2009-12-15
Resolution : 2.30 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)
Xtriage (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

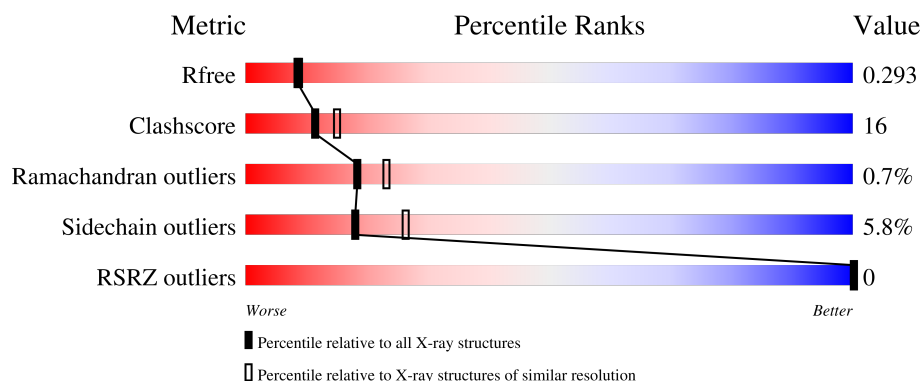
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

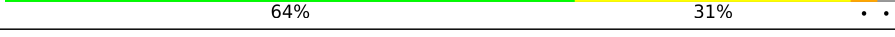
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	AA	390	
1	AB	390	
1	AC	390	
1	AD	390	
1	AE	390	

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Mol	Chain	Length	Quality of chain
1	AF	390	
1	AG	390	
1	AH	390	
1	AI	390	
1	AJ	390	
1	AK	390	
1	AL	390	
1	AM	390	
1	AN	390	
1	AO	390	
1	AP	390	
1	AQ	390	
1	AR	390	
1	BA	390	
1	BB	390	
1	BC	390	
1	BD	390	
1	BE	390	
1	BF	390	
1	BG	390	
1	BH	390	
1	BI	390	
1	BJ	390	
1	BK	390	
1	BL	390	

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Mol	Chain	Length	Quality of chain
1	BM	390	 63% 28% • 6%
1	BN	390	 62% 32% • •
1	BO	390	 66% 25% • 6%
1	BP	390	 67% 29% • •
1	BQ	390	 59% 33% • 6%
1	BR	390	 66% 30% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 113311 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 Glycocyamine kinase beta chain.

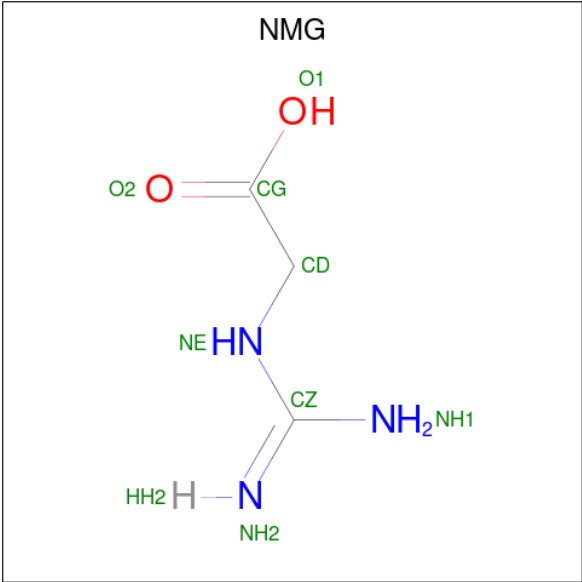
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AB	387	Total	C	N	O	S	0	0	0
			3074	1939	543	571	21			
1	AC	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AD	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	AE	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AF	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	AG	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AH	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	AI	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AJ	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	AK	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AL	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	AM	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AN	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	AO	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AP	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AR	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			
1	BA	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BB	388	Total	C	N	O	S	0	0	0
			3080	1942	544	573	21			
1	BC	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BD	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	BE	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BF	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BG	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BH	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BI	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BJ	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	BK	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BL	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			
1	BM	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BN	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BO	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BP	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BQ	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	BR	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

- Molecule 2 is GUANIDINO ACETATE (CCD ID: NMG) (formula: C₃H₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AA	1	Total	C	N	O	0	0
			8	3	3	2		
2	AB	1	Total	C	N	O	0	0
			8	3	3	2		
2	AC	1	Total	C	N	O	0	0
			8	3	3	2		
2	AD	1	Total	C	N	O	0	0
			8	3	3	2		
2	AE	1	Total	C	N	O	0	0
			8	3	3	2		
2	AF	1	Total	C	N	O	0	0
			8	3	3	2		
2	AG	1	Total	C	N	O	0	0
			8	3	3	2		
2	AH	1	Total	C	N	O	0	0
			8	3	3	2		
2	AI	1	Total	C	N	O	0	0
			8	3	3	2		
2	AJ	1	Total	C	N	O	0	0
			8	3	3	2		
2	AK	1	Total	C	N	O	0	0
			8	3	3	2		
2	AL	1	Total	C	N	O	0	0
			8	3	3	2		
2	AM	1	Total	C	N	O	0	0
			8	3	3	2		
2	AN	1	Total	C	N	O	0	0
			8	3	3	2		

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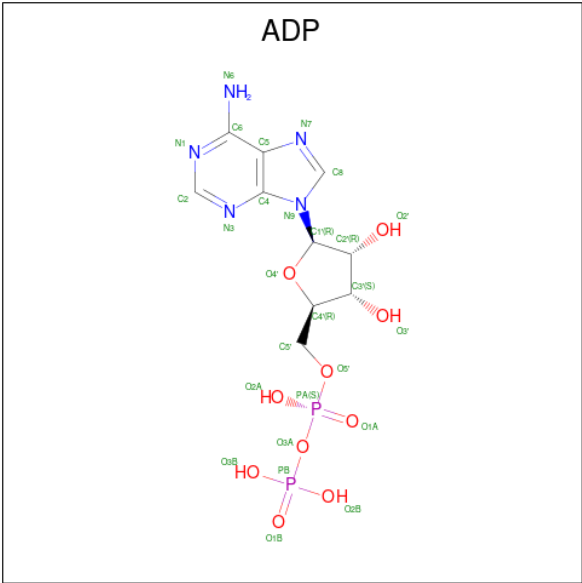
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AO	1	Total 8	C 3	N 3	O 2	0	0
2	AP	1	Total 8	C 3	N 3	O 2	0	0
2	AQ	1	Total 8	C 3	N 3	O 2	0	0
2	AR	1	Total 8	C 3	N 3	O 2	0	0
2	BA	1	Total 8	C 3	N 3	O 2	0	0
2	BB	1	Total 8	C 3	N 3	O 2	0	0
2	BC	1	Total 8	C 3	N 3	O 2	0	0
2	BD	1	Total 8	C 3	N 3	O 2	0	0
2	BE	1	Total 8	C 3	N 3	O 2	0	0
2	BF	1	Total 8	C 3	N 3	O 2	0	0
2	BG	1	Total 8	C 3	N 3	O 2	0	0
2	BH	1	Total 8	C 3	N 3	O 2	0	0
2	BI	1	Total 8	C 3	N 3	O 2	0	0
2	BJ	1	Total 8	C 3	N 3	O 2	0	0
2	BK	1	Total 8	C 3	N 3	O 2	0	0
2	BL	1	Total 8	C 3	N 3	O 2	0	0
2	BM	1	Total 8	C 3	N 3	O 2	0	0
2	BN	1	Total 8	C 3	N 3	O 2	0	0
2	BO	1	Total 8	C 3	N 3	O 2	0	0
2	BP	1	Total 8	C 3	N 3	O 2	0	0
2	BQ	1	Total 8	C 3	N 3	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	BR	1	Total	C	N	O	0	0
			8	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AC	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AF	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AI	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AJ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AK	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AL	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AM	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AN	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AO	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AP	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	AR	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BC	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BF	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BI	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BJ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BK	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BL	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BM	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	BN	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BO	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BP	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BR	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AA	1	Total	Mg	0	0
			1	1		
4	AB	1	Total	Mg	0	0
			1	1		
4	AC	1	Total	Mg	0	0
			1	1		
4	AD	1	Total	Mg	0	0
			1	1		
4	AE	1	Total	Mg	0	0
			1	1		
4	AF	1	Total	Mg	0	0
			1	1		
4	AG	1	Total	Mg	0	0
			1	1		
4	AH	1	Total	Mg	0	0
			1	1		
4	AI	1	Total	Mg	0	0
			1	1		
4	AJ	1	Total	Mg	0	0
			1	1		
4	AK	1	Total	Mg	0	0
			1	1		
4	AL	1	Total	Mg	0	0
			1	1		
4	AM	1	Total	Mg	0	0
			1	1		
4	AN	1	Total	Mg	0	0
			1	1		

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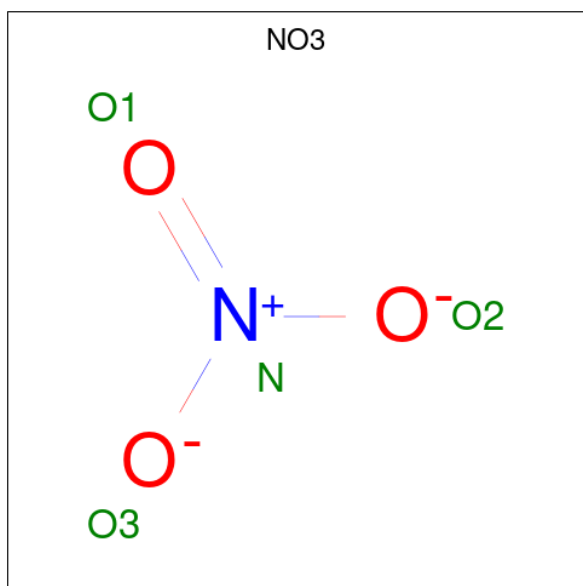
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AO	1	Total 1	Mg 1	0	0
4	AP	1	Total 1	Mg 1	0	0
4	AQ	1	Total 1	Mg 1	0	0
4	AR	1	Total 1	Mg 1	0	0
4	BA	1	Total 1	Mg 1	0	0
4	BB	1	Total 1	Mg 1	0	0
4	BC	1	Total 1	Mg 1	0	0
4	BD	1	Total 1	Mg 1	0	0
4	BE	1	Total 1	Mg 1	0	0
4	BF	1	Total 1	Mg 1	0	0
4	BG	1	Total 1	Mg 1	0	0
4	BH	1	Total 1	Mg 1	0	0
4	BI	1	Total 1	Mg 1	0	0
4	BJ	1	Total 1	Mg 1	0	0
4	BK	1	Total 1	Mg 1	0	0
4	BL	1	Total 1	Mg 1	0	0
4	BM	1	Total 1	Mg 1	0	0
4	BN	1	Total 1	Mg 1	0	0
4	BO	1	Total 1	Mg 1	0	0
4	BP	1	Total 1	Mg 1	0	0
4	BQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BR	1	Total	Mg	0	0
			1	1		

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AA	1	Total	N	O	0	0
			4	1	3		
5	AB	1	Total	N	O	0	0
			4	1	3		
5	AC	1	Total	N	O	0	0
			4	1	3		
5	AD	1	Total	N	O	0	0
			4	1	3		
5	AE	1	Total	N	O	0	0
			4	1	3		
5	AF	1	Total	N	O	0	0
			4	1	3		
5	AG	1	Total	N	O	0	0
			4	1	3		
5	AH	1	Total	N	O	0	0
			4	1	3		
5	AI	1	Total	N	O	0	0
			4	1	3		
5	AJ	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AK	1	Total	N	O	0	0
			4	1	3		
5	AL	1	Total	N	O	0	0
			4	1	3		
5	AM	1	Total	N	O	0	0
			4	1	3		
5	AN	1	Total	N	O	0	0
			4	1	3		
5	AO	1	Total	N	O	0	0
			4	1	3		
5	AP	1	Total	N	O	0	0
			4	1	3		
5	AQ	1	Total	N	O	0	0
			4	1	3		
5	AR	1	Total	N	O	0	0
			4	1	3		
5	BA	1	Total	N	O	0	0
			4	1	3		
5	BB	1	Total	N	O	0	0
			4	1	3		
5	BC	1	Total	N	O	0	0
			4	1	3		
5	BD	1	Total	N	O	0	0
			4	1	3		
5	BE	1	Total	N	O	0	0
			4	1	3		
5	BF	1	Total	N	O	0	0
			4	1	3		
5	BG	1	Total	N	O	0	0
			4	1	3		
5	BH	1	Total	N	O	0	0
			4	1	3		
5	BI	1	Total	N	O	0	0
			4	1	3		
5	BJ	1	Total	N	O	0	0
			4	1	3		
5	BK	1	Total	N	O	0	0
			4	1	3		
5	BL	1	Total	N	O	0	0
			4	1	3		
5	BM	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BN	1	Total	N	O	0	0
			4	1	3		
5	BO	1	Total	N	O	0	0
			4	1	3		
5	BP	1	Total	N	O	0	0
			4	1	3		
5	BQ	1	Total	N	O	0	0
			4	1	3		
5	BR	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AA	106	Total	O	0	0
			106	106		
6	AB	138	Total	O	0	0
			138	138		
6	AC	116	Total	O	0	0
			116	116		
6	AD	149	Total	O	0	0
			149	149		
6	AE	154	Total	O	0	0
			154	154		
6	AF	117	Total	O	0	0
			117	117		
6	AG	131	Total	O	0	0
			131	131		
6	AH	88	Total	O	0	0
			88	88		
6	AI	111	Total	O	0	0
			111	111		
6	AJ	137	Total	O	0	0
			137	137		
6	AK	125	Total	O	0	0
			125	125		
6	AL	156	Total	O	0	0
			156	156		
6	AM	149	Total	O	0	0
			149	149		
6	AN	116	Total	O	0	0
			116	116		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AO	113	Total 113	O 113	0	0
6	AP	172	Total 172	O 172	0	0
6	AQ	167	Total 167	O 167	0	0
6	AR	166	Total 166	O 166	0	0
6	BA	99	Total 99	O 99	0	0
6	BB	130	Total 130	O 130	0	0
6	BC	155	Total 155	O 155	0	0
6	BD	110	Total 110	O 110	0	0
6	BE	117	Total 117	O 117	0	0
6	BF	144	Total 144	O 144	0	0
6	BG	131	Total 131	O 131	0	0
6	BH	145	Total 145	O 145	0	0
6	BI	118	Total 118	O 118	0	0
6	BJ	145	Total 145	O 145	0	0
6	BK	127	Total 127	O 127	0	0
6	BL	90	Total 90	O 90	0	0
6	BM	141	Total 141	O 141	0	0
6	BN	116	Total 116	O 116	0	0
6	BO	173	Total 173	O 173	0	0
6	BP	151	Total 151	O 151	0	0
6	BQ	105	Total 105	O 105	0	0

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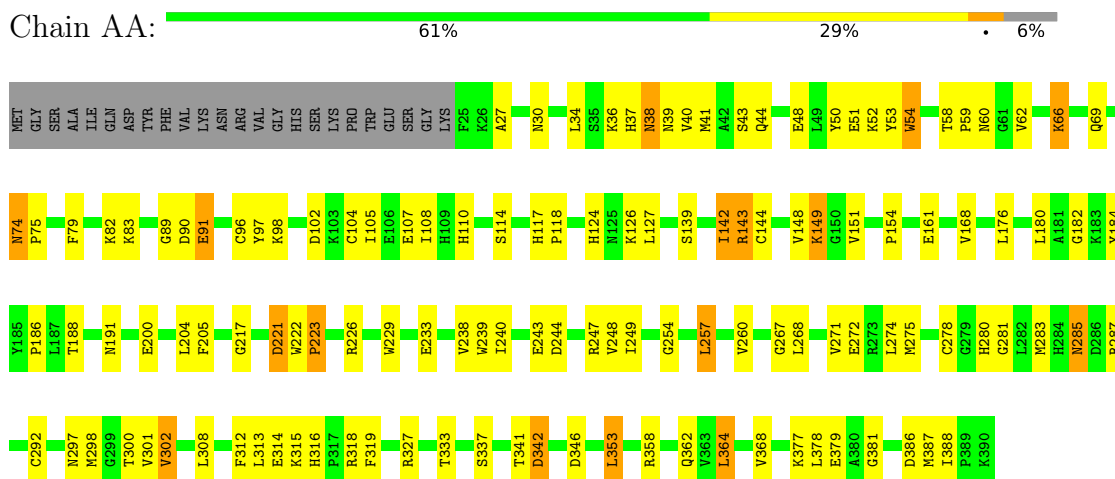
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BR	166	Total 166	O 166	0	0

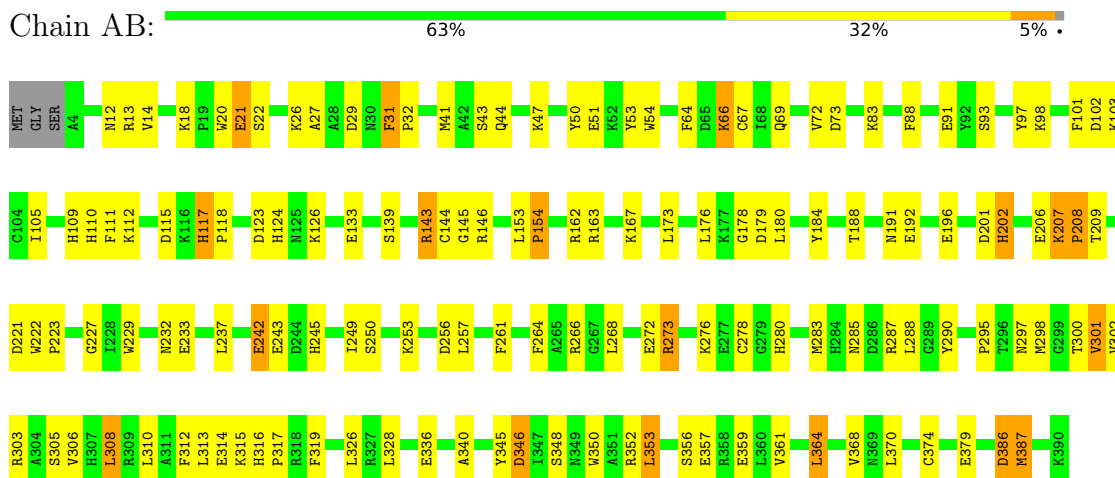
3 Residue-property plots

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: Glycocyamine kinase beta chain

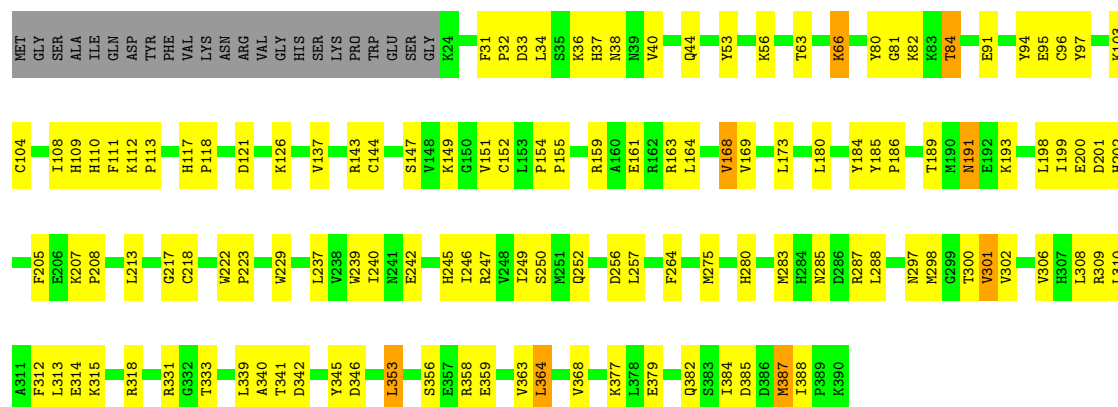


- Molecule 1: Glycocyamine kinase beta chain



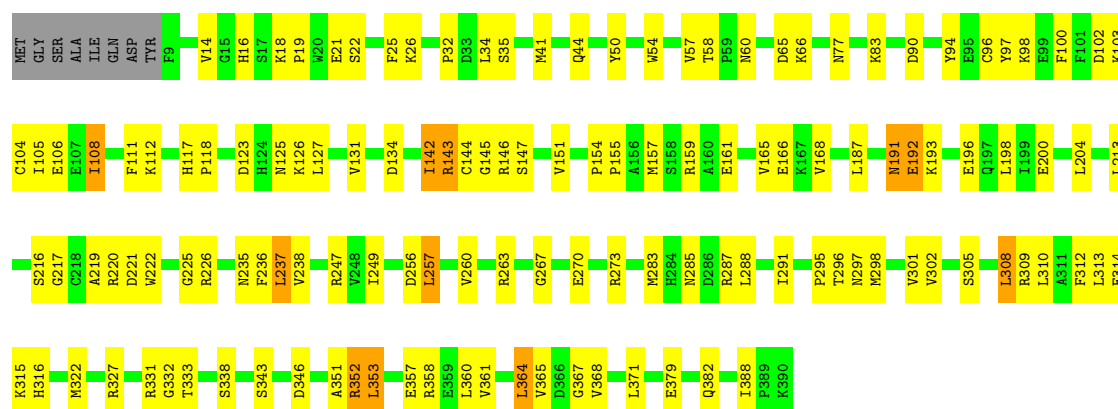
- Molecule 1: Glycocyamine kinase beta chain





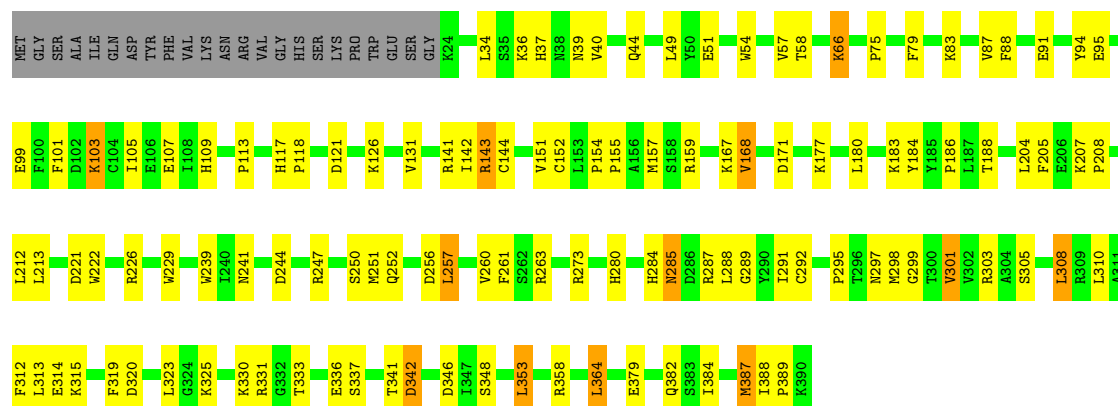
• Molecule 1: Glycocyamine kinase beta chain

Chain AD: 64% 31%



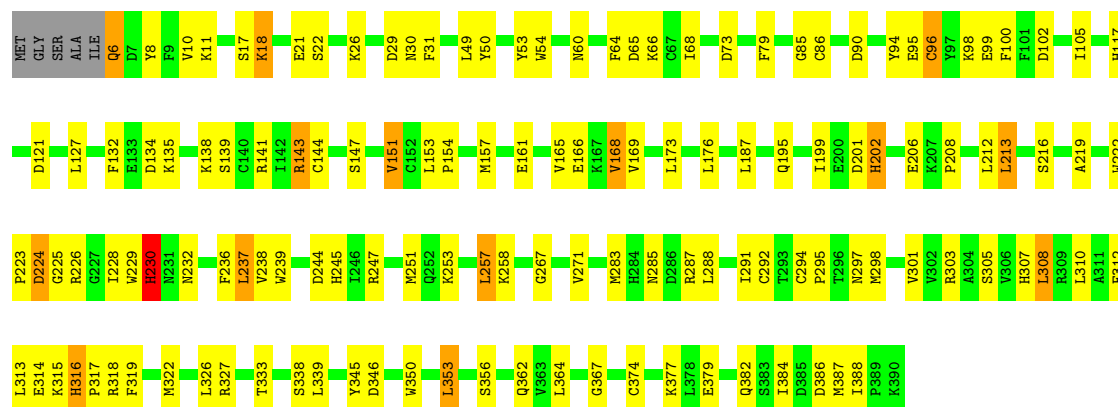
• Molecule 1: Glycocyamine kinase beta chain

Chain AE: 64% 27% 6%



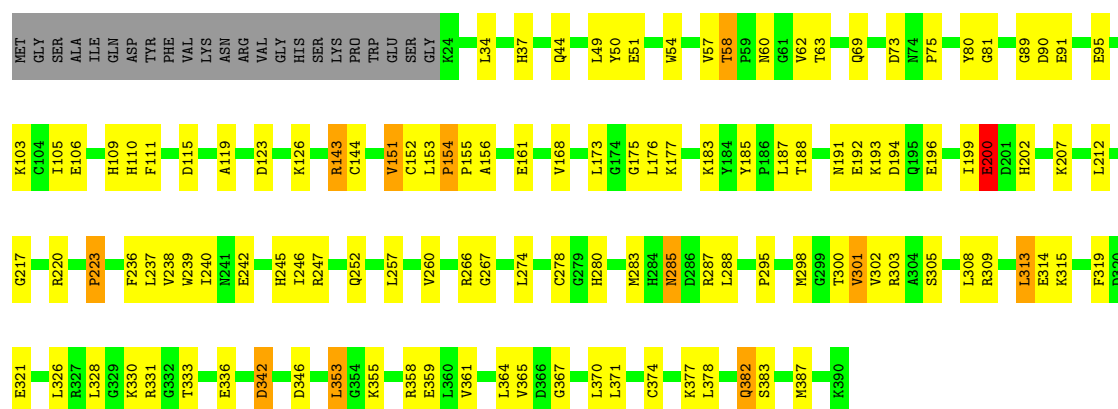
• Molecule 1: Glycocyamine kinase beta chain

Chain AF: 64% 31%



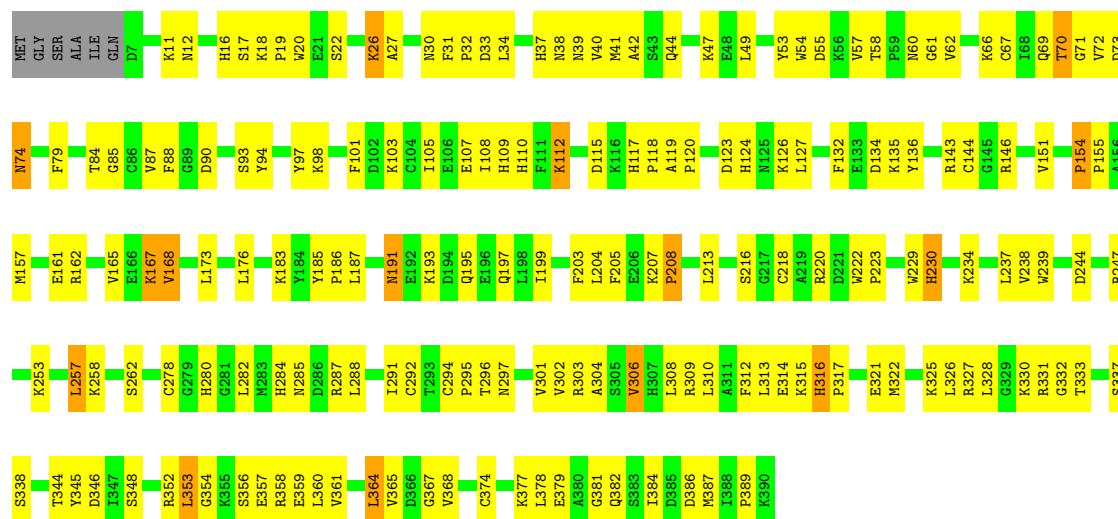
- Molecule 1: Glycocyamine kinase beta chain

Chain AG: 63% 28% 6%



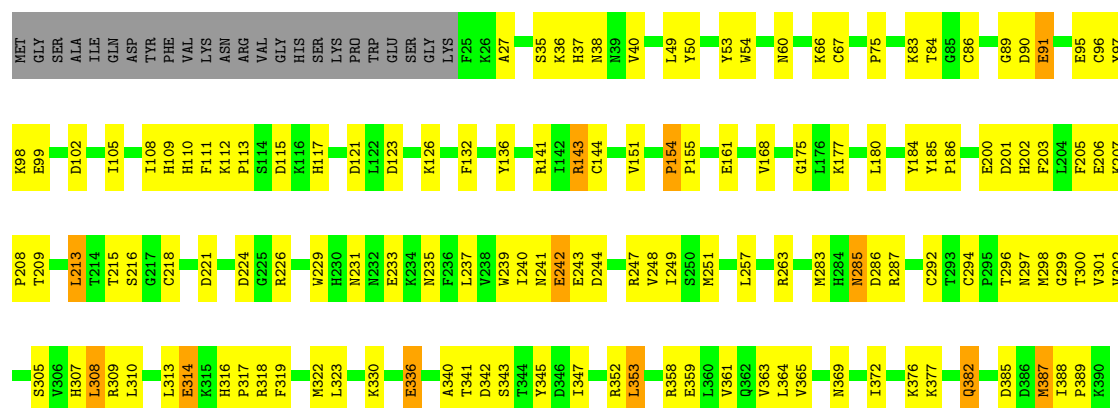
- Molecule 1: Glycocyamine kinase beta chain

Chain AH: 52% 43% 5%



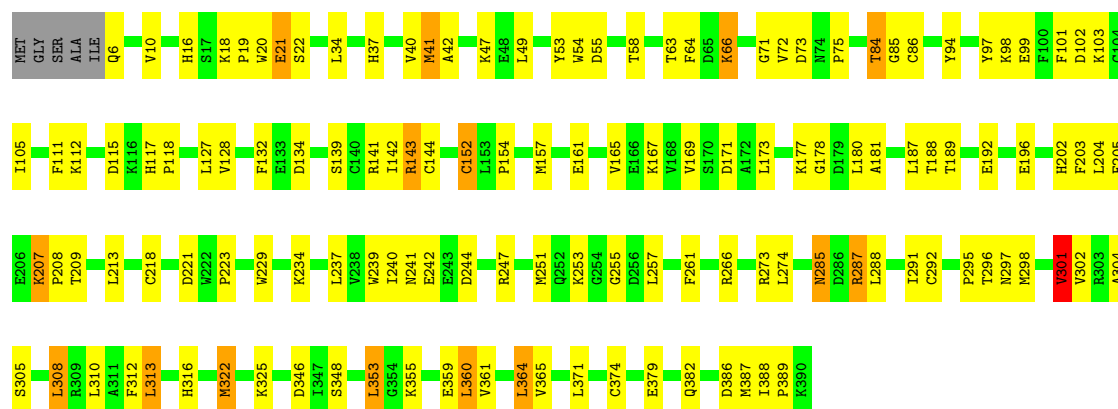
- Molecule 1: Glycocyamine kinase beta chain

Chain AI:  58% 32% 6%



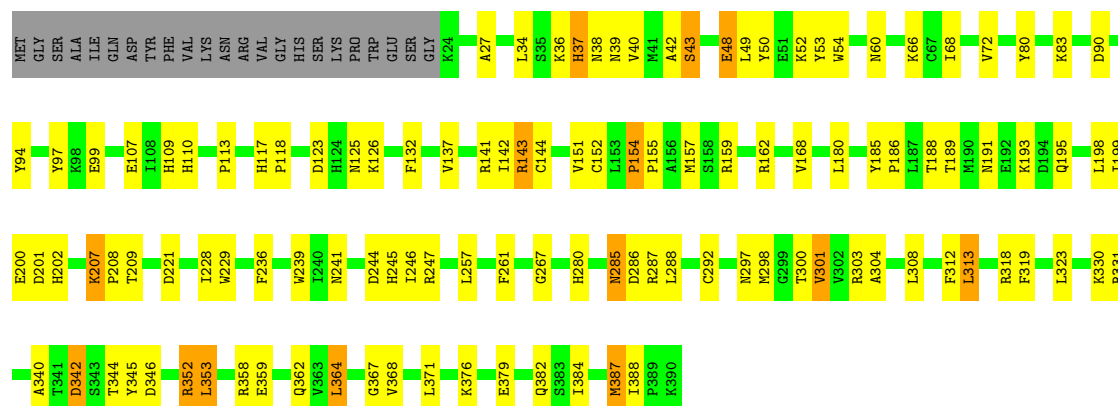
• Molecule 1: Glycocyamine kinase beta chain

Chain AJ:  64% 30% 6%



• Molecule 1: Glycocyamine kinase beta chain

Chain AK:  64% 26% 6%



• Molecule 1: Glycocyamine kinase beta chain

Response	Percentage
Yes	69%
No	26%



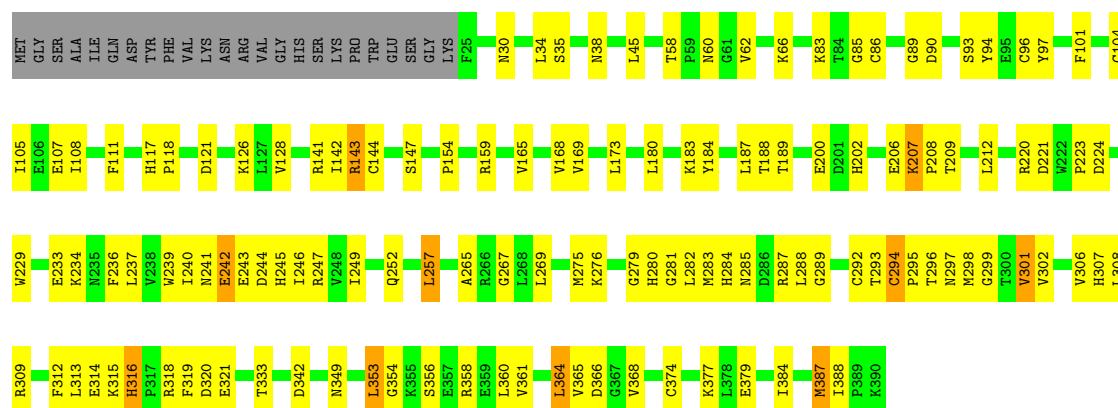
63% 27% 6%



Response	Percentage
Yes	65%
No	29%
Don't know	6%

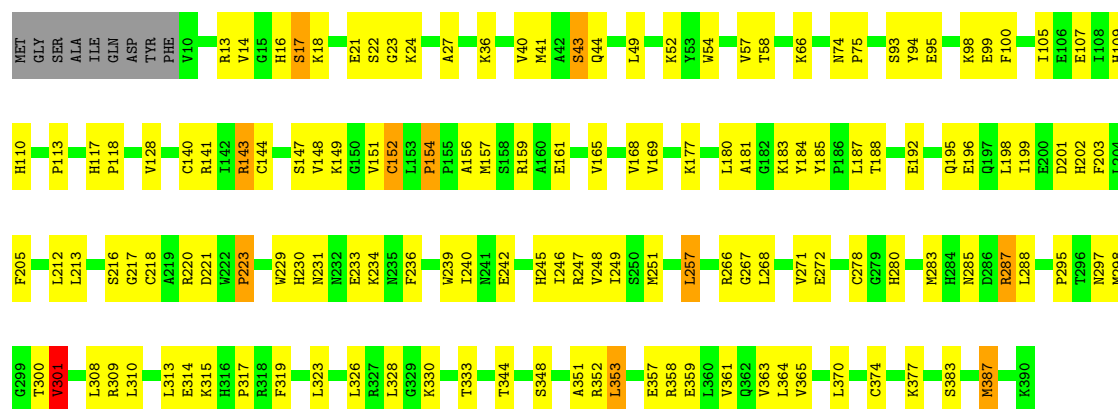


Chain AO:  60% 31% 6%



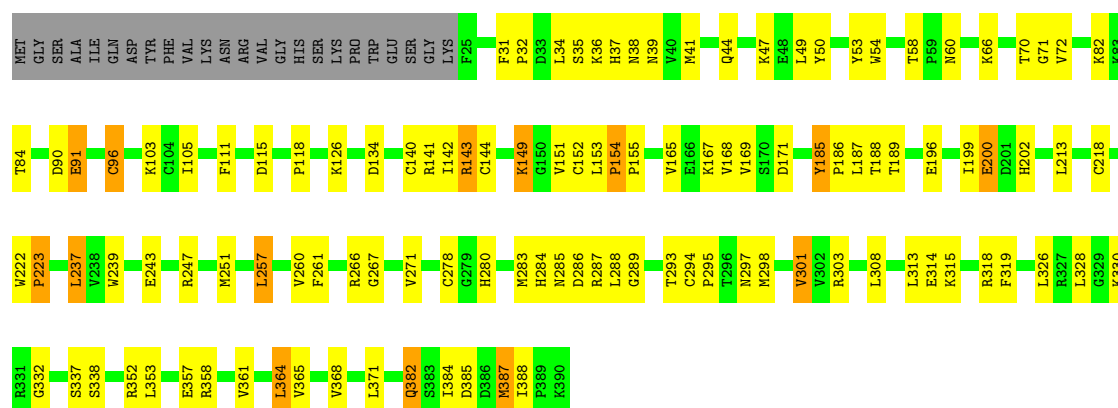
• Molecule 1: Glycocyamine kinase beta chain

Chain AP:  62% 33% 2%



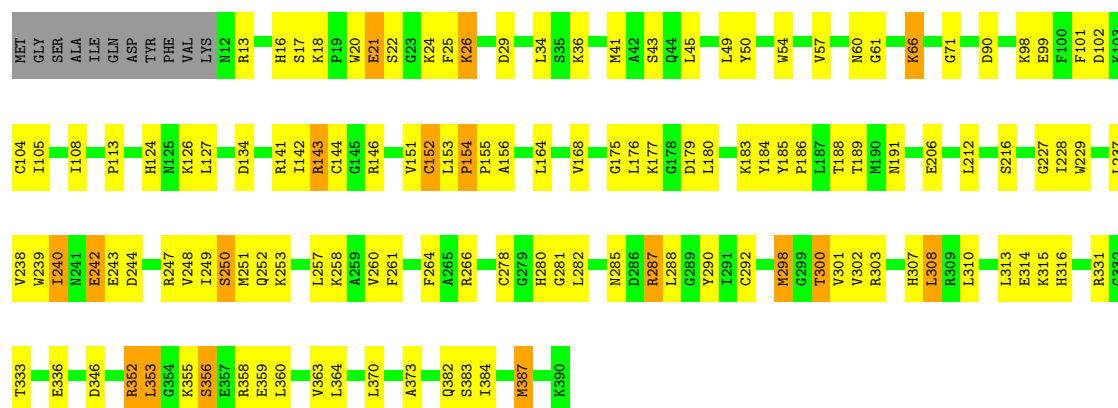
• Molecule 1: Glycocyamine kinase beta chain

Chain AQ:  64% 26% 6%



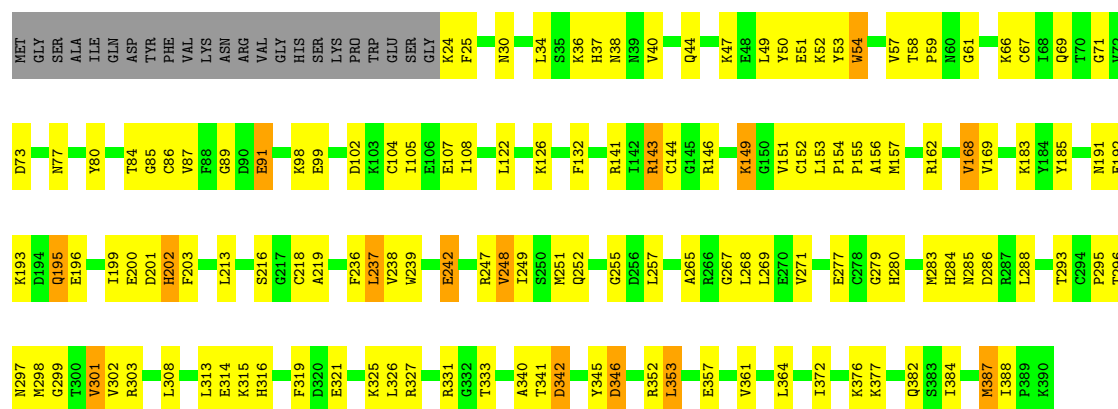
• Molecule 1: Glycocyamine kinase beta chain

Chain AR:  64% 28%



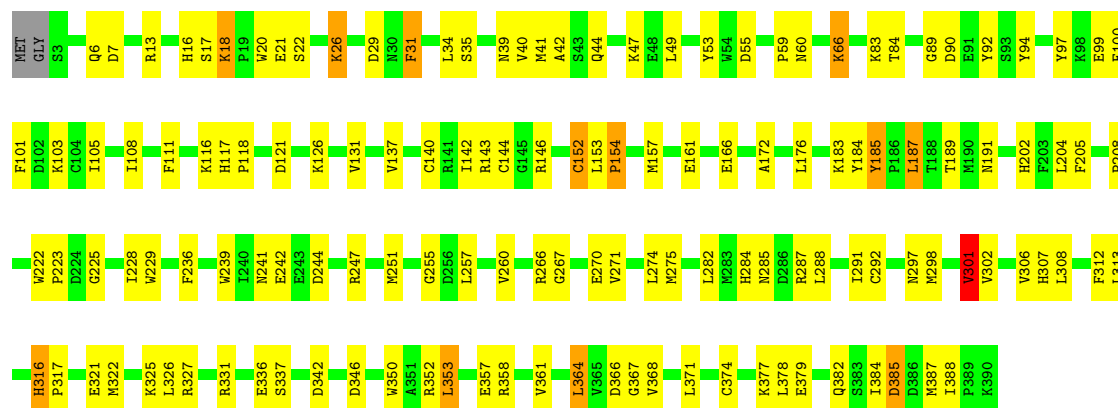
• Molecule 1: Glycocyamine kinase beta chain

Chain BA:  59% 31% 6%



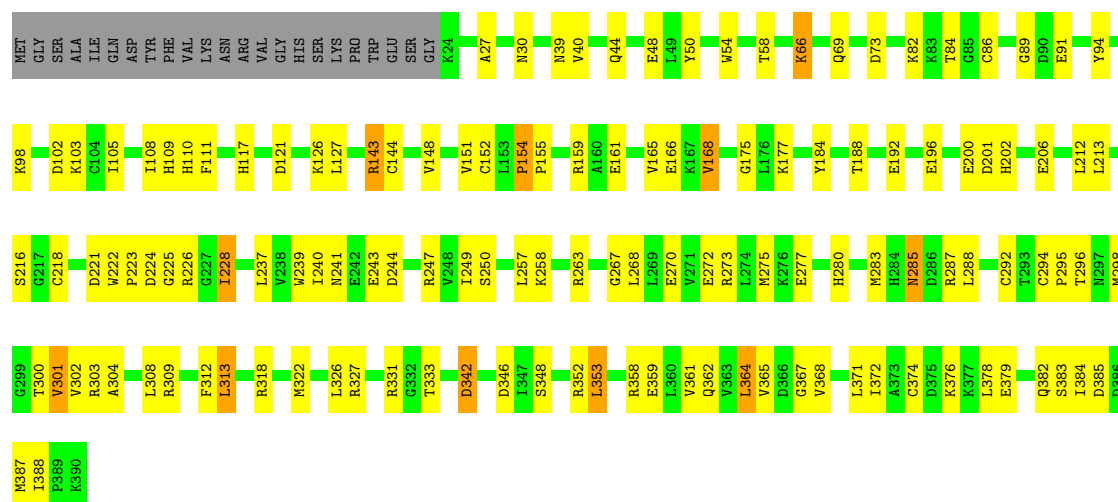
• Molecule 1: Glycocyamine kinase beta chain

Chain BB:  64% 32%



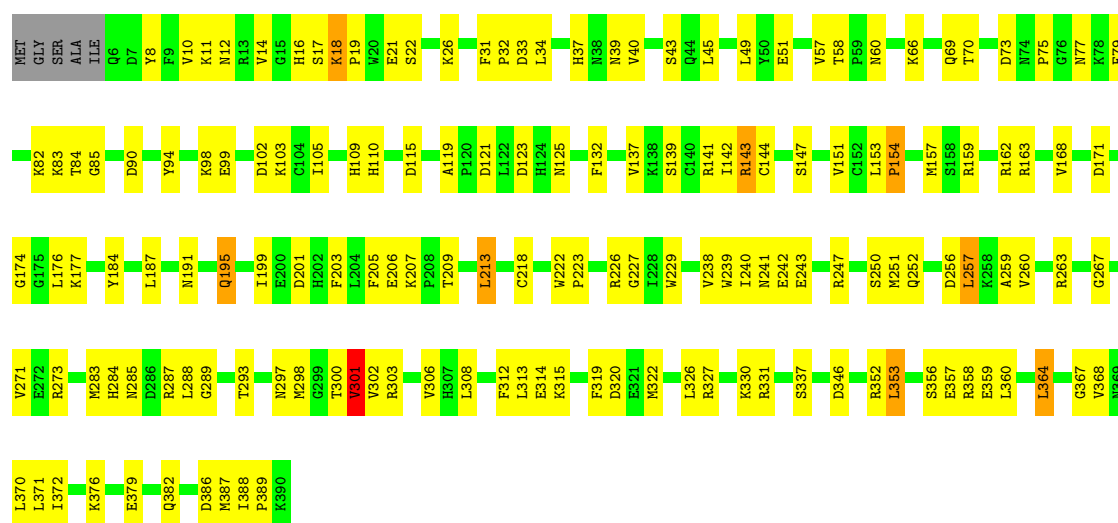
• Molecule 1: Glycocyamine kinase beta chain

Chain BC:  60% 31% 6%



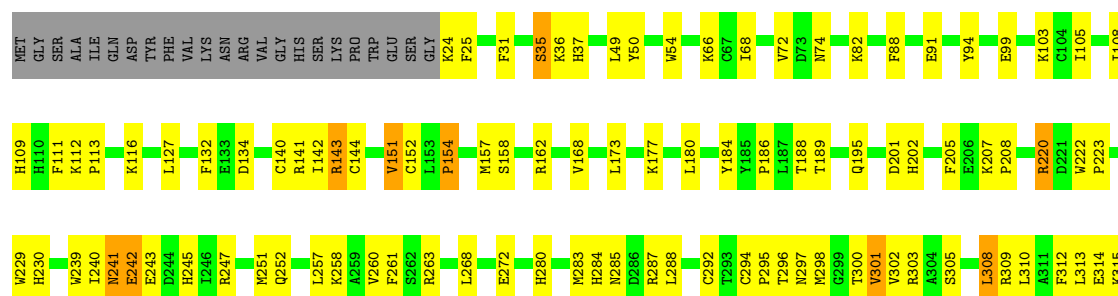
• Molecule 1: Glycocyamine kinase beta chain

Chain BD:  59% 37% 2%



• Molecule 1: Glycocyamine kinase beta chain

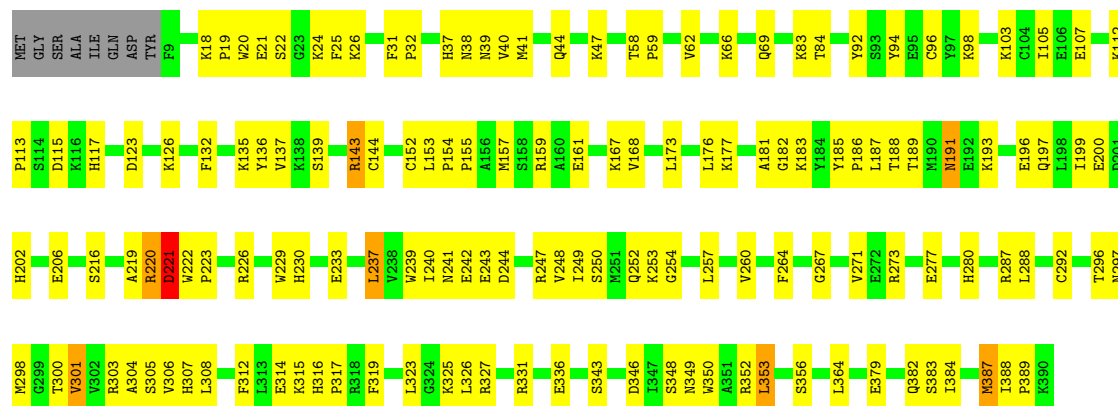
Chain BE:  62% 29% 6%





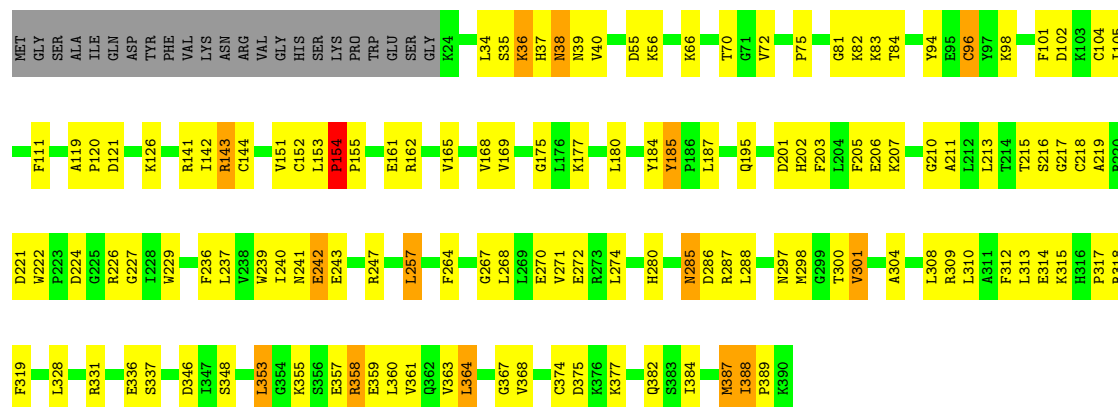
• Molecule 1: Glycocyamine kinase beta chain

Chain BF: 61% 35%



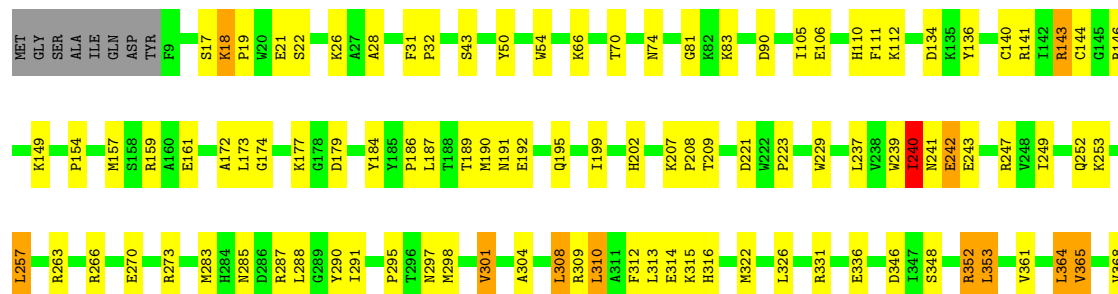
• Molecule 1: Glycocyamine kinase beta chain

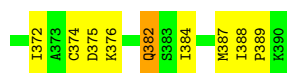
Chain BG: 61% 30% 6%



• Molecule 1: Glycocyamine kinase beta chain

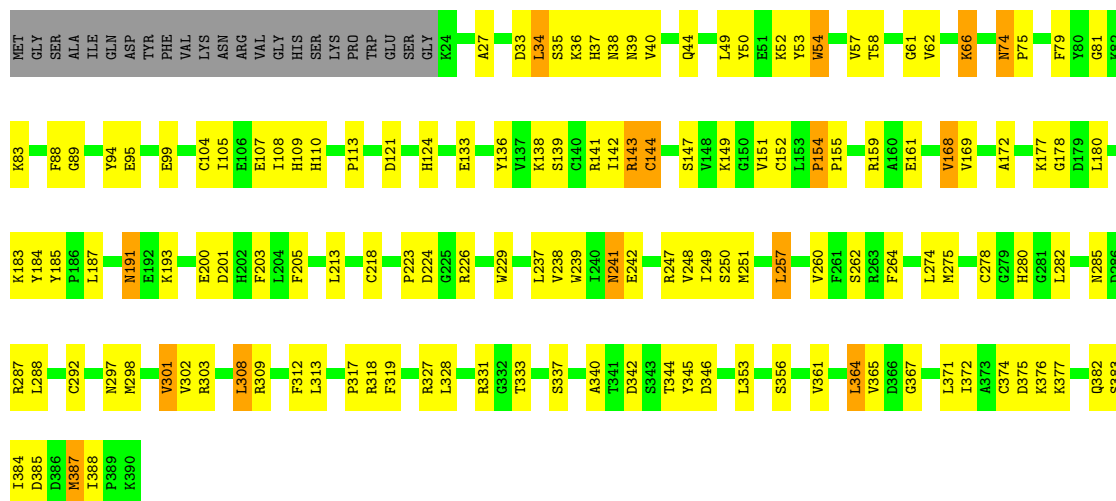
Chain BH: 69% 25%





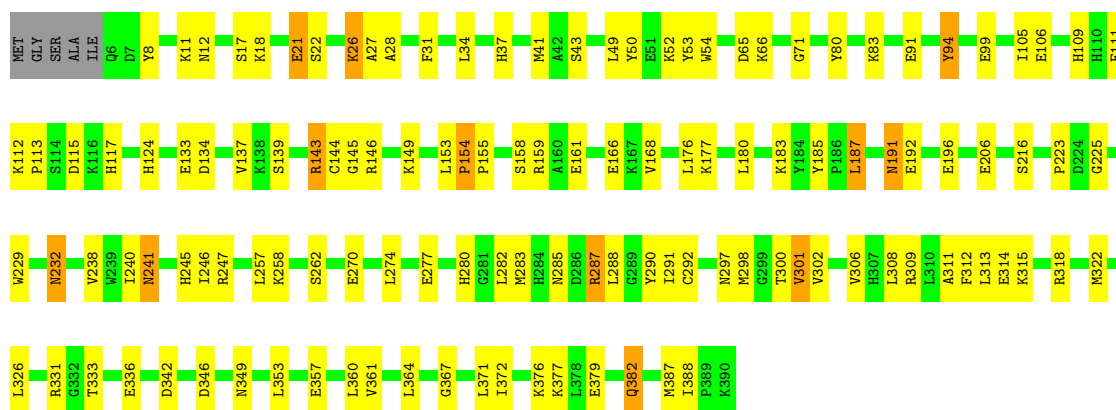
• Molecule 1: Glycocyamine kinase beta chain

Chain BI: 58% 32% 6%



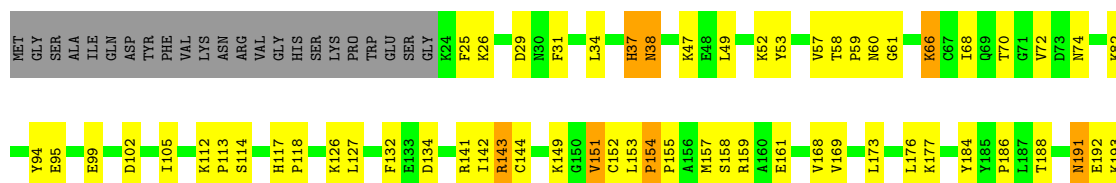
• Molecule 1: Glycocyamine kinase beta chain

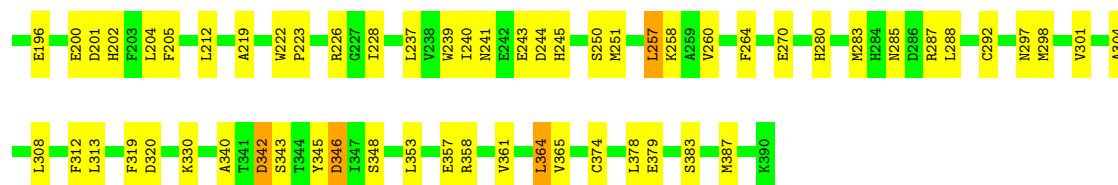
Chain BJ: 66% 29% 2%



• Molecule 1: Glycocyamine kinase beta chain

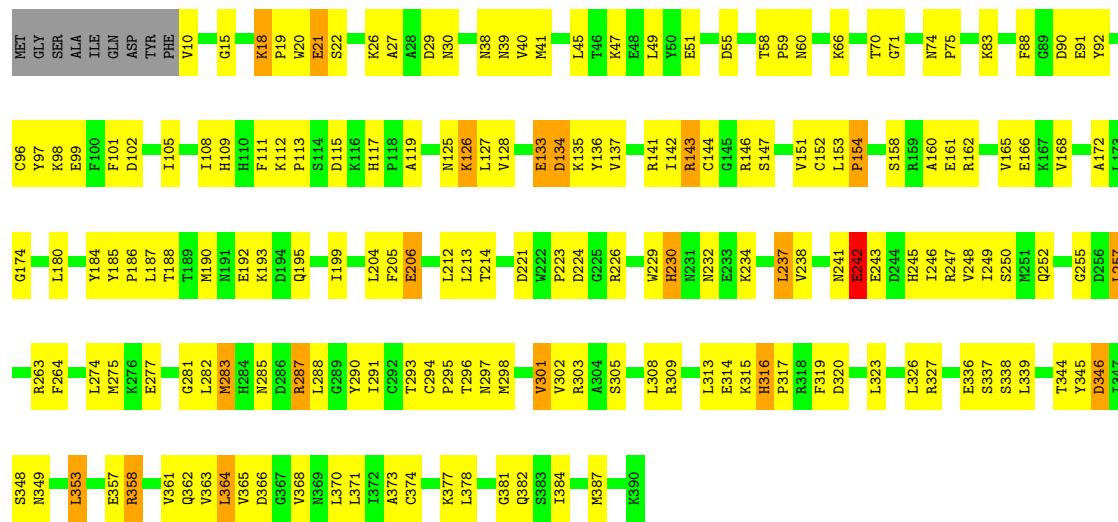
Chain BK: 63% 28% 6%





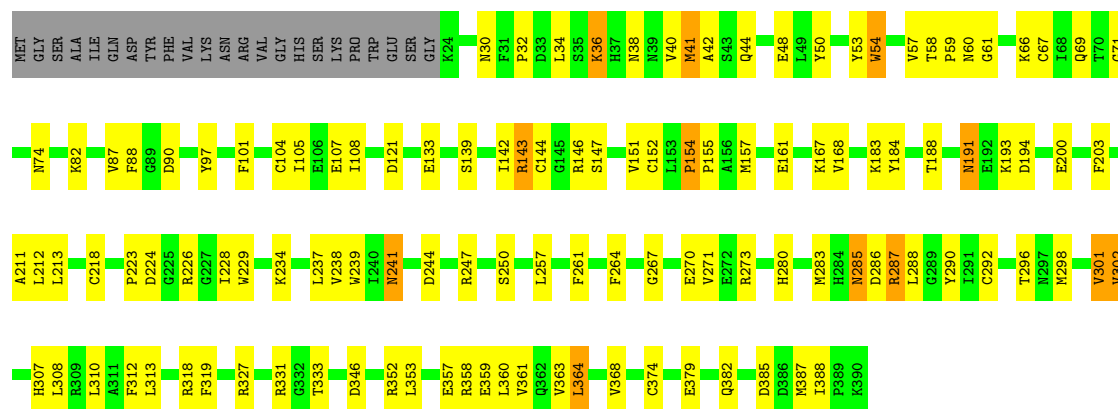
• Molecule 1: Glycocyamine kinase beta chain

Chain BL: 52% 41% 5% .



• Molecule 1: Glycocyamine kinase beta chain

Chain BM: 63% 28% 6% .



• Molecule 1: Glycocyamine kinase beta chain

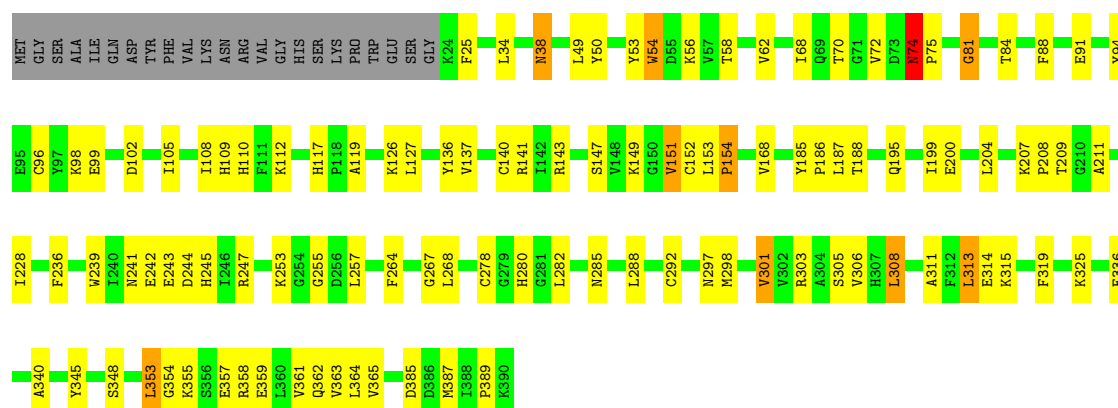
Chain BN: 62% 32% . .





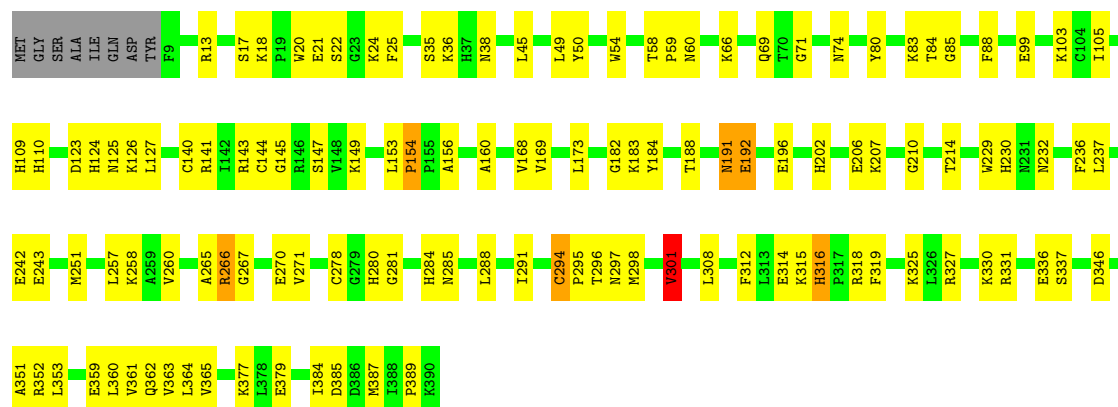
• Molecule 1: Glycocyamine kinase beta chain

Chain BO: 66% 25% 6%



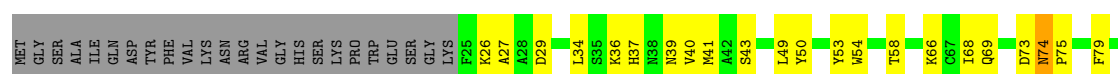
• Molecule 1: Glycocyamine kinase beta chain

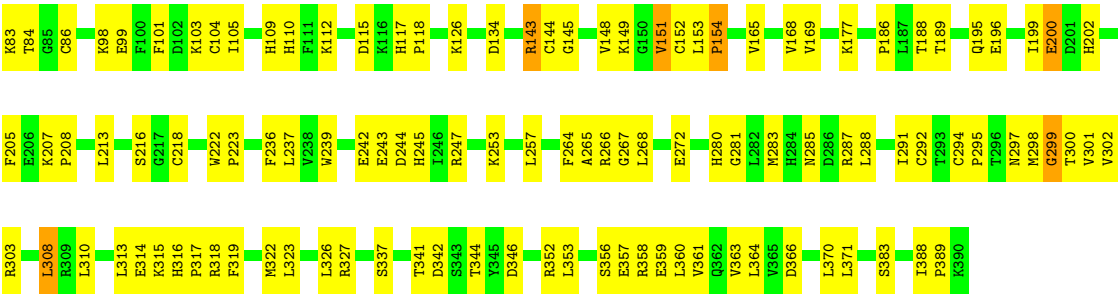
Chain BP: 67% 29% 4%



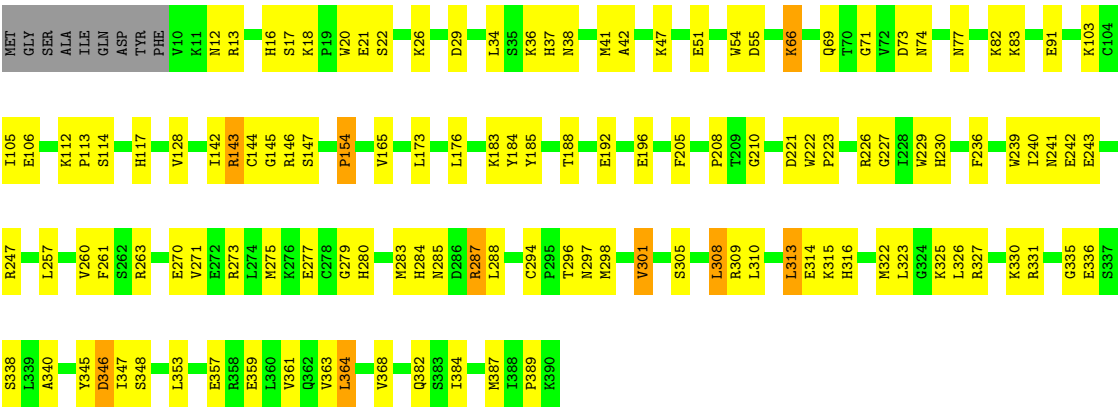
• Molecule 1: Glycocyamine kinase beta chain

Chain BQ: 59% 33% 6%





• Molecule 1: Glycocyamine kinase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	243.11Å 114.27Å 259.90Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 92.1 (20.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.263 0.235 , 0.293	Depositor DCC
R_{free} test set	30531 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.430 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	113311	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6308e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMG, MG, ADP, NO3

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	AA	0.41	0/2963	0.85	5/3986 (0.1%)
1	AB	0.45	0/3142	0.88	10/4227 (0.2%)
1	AC	0.42	0/2972	0.82	4/3997 (0.1%)
1	AD	0.46	0/3099	0.85	4/4168 (0.1%)
1	AE	0.43	0/2972	0.82	2/3997 (0.1%)
1	AF	0.45	0/3129	0.89	10/4209 (0.2%)
1	AG	0.43	0/2972	0.83	6/3997 (0.2%)
1	AH	0.43	0/3120	0.88	11/4197 (0.3%)
1	AI	0.42	0/2963	0.82	1/3986 (0.0%)
1	AJ	0.46	0/3129	0.85	6/4209 (0.1%)
1	AK	0.43	0/2972	0.83	7/3997 (0.2%)
1	AL	0.47	0/3120	0.88	8/4197 (0.2%)
1	AM	0.43	0/2972	0.86	5/3997 (0.1%)
1	AN	0.45	0/3099	0.85	4/4168 (0.1%)
1	AO	0.42	0/2963	0.86	9/3986 (0.2%)
1	AP	0.49	0/3087	0.84	3/4152 (0.1%)
1	AQ	0.44	0/2963	0.84	3/3986 (0.1%)
1	AR	0.47	0/3071	0.87	6/4131 (0.1%)
1	BA	0.40	0/2972	0.81	2/3997 (0.1%)
1	BB	0.45	0/3148	0.88	14/4235 (0.3%)
1	BC	0.43	0/2972	0.84	5/3997 (0.1%)
1	BD	0.44	0/3129	0.86	6/4209 (0.1%)
1	BE	0.42	0/2972	0.86	11/3997 (0.3%)
1	BF	0.46	0/3099	0.85	1/4168 (0.0%)
1	BG	0.44	0/2972	0.82	6/3997 (0.2%)
1	BH	0.46	0/3099	0.87	8/4168 (0.2%)
1	BI	0.45	0/2972	0.85	5/3997 (0.1%)
1	BJ	0.46	0/3129	0.89	8/4209 (0.2%)
1	BK	0.44	0/2972	0.84	2/3997 (0.1%)
1	BL	0.44	0/3087	0.90	13/4152 (0.3%)
1	BM	0.43	0/2972	0.84	2/3997 (0.1%)
1	BN	0.43	0/3099	0.87	9/4168 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BO	0.45	0/2972	0.87	12/3997 (0.3%)
1	BP	0.46	0/3099	0.88	7/4168 (0.2%)
1	BQ	0.42	0/2963	0.84	4/3986 (0.1%)
1	BR	0.47	0/3087	0.87	6/4152 (0.1%)
All	All	0.44	0/109423	0.86	225/147178 (0.2%)

There are no bond length outliers.

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AF	316	HIS	CA-C-N	9.95	129.57	119.82
1	AF	316	HIS	C-N-CA	9.95	129.57	119.82
1	BL	117	HIS	CA-C-N	9.10	129.04	120.03
1	BL	117	HIS	C-N-CA	9.10	129.04	120.03
1	BH	18	LYS	CA-C-N	8.28	127.94	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2901	0	2866	101	0
1	AB	3074	0	3034	114	0
1	AC	2910	0	2879	92	0
1	AD	3032	0	2997	86	0
1	AE	2910	0	2879	83	0
1	AF	3061	0	3018	107	0
1	AG	2910	0	2879	90	0
1	AH	3052	0	3010	151	0
1	AI	2901	0	2866	93	0
1	AJ	3061	0	3018	89	0
1	AK	2910	0	2879	92	0
1	AL	3052	0	3010	86	0
1	AM	2910	0	2879	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	3032	0	2997	97	0
1	AO	2901	0	2866	98	0
1	AP	3021	0	2988	112	0
1	AQ	2901	0	2866	89	0
1	AR	3005	0	2966	99	0
1	BA	2910	0	2879	97	0
1	BB	3080	0	3039	99	0
1	BC	2910	0	2879	94	0
1	BD	3061	0	3018	125	0
1	BE	2910	0	2879	102	0
1	BF	3032	0	2997	118	0
1	BG	2910	0	2879	95	0
1	BH	3032	0	2997	85	0
1	BI	2910	0	2879	109	0
1	BJ	3061	0	3018	84	0
1	BK	2910	0	2879	95	0
1	BL	3021	0	2988	132	0
1	BM	2910	0	2879	87	0
1	BN	3032	0	2997	101	0
1	BO	2910	0	2879	73	0
1	BP	3032	0	2997	83	0
1	BQ	2901	0	2866	99	0
1	BR	3021	0	2988	88	0
2	AA	8	0	5	0	0
2	AB	8	0	5	3	0
2	AC	8	0	5	0	0
2	AD	8	0	5	0	0
2	AE	8	0	5	1	0
2	AF	8	0	5	0	0
2	AG	8	0	5	2	0
2	AH	8	0	5	0	0
2	AI	8	0	5	1	0
2	AJ	8	0	5	0	0
2	AK	8	0	5	0	0
2	AL	8	0	5	0	0
2	AM	8	0	5	1	0
2	AN	8	0	5	1	0
2	AO	8	0	5	1	0
2	AP	8	0	5	0	0
2	AQ	8	0	5	0	0
2	AR	8	0	5	0	0
2	BA	8	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BB	8	0	5	1	0
2	BC	8	0	5	0	0
2	BD	8	0	5	1	0
2	BE	8	0	5	0	0
2	BF	8	0	5	0	0
2	BG	8	0	5	0	0
2	BH	8	0	5	1	0
2	BI	8	0	5	0	0
2	BJ	8	0	5	1	0
2	BK	8	0	5	0	0
2	BL	8	0	5	0	0
2	BM	8	0	5	0	0
2	BN	8	0	5	0	0
2	BO	8	0	5	2	0
2	BP	8	0	5	0	0
2	BQ	8	0	5	0	0
2	BR	8	0	5	1	0
3	AA	27	0	12	1	0
3	AB	27	0	12	2	0
3	AC	27	0	12	1	0
3	AD	27	0	12	0	0
3	AE	27	0	12	4	0
3	AF	27	0	12	7	0
3	AG	27	0	12	2	0
3	AH	27	0	12	3	0
3	AI	27	0	12	3	0
3	AJ	27	0	12	3	0
3	AK	27	0	12	5	0
3	AL	27	0	12	1	0
3	AM	27	0	12	2	0
3	AN	27	0	12	1	0
3	AO	27	0	12	4	0
3	AP	27	0	12	5	0
3	AQ	27	0	12	3	0
3	AR	27	0	12	2	0
3	BA	27	0	12	3	0
3	BB	27	0	12	4	0
3	BC	27	0	12	1	0
3	BD	27	0	12	3	0
3	BE	27	0	12	4	0
3	BF	27	0	12	4	0
3	BG	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BH	27	0	12	2	0
3	BI	27	0	12	2	0
3	BJ	27	0	12	2	0
3	BK	27	0	12	1	0
3	BL	27	0	12	2	0
3	BM	27	0	12	4	0
3	BN	27	0	12	3	0
3	BO	27	0	12	2	0
3	BP	27	0	12	2	0
3	BQ	27	0	12	3	0
3	BR	27	0	12	3	0
4	AA	1	0	0	0	0
4	AB	1	0	0	0	0
4	AC	1	0	0	0	0
4	AD	1	0	0	0	0
4	AE	1	0	0	0	0
4	AF	1	0	0	0	0
4	AG	1	0	0	0	0
4	AH	1	0	0	0	0
4	AI	1	0	0	0	0
4	AJ	1	0	0	0	0
4	AK	1	0	0	0	0
4	AL	1	0	0	0	0
4	AM	1	0	0	0	0
4	AN	1	0	0	0	0
4	AO	1	0	0	0	0
4	AP	1	0	0	0	0
4	AQ	1	0	0	0	0
4	AR	1	0	0	0	0
4	BA	1	0	0	0	0
4	BB	1	0	0	0	0
4	BC	1	0	0	0	0
4	BD	1	0	0	0	0
4	BE	1	0	0	0	0
4	BF	1	0	0	0	0
4	BG	1	0	0	0	0
4	BH	1	0	0	0	0
4	BI	1	0	0	0	0
4	BJ	1	0	0	0	0
4	BK	1	0	0	0	0
4	BL	1	0	0	0	0
4	BM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BN	1	0	0	0	0
4	BO	1	0	0	0	0
4	BP	1	0	0	0	0
4	BQ	1	0	0	0	0
4	BR	1	0	0	0	0
5	AA	4	0	0	0	0
5	AB	4	0	0	0	0
5	AC	4	0	0	0	0
5	AD	4	0	0	1	0
5	AE	4	0	0	0	0
5	AF	4	0	0	0	0
5	AG	4	0	0	0	0
5	AH	4	0	0	0	0
5	AI	4	0	0	0	0
5	AJ	4	0	0	0	0
5	AK	4	0	0	0	0
5	AL	4	0	0	0	0
5	AM	4	0	0	0	0
5	AN	4	0	0	0	0
5	AO	4	0	0	1	0
5	AP	4	0	0	0	0
5	AQ	4	0	0	0	0
5	AR	4	0	0	1	0
5	BA	4	0	0	0	0
5	BB	4	0	0	1	0
5	BC	4	0	0	0	0
5	BD	4	0	0	1	0
5	BE	4	0	0	0	0
5	BF	4	0	0	0	0
5	BG	4	0	0	0	0
5	BH	4	0	0	1	0
5	BI	4	0	0	0	0
5	BJ	4	0	0	0	0
5	BK	4	0	0	1	0
5	BL	4	0	0	0	0
5	BM	4	0	0	0	0
5	BN	4	0	0	0	0
5	BO	4	0	0	0	0
5	BP	4	0	0	0	0
5	BQ	4	0	0	0	0
5	BR	4	0	0	1	0
6	AA	106	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AB	138	0	0	12	0
6	AC	116	0	0	5	0
6	AD	149	0	0	3	0
6	AE	154	0	0	6	0
6	AF	117	0	0	9	0
6	AG	131	0	0	5	0
6	AH	88	0	0	5	0
6	AI	111	0	0	3	0
6	AJ	137	0	0	5	0
6	AK	125	0	0	8	0
6	AL	156	0	0	5	0
6	AM	149	0	0	8	0
6	AN	116	0	0	7	0
6	AO	113	0	0	7	0
6	AP	172	0	0	15	0
6	AQ	167	0	0	10	0
6	AR	166	0	0	5	0
6	BA	99	0	0	2	0
6	BB	130	0	0	2	0
6	BC	155	0	0	4	0
6	BD	110	0	0	12	0
6	BE	117	0	0	7	0
6	BF	144	0	0	6	0
6	BG	131	0	0	5	0
6	BH	145	0	0	13	0
6	BI	118	0	0	9	0
6	BJ	145	0	0	7	0
6	BK	127	0	0	4	0
6	BL	90	0	0	6	0
6	BM	141	0	0	9	0
6	BN	116	0	0	6	0
6	BO	173	0	0	6	0
6	BP	151	0	0	9	0
6	BQ	105	0	0	13	0
6	BR	166	0	0	10	0
All	All	113311	0	106446	3462	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 16.

The worst 5 of 3462 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:AK:126:LYS:HB2	1:AK:358:ARG:HD2	1.38	1.04
1:AD:285:ASN:HB2	1:AD:291:ILE:HD11	1.40	1.02
1:BC:126:LYS:HB2	1:BC:358:ARG:HD2	1.39	1.02
1:BB:285:ASN:HD22	1:BB:288:LEU:H	1.06	1.00
1:AL:285:ASN:HD22	1:AL:288:LEU:H	1.03	0.99

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	AA	364/390 (93%)	335 (92%)	29 (8%)	0	100	100
1	AB	385/390 (99%)	360 (94%)	21 (6%)	4 (1%)	12	15
1	AC	365/390 (94%)	338 (93%)	26 (7%)	1 (0%)	36	46
1	AD	380/390 (97%)	359 (94%)	21 (6%)	0	100	100
1	AE	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	24	31
1	AF	383/390 (98%)	361 (94%)	20 (5%)	2 (0%)	24	31
1	AG	365/390 (94%)	338 (93%)	23 (6%)	4 (1%)	11	13
1	AH	382/390 (98%)	337 (88%)	41 (11%)	4 (1%)	12	15
1	AI	364/390 (93%)	340 (93%)	21 (6%)	3 (1%)	16	20
1	AJ	383/390 (98%)	352 (92%)	27 (7%)	4 (1%)	12	15
1	AK	365/390 (94%)	347 (95%)	17 (5%)	1 (0%)	36	46
1	AL	382/390 (98%)	362 (95%)	20 (5%)	0	100	100
1	AM	365/390 (94%)	336 (92%)	24 (7%)	5 (1%)	9	9
1	AN	380/390 (97%)	351 (92%)	26 (7%)	3 (1%)	16	20
1	AO	364/390 (93%)	342 (94%)	18 (5%)	4 (1%)	11	13
1	AP	379/390 (97%)	355 (94%)	21 (6%)	3 (1%)	16	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AQ	364/390 (93%)	342 (94%)	21 (6%)	1 (0%)	36	46
1	AR	377/390 (97%)	351 (93%)	22 (6%)	4 (1%)	11	13
1	BA	365/390 (94%)	337 (92%)	23 (6%)	5 (1%)	9	9
1	BB	386/390 (99%)	358 (93%)	24 (6%)	4 (1%)	12	15
1	BC	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	36	46
1	BD	383/390 (98%)	351 (92%)	29 (8%)	3 (1%)	16	20
1	BE	365/390 (94%)	337 (92%)	25 (7%)	3 (1%)	16	20
1	BF	380/390 (97%)	344 (90%)	33 (9%)	3 (1%)	16	20
1	BG	365/390 (94%)	334 (92%)	29 (8%)	2 (0%)	24	31
1	BH	380/390 (97%)	353 (93%)	23 (6%)	4 (1%)	11	13
1	BI	365/390 (94%)	342 (94%)	22 (6%)	1 (0%)	36	46
1	BJ	383/390 (98%)	355 (93%)	26 (7%)	2 (0%)	24	31
1	BK	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	36	46
1	BL	379/390 (97%)	331 (87%)	40 (11%)	8 (2%)	5	4
1	BM	365/390 (94%)	345 (94%)	19 (5%)	1 (0%)	36	46
1	BN	380/390 (97%)	349 (92%)	26 (7%)	5 (1%)	9	10
1	BO	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	24	31
1	BP	380/390 (97%)	348 (92%)	29 (8%)	3 (1%)	16	20
1	BQ	364/390 (93%)	342 (94%)	20 (6%)	2 (0%)	24	31
1	BR	379/390 (97%)	353 (93%)	24 (6%)	2 (0%)	24	31
All	All	13426/14040 (96%)	12455 (93%)	874 (6%)	97 (1%)	18	23

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AH	168	VAL
1	AM	54	TRP
1	AM	336	GLU
1	BG	242	GLU
1	BH	242	GLU

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	AA	315/335 (94%)	288 (91%)	27 (9%)	10	13
1	AB	333/335 (99%)	315 (95%)	18 (5%)	20	29
1	AC	316/335 (94%)	297 (94%)	19 (6%)	17	25
1	AD	329/335 (98%)	310 (94%)	19 (6%)	18	26
1	AE	316/335 (94%)	298 (94%)	18 (6%)	18	27
1	AF	332/335 (99%)	314 (95%)	18 (5%)	20	29
1	AG	316/335 (94%)	300 (95%)	16 (5%)	21	32
1	AH	331/335 (99%)	311 (94%)	20 (6%)	17	25
1	AI	315/335 (94%)	295 (94%)	20 (6%)	16	23
1	AJ	332/335 (99%)	308 (93%)	24 (7%)	13	18
1	AK	316/335 (94%)	299 (95%)	17 (5%)	20	29
1	AL	331/335 (99%)	315 (95%)	16 (5%)	23	35
1	AM	316/335 (94%)	291 (92%)	25 (8%)	11	15
1	AN	329/335 (98%)	308 (94%)	21 (6%)	16	23
1	AO	315/335 (94%)	299 (95%)	16 (5%)	21	32
1	AP	328/335 (98%)	313 (95%)	15 (5%)	24	36
1	AQ	315/335 (94%)	294 (93%)	21 (7%)	15	21
1	AR	326/335 (97%)	304 (93%)	22 (7%)	15	21
1	BA	316/335 (94%)	297 (94%)	19 (6%)	17	25
1	BB	334/335 (100%)	313 (94%)	21 (6%)	16	23
1	BC	316/335 (94%)	297 (94%)	19 (6%)	17	25
1	BD	332/335 (99%)	315 (95%)	17 (5%)	21	32
1	BE	316/335 (94%)	301 (95%)	15 (5%)	23	35
1	BF	329/335 (98%)	311 (94%)	18 (6%)	19	28
1	BG	316/335 (94%)	299 (95%)	17 (5%)	20	29
1	BH	329/335 (98%)	314 (95%)	15 (5%)	24	36
1	BI	316/335 (94%)	296 (94%)	20 (6%)	16	23
1	BJ	332/335 (99%)	313 (94%)	19 (6%)	18	27
1	BK	316/335 (94%)	299 (95%)	17 (5%)	20	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BL	328/335 (98%)	305 (93%)	23 (7%)	14	19
1	BM	316/335 (94%)	298 (94%)	18 (6%)	18	27
1	BN	329/335 (98%)	309 (94%)	20 (6%)	17	24
1	BO	316/335 (94%)	302 (96%)	14 (4%)	25	38
1	BP	329/335 (98%)	315 (96%)	14 (4%)	26	39
1	BQ	315/335 (94%)	300 (95%)	15 (5%)	23	35
1	BR	328/335 (98%)	307 (94%)	21 (6%)	16	23
All	All	11624/12060 (96%)	10950 (94%)	674 (6%)	18	26

5 of 674 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BG	96	CYS
1	BM	36	LYS
1	BG	364	LEU
1	BG	38	ASN
1	BJ	191	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 209 such sidechains are listed below:

Mol	Chain	Res	Type
1	AR	280	HIS
1	BF	195	GLN
1	BQ	195	GLN
1	BA	38	ASN
1	BB	307	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 144 ligands modelled in this entry, 36 are monoatomic - leaving 108 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
5	NO3	BB	404	4	1,3,3	3.46	1 (100%)	0,3,3	-	-
5	NO3	AH	404	4	1,3,3	3.26	1 (100%)	0,3,3	-	-
5	NO3	BN	404	4	1,3,3	3.26	1 (100%)	0,3,3	-	-
5	NO3	BQ	404	4	1,3,3	3.31	1 (100%)	0,3,3	-	-
3	ADP	AQ	402	4	28,29,29	1.37	5 (17%)	43,45,45	1.82	12 (27%)
3	ADP	BH	402	4	28,29,29	1.57	6 (21%)	43,45,45	1.69	7 (16%)
3	ADP	BA	502	4	28,29,29	1.43	5 (17%)	43,45,45	1.90	15 (34%)
5	NO3	BG	404	4	1,3,3	3.25	1 (100%)	0,3,3	-	-
3	ADP	AA	502	4	28,29,29	1.48	5 (17%)	43,45,45	1.79	9 (20%)
3	ADP	BM	402	4	28,29,29	1.49	5 (17%)	43,45,45	1.86	12 (27%)
3	ADP	AR	402	4	28,29,29	1.44	5 (17%)	43,45,45	1.76	10 (23%)
2	NMG	BB	401	-	7,7,7	0.79	0	8,8,8	2.93	1 (12%)
3	ADP	BK	402	4	28,29,29	1.56	5 (17%)	43,45,45	1.79	10 (23%)
3	ADP	BF	402	4	28,29,29	1.45	5 (17%)	43,45,45	1.93	13 (30%)
5	NO3	AP	404	4	1,3,3	3.24	1 (100%)	0,3,3	-	-
5	NO3	AL	404	4	1,3,3	3.34	1 (100%)	0,3,3	-	-
2	NMG	BP	401	-	7,7,7	0.83	0	8,8,8	2.67	1 (12%)
2	NMG	BM	401	-	7,7,7	0.75	0	8,8,8	1.88	1 (12%)
5	NO3	AA	504	4	1,3,3	3.28	1 (100%)	0,3,3	-	-
3	ADP	BQ	402	4	28,29,29	1.45	5 (17%)	43,45,45	1.80	9 (20%)
3	ADP	AK	402	4	28,29,29	1.42	5 (17%)	43,45,45	1.87	12 (27%)
5	NO3	BA	504	4	1,3,3	3.29	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	AC	402	4	28,29,29	1.56	6 (21%)	43,45,45	1.80	9 (20%)
3	ADP	AG	402	4	28,29,29	1.38	5 (17%)	43,45,45	1.85	10 (23%)
3	ADP	AN	402	4	28,29,29	1.56	5 (17%)	43,45,45	1.85	11 (25%)
2	NMG	BI	401	-	7,7,7	0.81	0	8,8,8	2.45	1 (12%)
5	NO3	AR	404	4	1,3,3	3.45	1 (100%)	0,3,3	-	-
3	ADP	BJ	402	4	28,29,29	1.58	5 (17%)	43,45,45	1.80	12 (27%)
2	NMG	AO	401	-	7,7,7	0.79	0	8,8,8	1.67	1 (12%)
5	NO3	AF	404	4	1,3,3	3.25	1 (100%)	0,3,3	-	-
2	NMG	AB	401	-	7,7,7	0.81	0	8,8,8	2.66	1 (12%)
2	NMG	AH	401	-	7,7,7	0.78	0	8,8,8	1.89	1 (12%)
3	ADP	BP	402	4	28,29,29	1.51	6 (21%)	43,45,45	1.99	14 (32%)
2	NMG	AJ	401	-	7,7,7	0.77	0	8,8,8	1.88	1 (12%)
2	NMG	BE	401	-	7,7,7	0.78	0	8,8,8	1.96	1 (12%)
2	NMG	BK	401	-	7,7,7	0.77	0	8,8,8	2.03	1 (12%)
3	ADP	AP	402	4	28,29,29	1.43	4 (14%)	43,45,45	1.91	10 (23%)
3	ADP	AL	402	4	28,29,29	1.53	5 (17%)	43,45,45	1.72	9 (20%)
5	NO3	AK	404	4	1,3,3	3.32	1 (100%)	0,3,3	-	-
3	ADP	BI	402	4	28,29,29	1.41	5 (17%)	43,45,45	1.88	10 (23%)
2	NMG	AE	401	-	7,7,7	0.77	0	8,8,8	2.50	2 (25%)
3	ADP	BE	402	4	28,29,29	1.53	5 (17%)	43,45,45	1.91	11 (25%)
5	NO3	BM	404	4	1,3,3	3.28	1 (100%)	0,3,3	-	-
5	NO3	AI	404	4	1,3,3	3.50	1 (100%)	0,3,3	-	-
3	ADP	AH	402	4	28,29,29	1.43	4 (14%)	43,45,45	1.75	9 (20%)
3	ADP	BN	402	4	28,29,29	1.51	5 (17%)	43,45,45	1.84	10 (23%)
3	ADP	BC	402	4	28,29,29	1.42	6 (21%)	43,45,45	1.77	11 (25%)
5	NO3	AD	404	4	1,3,3	3.26	1 (100%)	0,3,3	-	-
2	NMG	BN	401	-	7,7,7	0.83	0	8,8,8	1.81	1 (12%)
3	ADP	AB	402	4	28,29,29	1.45	5 (17%)	43,45,45	1.86	12 (27%)
2	NMG	AF	401	-	7,7,7	0.94	0	8,8,8	2.21	1 (12%)
2	NMG	BG	401	-	7,7,7	0.80	0	8,8,8	1.56	1 (12%)
3	ADP	AJ	402	4	28,29,29	1.52	5 (17%)	43,45,45	1.87	11 (25%)
5	NO3	AQ	404	4	1,3,3	3.30	1 (100%)	0,3,3	-	-
5	NO3	AM	404	4	1,3,3	3.22	1 (100%)	0,3,3	-	-
2	NMG	BF	401	-	7,7,7	0.81	0	8,8,8	2.28	1 (12%)
5	NO3	BP	404	-	1,3,3	3.29	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NO3	BH	404	4	1,3,3	3.31	1 (100%)	0,3,3	-	-
5	NO3	BJ	404	4	1,3,3	3.20	1 (100%)	0,3,3	-	-
3	ADP	BO	402	4	28,29,29	1.54	6 (21%)	43,45,45	1.95	11 (25%)
3	ADP	AE	402	4	28,29,29	1.53	5 (17%)	43,45,45	1.80	9 (20%)
2	NMG	AA	501	-	7,7,7	0.77	0	8,8,8	2.18	1 (12%)
5	NO3	AC	404	4	1,3,3	3.28	1 (100%)	0,3,3	-	-
2	NMG	BD	401	-	7,7,7	0.83	0	8,8,8	2.00	1 (12%)
3	ADP	BR	402	4	28,29,29	1.58	5 (17%)	43,45,45	1.82	10 (23%)
2	NMG	AL	401	-	7,7,7	0.80	0	8,8,8	2.00	1 (12%)
5	NO3	BK	404	4	1,3,3	3.25	1 (100%)	0,3,3	-	-
5	NO3	BF	404	4	1,3,3	3.46	1 (100%)	0,3,3	-	-
3	ADP	BD	402	4	28,29,29	1.43	4 (14%)	43,45,45	1.86	10 (23%)
5	NO3	AB	404	4	1,3,3	3.12	1 (100%)	0,3,3	-	-
3	ADP	BB	402	4	28,29,29	1.47	4 (14%)	43,45,45	1.92	10 (23%)
2	NMG	BL	401	-	7,7,7	0.80	0	8,8,8	1.98	1 (12%)
3	ADP	BG	402	4	28,29,29	1.44	5 (17%)	43,45,45	1.88	10 (23%)
2	NMG	BA	501	-	7,7,7	0.78	0	8,8,8	2.10	1 (12%)
3	ADP	BL	402	4	28,29,29	1.47	6 (21%)	43,45,45	1.75	10 (23%)
3	ADP	AM	402	4	28,29,29	1.54	5 (17%)	43,45,45	1.79	11 (25%)
5	NO3	AN	404	4	1,3,3	3.25	1 (100%)	0,3,3	-	-
3	ADP	AO	402	4	28,29,29	1.40	5 (17%)	43,45,45	1.83	11 (25%)
5	NO3	BL	404	4	1,3,3	3.39	1 (100%)	0,3,3	-	-
2	NMG	AR	401	-	7,7,7	0.77	0	8,8,8	2.76	1 (12%)
5	NO3	AJ	404	4	1,3,3	3.27	1 (100%)	0,3,3	-	-
2	NMG	AC	401	-	7,7,7	0.80	0	8,8,8	1.98	1 (12%)
2	NMG	AM	401	-	7,7,7	0.91	0	8,8,8	1.86	1 (12%)
5	NO3	BD	404	4	1,3,3	3.23	1 (100%)	0,3,3	-	-
5	NO3	BI	404	4	1,3,3	3.41	1 (100%)	0,3,3	-	-
2	NMG	AK	401	-	7,7,7	0.76	0	8,8,8	1.32	1 (12%)
2	NMG	BQ	401	-	7,7,7	0.83	0	8,8,8	1.51	1 (12%)
2	NMG	BC	401	-	7,7,7	0.79	0	8,8,8	1.76	1 (12%)
2	NMG	BO	401	-	7,7,7	0.68	0	8,8,8	2.30	2 (25%)
2	NMG	AP	401	-	7,7,7	0.76	0	8,8,8	1.85	1 (12%)
5	NO3	BC	404	4	1,3,3	3.47	1 (100%)	0,3,3	-	-
2	NMG	AG	401	-	7,7,7	0.75	0	8,8,8	1.56	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	AF	402	4	28,29,29	1.50	5 (17%)	43,45,45	1.83	9 (20%)
5	NO3	AE	404	4	1,3,3	3.46	1 (100%)	0,3,3	-	-
2	NMG	AN	401	-	7,7,7	0.76	0	8,8,8	2.11	1 (12%)
2	NMG	BJ	401	-	7,7,7	0.79	0	8,8,8	2.18	1 (12%)
5	NO3	BO	404	4	1,3,3	3.33	1 (100%)	0,3,3	-	-
5	NO3	AG	404	4	1,3,3	3.45	1 (100%)	0,3,3	-	-
2	NMG	AD	401	-	7,7,7	0.76	0	8,8,8	1.75	1 (12%)
3	ADP	AI	402	4	28,29,29	1.59	6 (21%)	43,45,45	1.77	11 (25%)
5	NO3	BR	404	4	1,3,3	3.40	1 (100%)	0,3,3	-	-
2	NMG	BR	401	-	7,7,7	0.89	0	8,8,8	2.53	1 (12%)
5	NO3	BE	404	4	1,3,3	3.24	1 (100%)	0,3,3	-	-
2	NMG	AI	401	-	7,7,7	0.78	0	8,8,8	2.13	1 (12%)
3	ADP	AD	402	4	28,29,29	1.59	6 (21%)	43,45,45	1.76	9 (20%)
2	NMG	AQ	401	-	7,7,7	0.79	0	8,8,8	3.01	1 (12%)
5	NO3	AO	404	4	1,3,3	3.24	1 (100%)	0,3,3	-	-
2	NMG	BH	401	-	7,7,7	0.87	0	8,8,8	1.71	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	AA	501	-	-	1/5/5/5	-
3	ADP	BJ	402	4	-	4/16/32/32	0/3/3/3
2	NMG	AO	401	-	-	2/5/5/5	-
2	NMG	AB	401	-	-	0/5/5/5	-
2	NMG	BD	401	-	-	0/5/5/5	-
3	ADP	AQ	402	4	-	5/16/32/32	0/3/3/3
3	ADP	BR	402	4	-	3/16/32/32	0/3/3/3
2	NMG	AL	401	-	-	1/5/5/5	-
3	ADP	BH	402	4	-	4/16/32/32	0/3/3/3
2	NMG	AH	401	-	-	0/5/5/5	-
2	NMG	AK	401	-	-	1/5/5/5	-
3	ADP	BA	502	4	-	5/16/32/32	0/3/3/3
2	NMG	BQ	401	-	-	0/5/5/5	-
3	ADP	BO	402	4	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	AJ	401	-	-	0/5/5/5	-
3	ADP	BP	402	4	-	5/16/32/32	0/3/3/3
3	ADP	AA	502	4	-	2/16/32/32	0/3/3/3
2	NMG	BC	401	-	-	1/5/5/5	-
2	NMG	BE	401	-	-	2/5/5/5	-
2	NMG	BK	401	-	-	1/5/5/5	-
2	NMG	BO	401	-	-	0/5/5/5	-
2	NMG	AP	401	-	-	0/5/5/5	-
3	ADP	BM	402	4	-	6/16/32/32	0/3/3/3
2	NMG	BI	401	-	-	1/5/5/5	-
2	NMG	AG	401	-	-	0/5/5/5	-
3	ADP	AP	402	4	-	5/16/32/32	0/3/3/3
3	ADP	AR	402	4	-	5/16/32/32	0/3/3/3
2	NMG	BB	401	-	-	0/5/5/5	-
3	ADP	BB	402	4	-	2/16/32/32	0/3/3/3
3	ADP	BD	402	4	-	6/16/32/32	0/3/3/3
3	ADP	AF	402	4	-	2/16/32/32	0/3/3/3
3	ADP	AL	402	4	-	2/16/32/32	0/3/3/3
2	NMG	AN	401	-	-	0/5/5/5	-
2	NMG	BL	401	-	-	0/5/5/5	-
3	ADP	BI	402	4	-	5/16/32/32	0/3/3/3
2	NMG	AE	401	-	-	0/5/5/5	-
3	ADP	BE	402	4	-	5/16/32/32	0/3/3/3
2	NMG	BJ	401	-	-	0/5/5/5	-
3	ADP	BG	402	4	-	3/16/32/32	0/3/3/3
3	ADP	BK	402	4	-	6/16/32/32	0/3/3/3
3	ADP	BF	402	4	-	0/16/32/32	0/3/3/3
3	ADP	AH	402	4	-	3/16/32/32	0/3/3/3
3	ADP	BN	402	4	-	5/16/32/32	0/3/3/3
2	NMG	BA	501	-	-	0/5/5/5	-
3	ADP	BL	402	4	-	0/16/32/32	0/3/3/3
3	ADP	BC	402	4	-	3/16/32/32	0/3/3/3
2	NMG	BP	401	-	-	0/5/5/5	-
3	ADP	AM	402	4	-	8/16/32/32	0/3/3/3
2	NMG	BN	401	-	-	1/5/5/5	-
3	ADP	AB	402	4	-	3/16/32/32	0/3/3/3
2	NMG	BM	401	-	-	0/5/5/5	-
2	NMG	AD	401	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	AO	402	4	-	5/16/32/32	0/3/3/3
3	ADP	BQ	402	4	-	9/16/32/32	0/3/3/3
3	ADP	AK	402	4	-	1/16/32/32	0/3/3/3
2	NMG	AR	401	-	-	0/5/5/5	-
3	ADP	AE	402	4	-	5/16/32/32	0/3/3/3
2	NMG	AF	401	-	-	0/5/5/5	-
2	NMG	BG	401	-	-	0/5/5/5	-
3	ADP	AJ	402	4	-	6/16/32/32	0/3/3/3
3	ADP	AI	402	4	-	1/16/32/32	0/3/3/3
2	NMG	AC	401	-	-	0/5/5/5	-
3	ADP	AC	402	4	-	2/16/32/32	0/3/3/3
3	ADP	AG	402	4	-	4/16/32/32	0/3/3/3
2	NMG	BF	401	-	-	0/5/5/5	-
2	NMG	BR	401	-	-	0/5/5/5	-
2	NMG	AI	401	-	-	0/5/5/5	-
3	ADP	AD	402	4	-	5/16/32/32	0/3/3/3
3	ADP	AN	402	4	-	3/16/32/32	0/3/3/3
2	NMG	AQ	401	-	-	0/5/5/5	-
2	NMG	AM	401	-	-	0/5/5/5	-
2	NMG	BH	401	-	-	0/5/5/5	-

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AM	402	ADP	C5-C4	5.02	1.48	1.39
3	AL	402	ADP	C5-C4	4.96	1.47	1.39
3	AR	402	ADP	C5-C4	4.92	1.47	1.39
3	BE	402	ADP	C5-C4	4.92	1.47	1.39
3	AD	402	ADP	C5-C4	4.91	1.47	1.39

The worst 5 of 417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AQ	401	NMG	CD-NE-CZ	8.19	130.02	122.39
2	BB	401	NMG	CD-NE-CZ	7.81	129.66	122.39
2	AR	401	NMG	CD-NE-CZ	7.55	129.42	122.39
2	BP	401	NMG	CD-NE-CZ	7.28	129.17	122.39
2	AB	401	NMG	CD-NE-CZ	7.05	128.96	122.39

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AB	402	ADP	C5'-O5'-PA-O1A
3	AD	402	ADP	O4'-C4'-C5'-O5'
3	AE	402	ADP	C5'-O5'-PA-O2A
3	AG	402	ADP	C5'-O5'-PA-O2A
3	AG	402	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

56 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BB	404	NO3	1	0
3	AQ	402	ADP	3	0
3	BH	402	ADP	2	0
3	BA	502	ADP	3	0
3	AA	502	ADP	1	0
3	BM	402	ADP	4	0
3	AR	402	ADP	2	0
2	BB	401	NMG	1	0
3	BK	402	ADP	1	0
3	BF	402	ADP	4	0
3	BQ	402	ADP	3	0
3	AK	402	ADP	5	0
3	AC	402	ADP	1	0
3	AG	402	ADP	2	0
3	AN	402	ADP	1	0
5	AR	404	NO3	1	0
3	BJ	402	ADP	2	0
2	AO	401	NMG	1	0
2	AB	401	NMG	3	0
3	BP	402	ADP	2	0
3	AP	402	ADP	5	0
3	AL	402	ADP	1	0
3	BI	402	ADP	2	0
2	AE	401	NMG	1	0
3	BE	402	ADP	4	0
3	AH	402	ADP	3	0
3	BN	402	ADP	3	0
3	BC	402	ADP	1	0
5	AD	404	NO3	1	0
3	AB	402	ADP	2	0
3	AJ	402	ADP	3	0

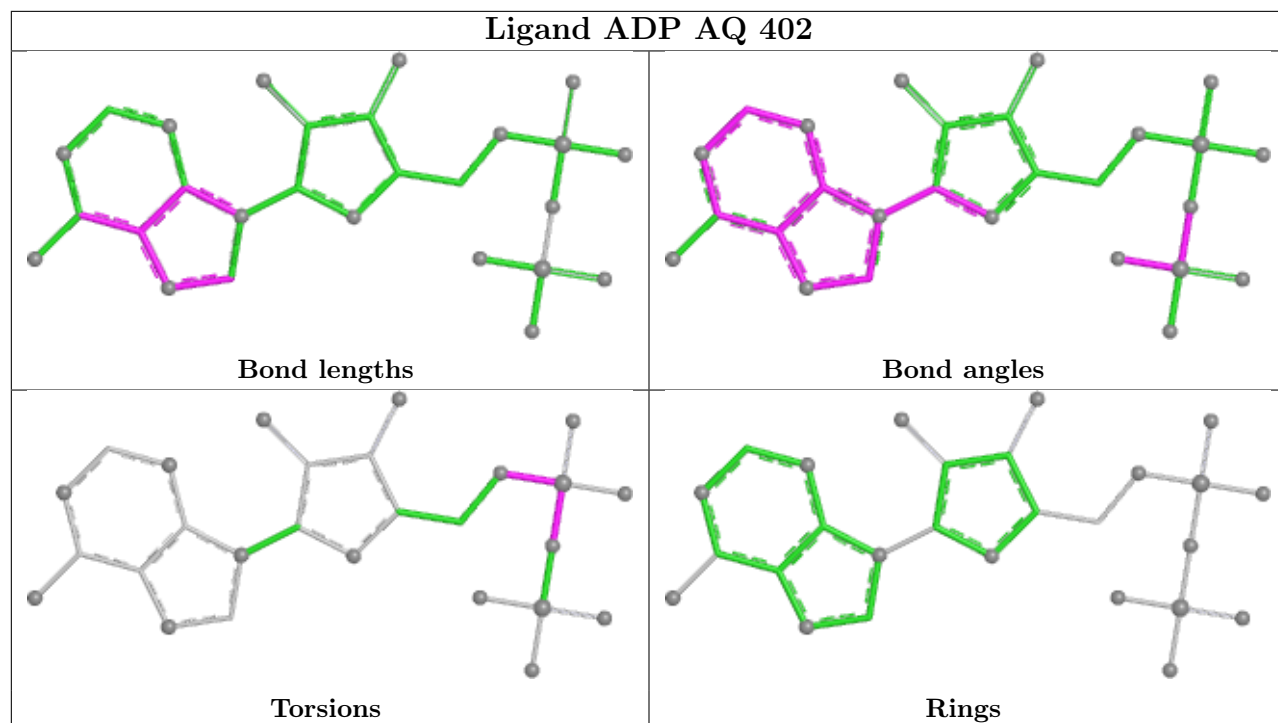
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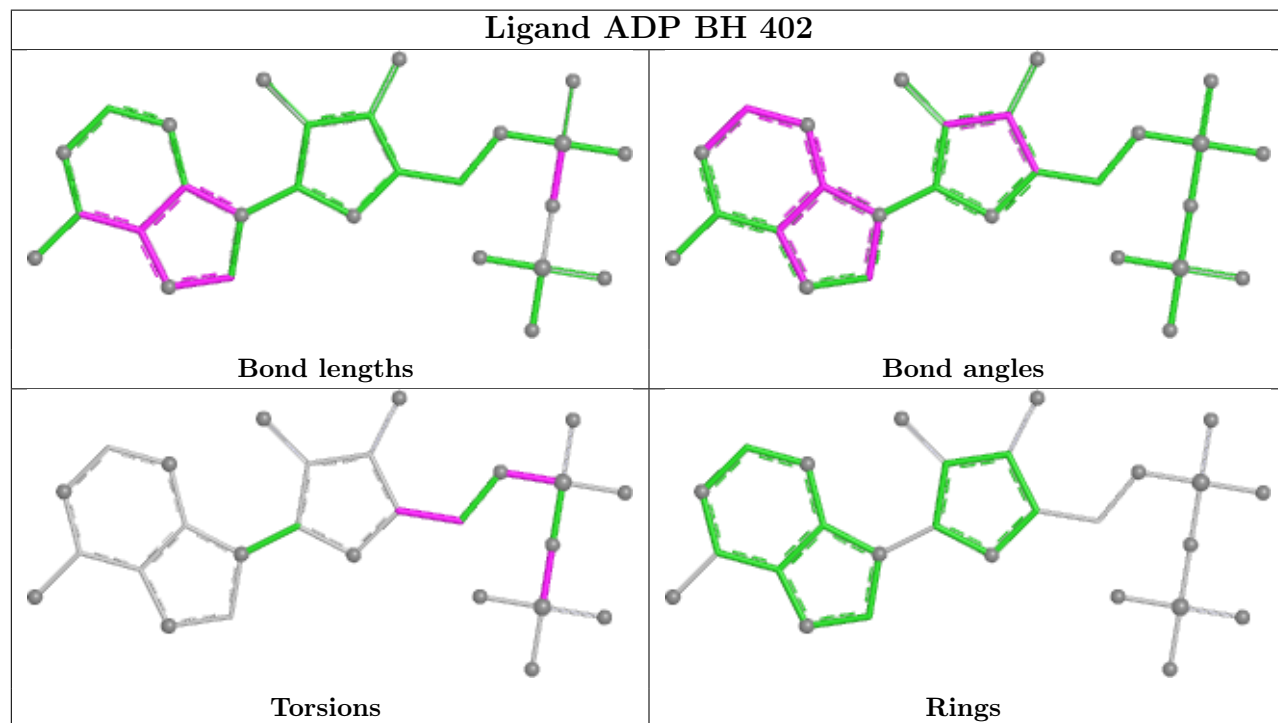
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BH	404	NO3	1	0
3	BO	402	ADP	2	0
3	AE	402	ADP	4	0
2	BD	401	NMG	1	0
3	BR	402	ADP	3	0
5	BK	404	NO3	1	0
3	BD	402	ADP	3	0
3	BB	402	ADP	4	0
3	BG	402	ADP	3	0
3	BL	402	ADP	2	0
3	AM	402	ADP	2	0
3	AO	402	ADP	4	0
2	AM	401	NMG	1	0
5	BD	404	NO3	1	0
2	BO	401	NMG	2	0
2	AG	401	NMG	2	0
3	AF	402	ADP	7	0
2	AN	401	NMG	1	0
2	BJ	401	NMG	1	0
3	AI	402	ADP	3	0
5	BR	404	NO3	1	0
2	BR	401	NMG	1	0
2	AI	401	NMG	1	0
5	AO	404	NO3	1	0
2	BH	401	NMG	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.

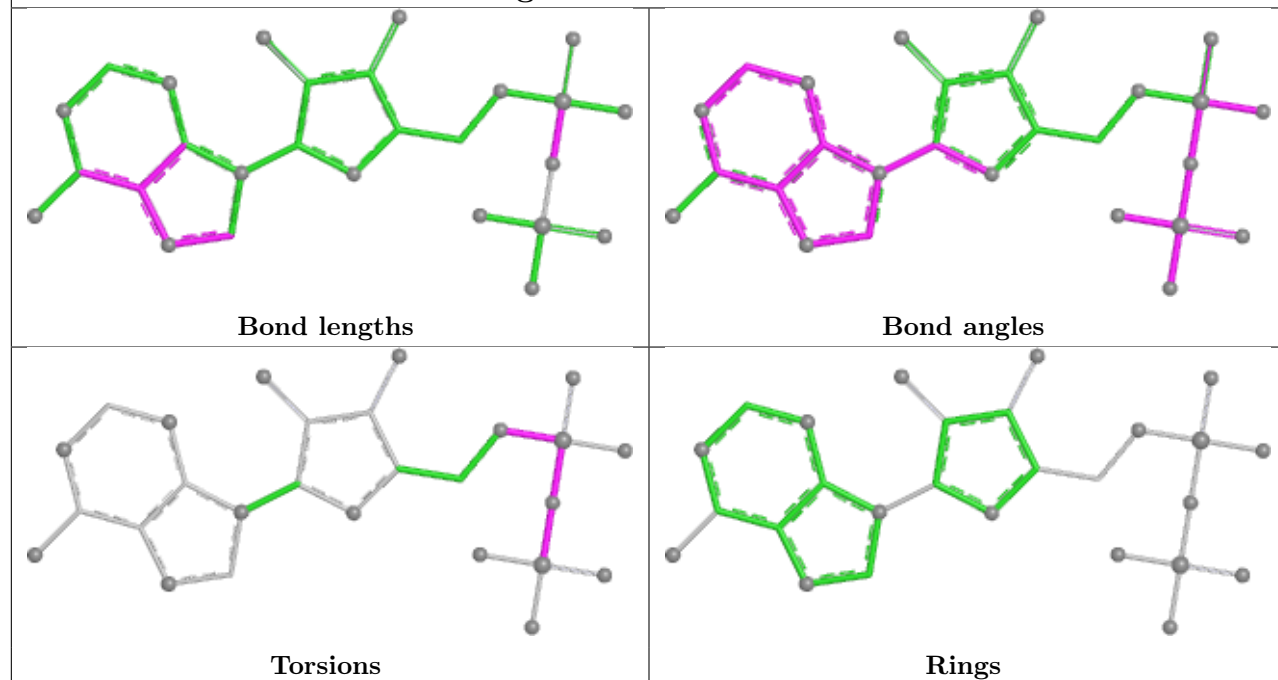
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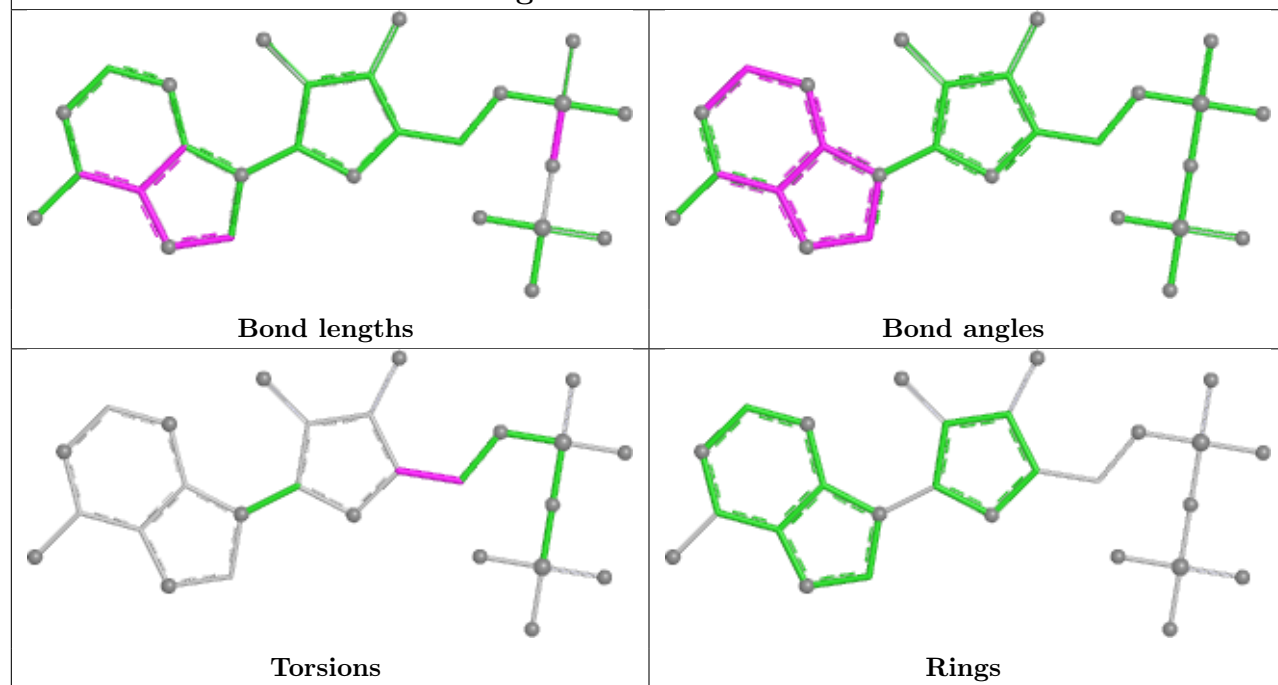
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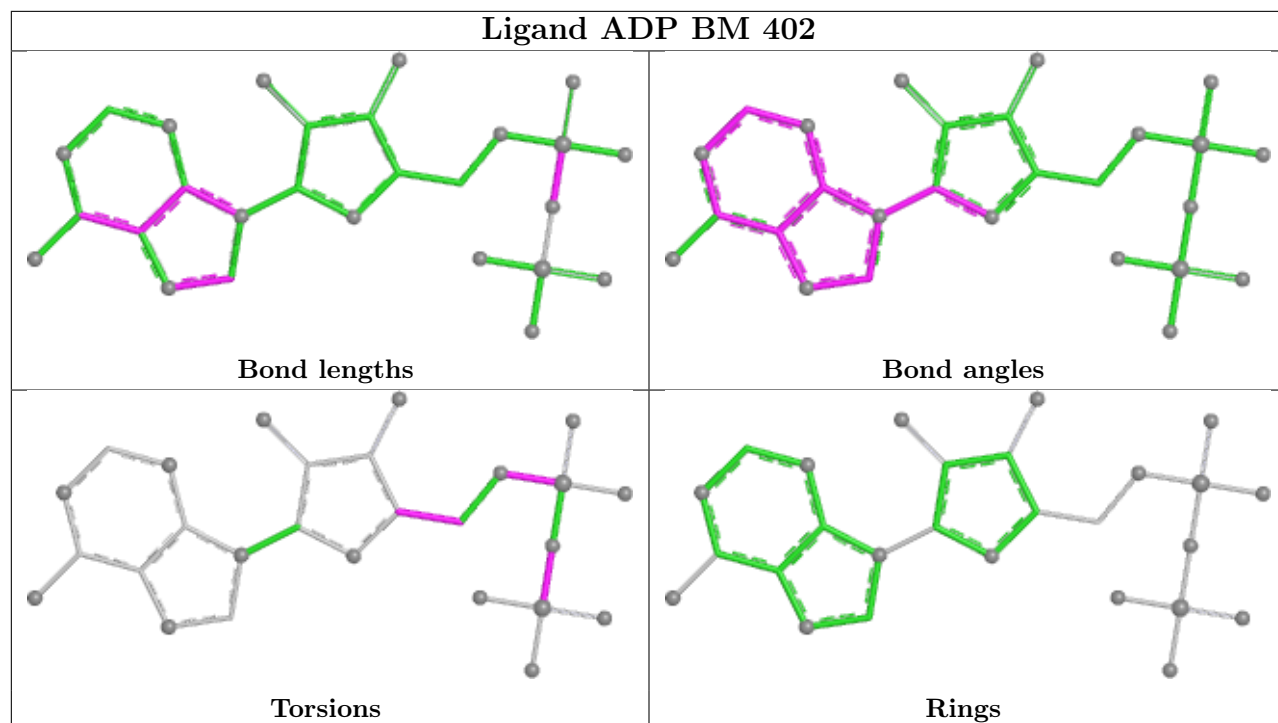
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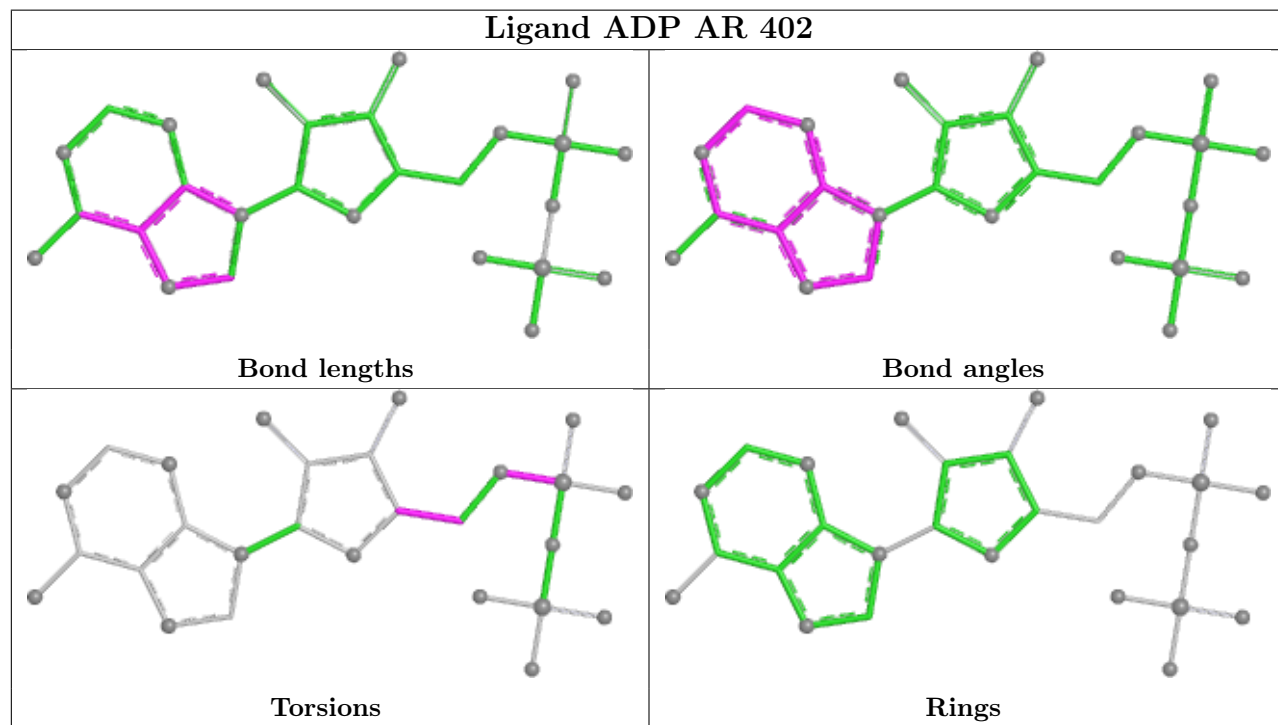
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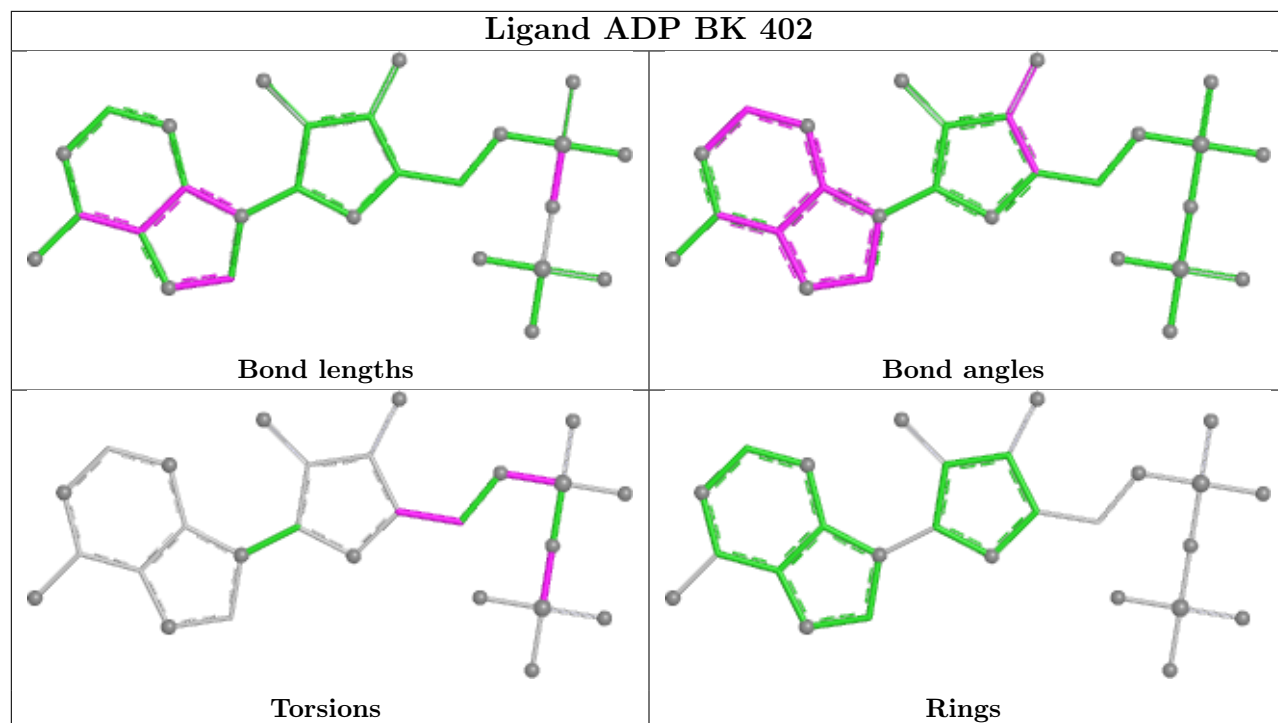
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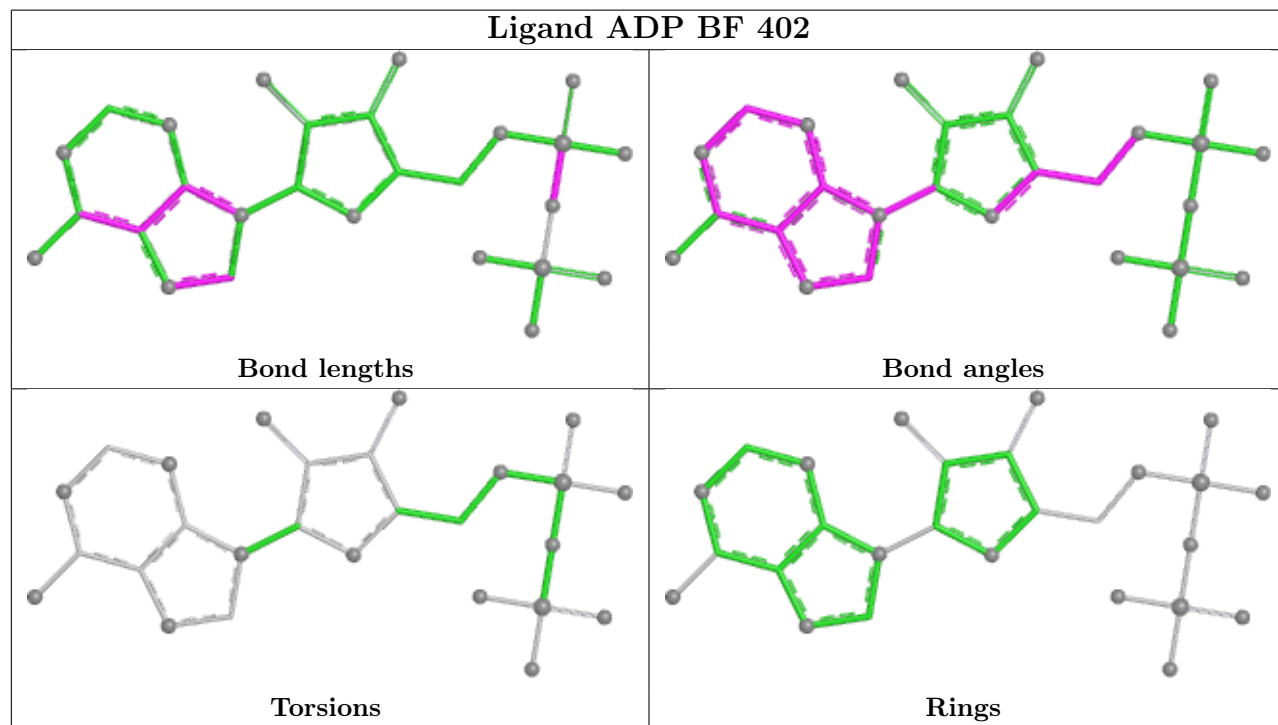
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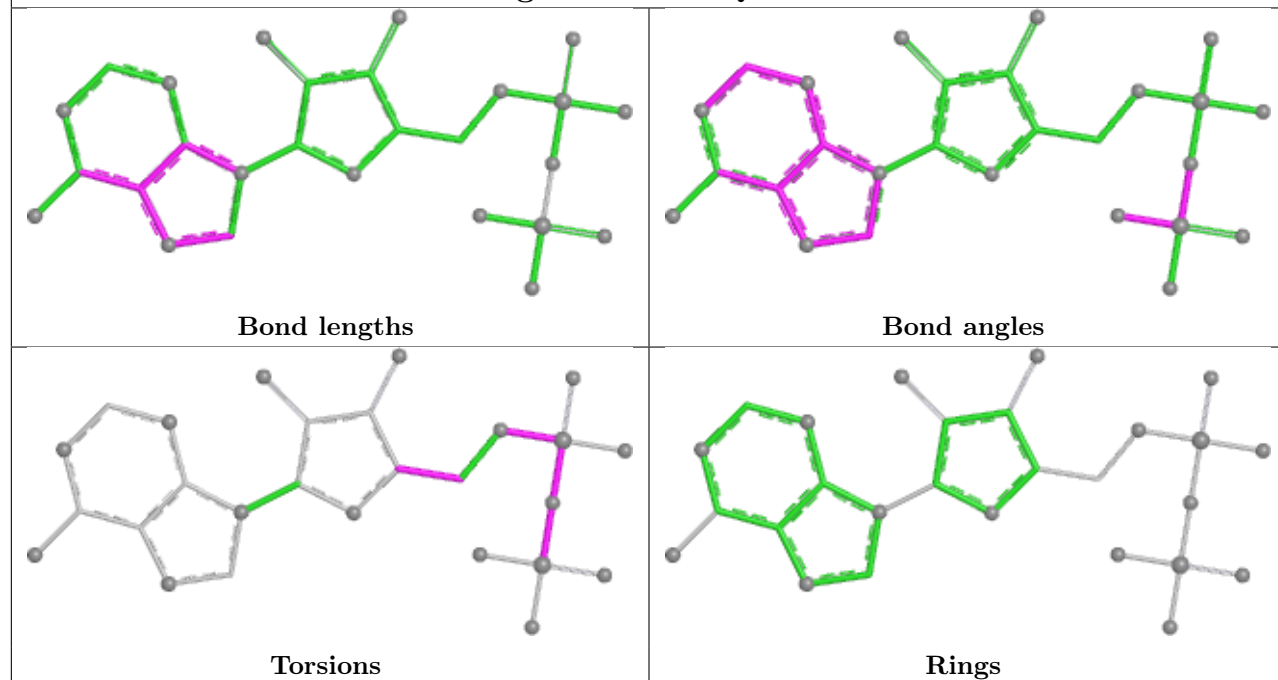
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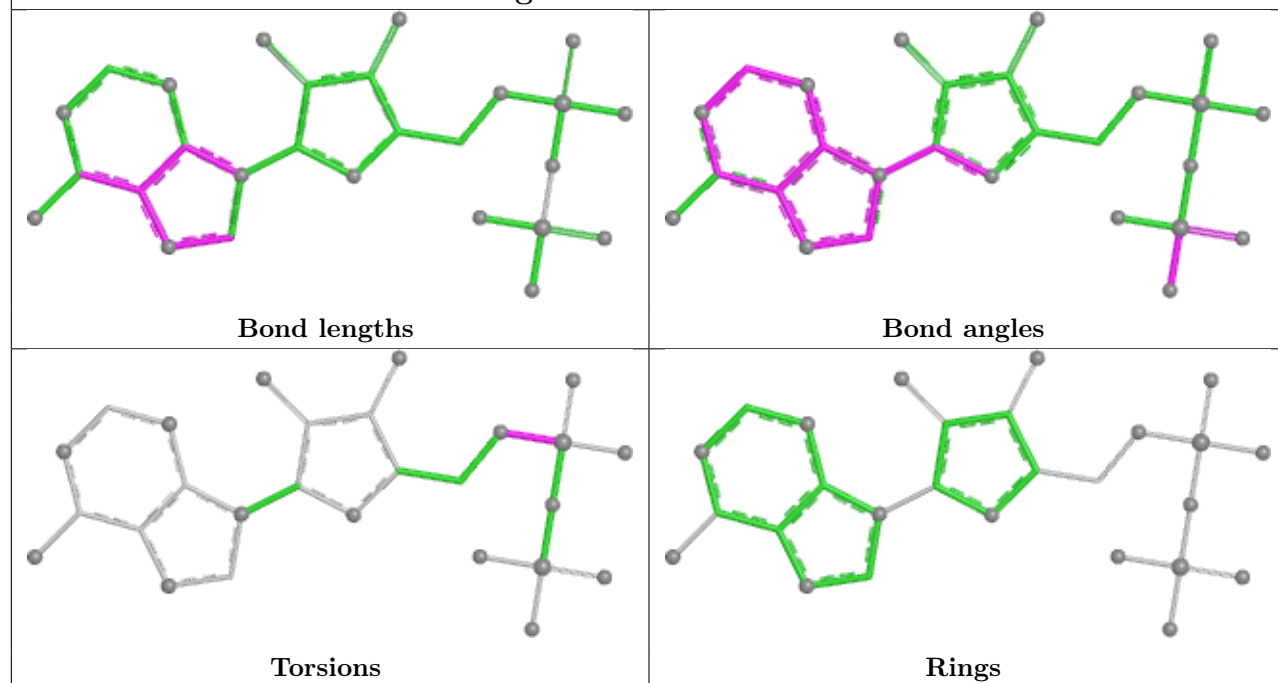
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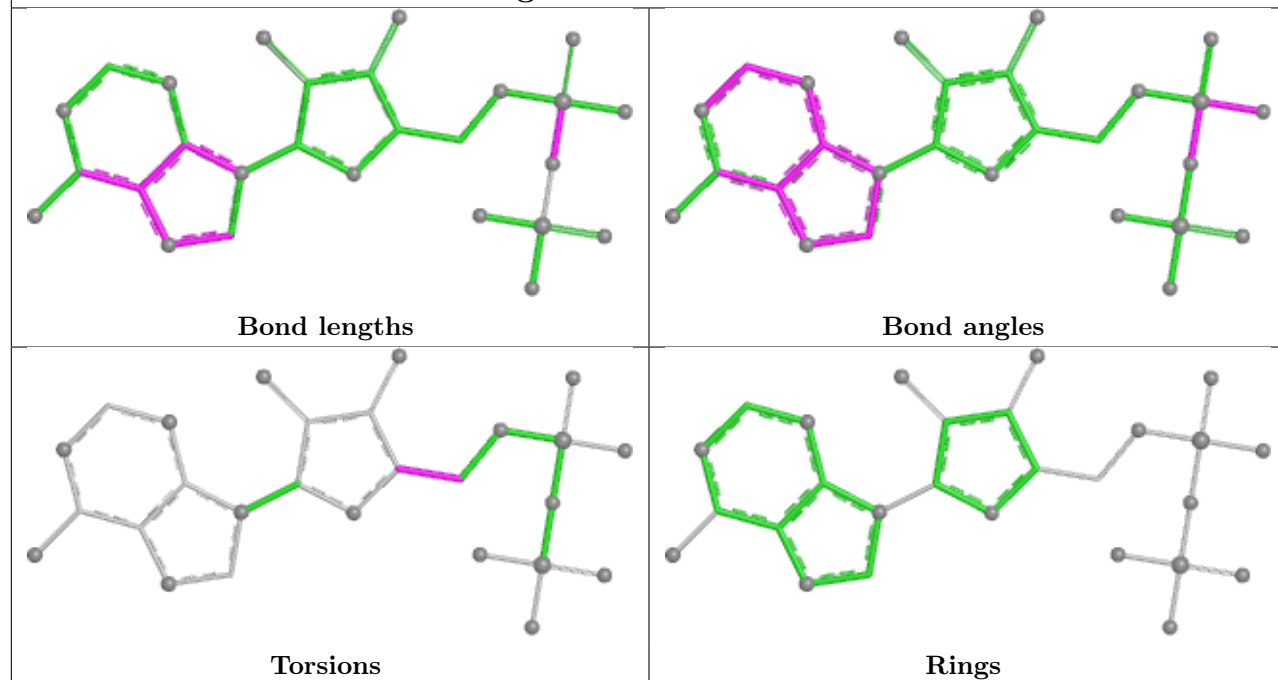
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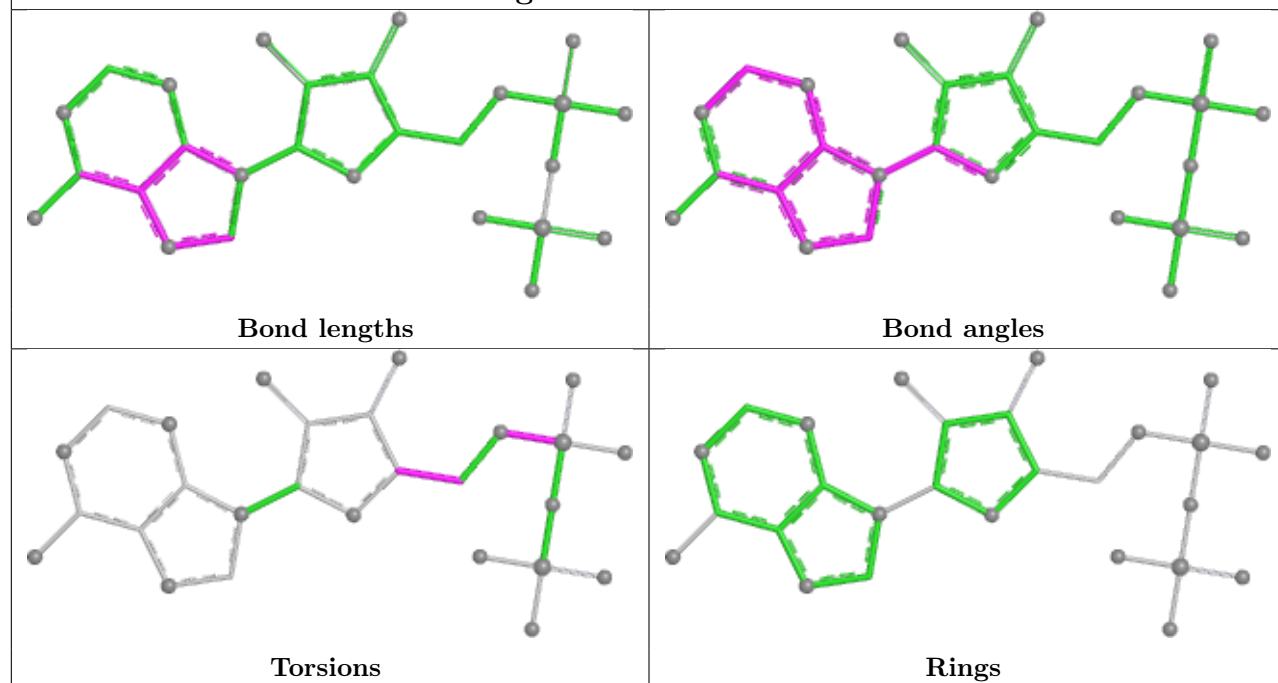
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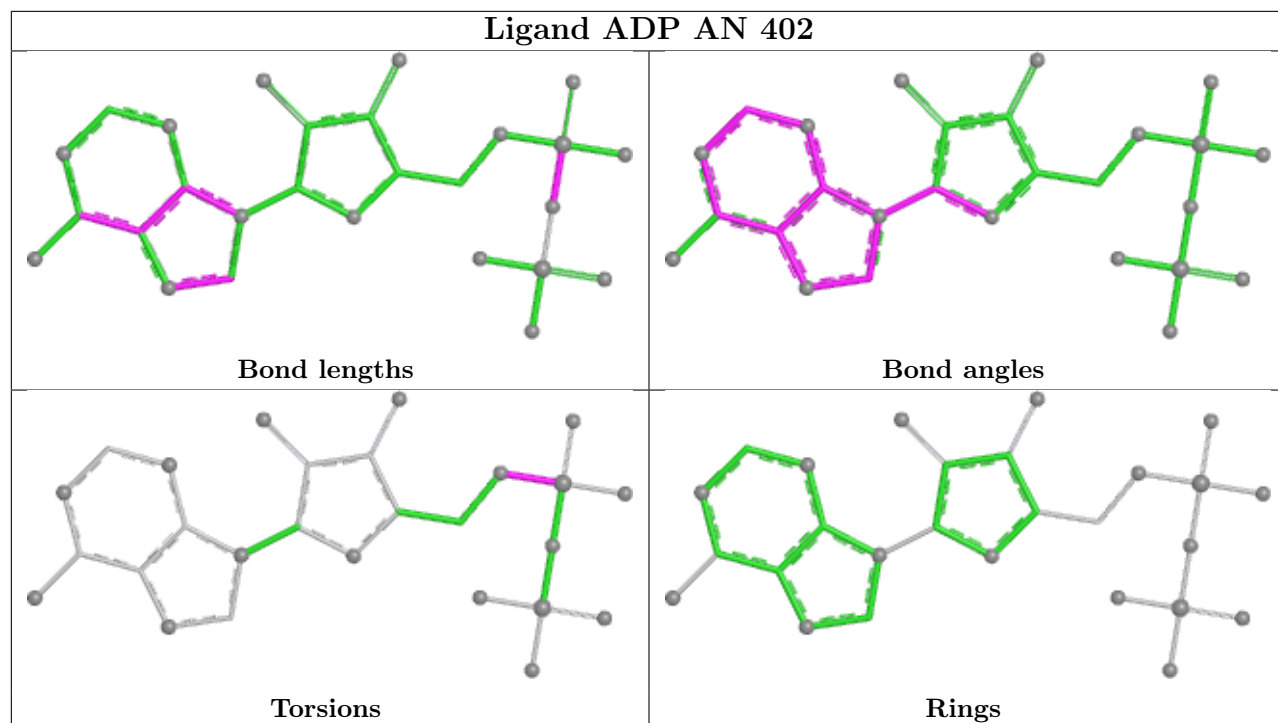
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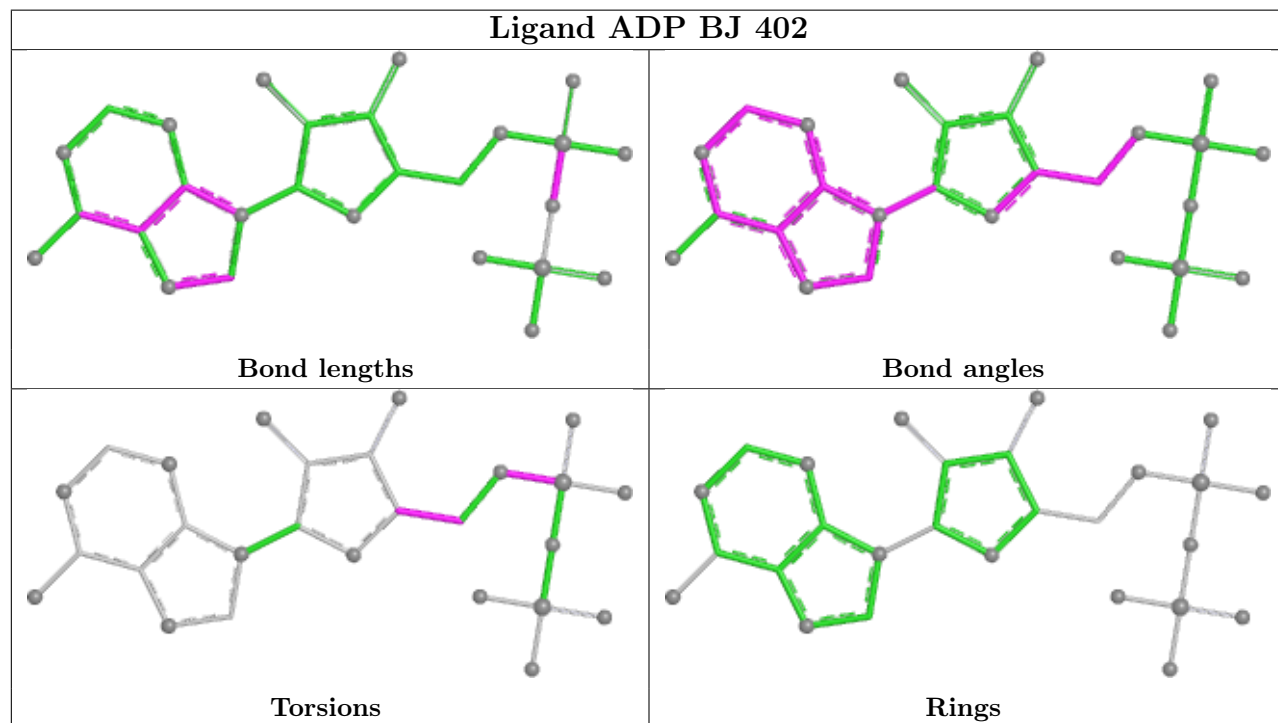
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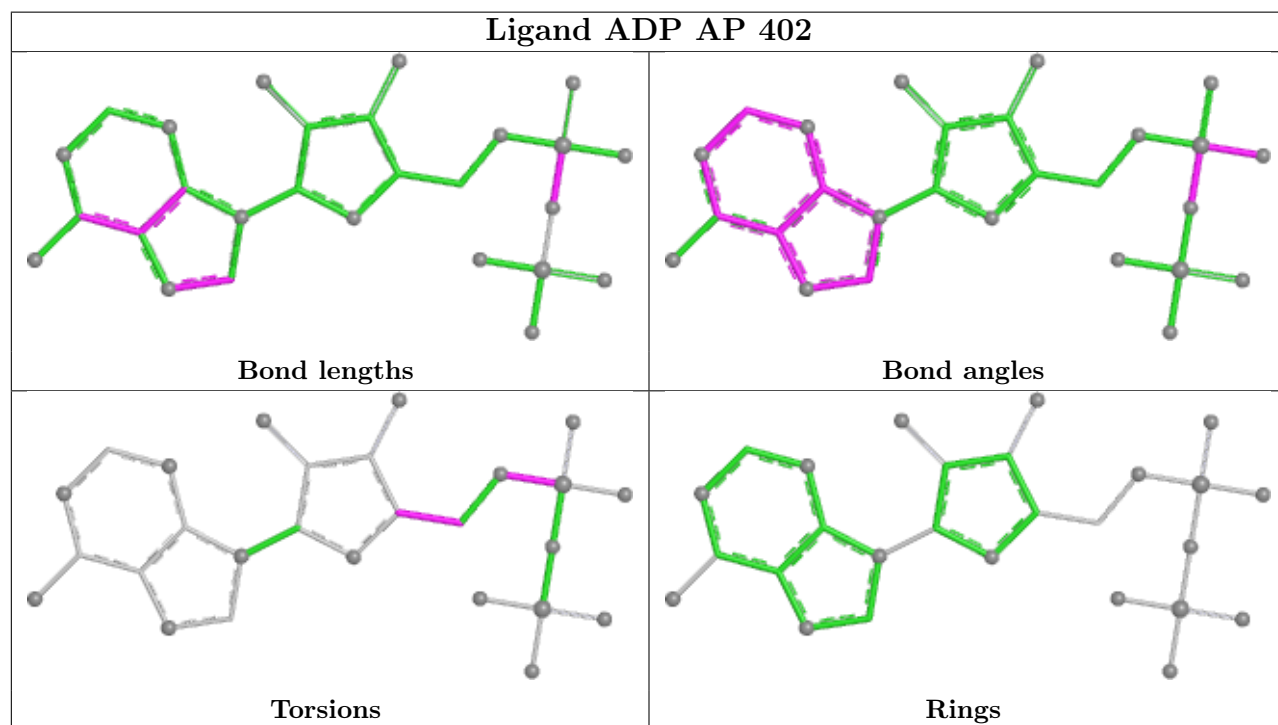
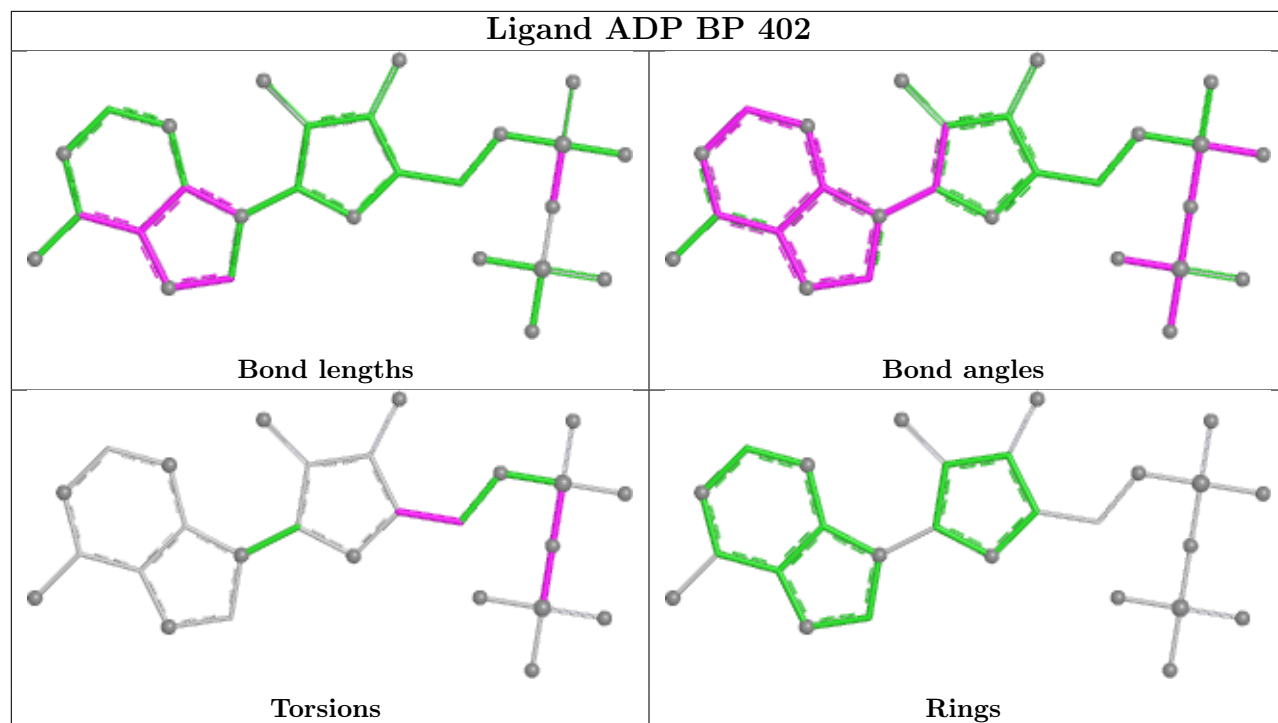


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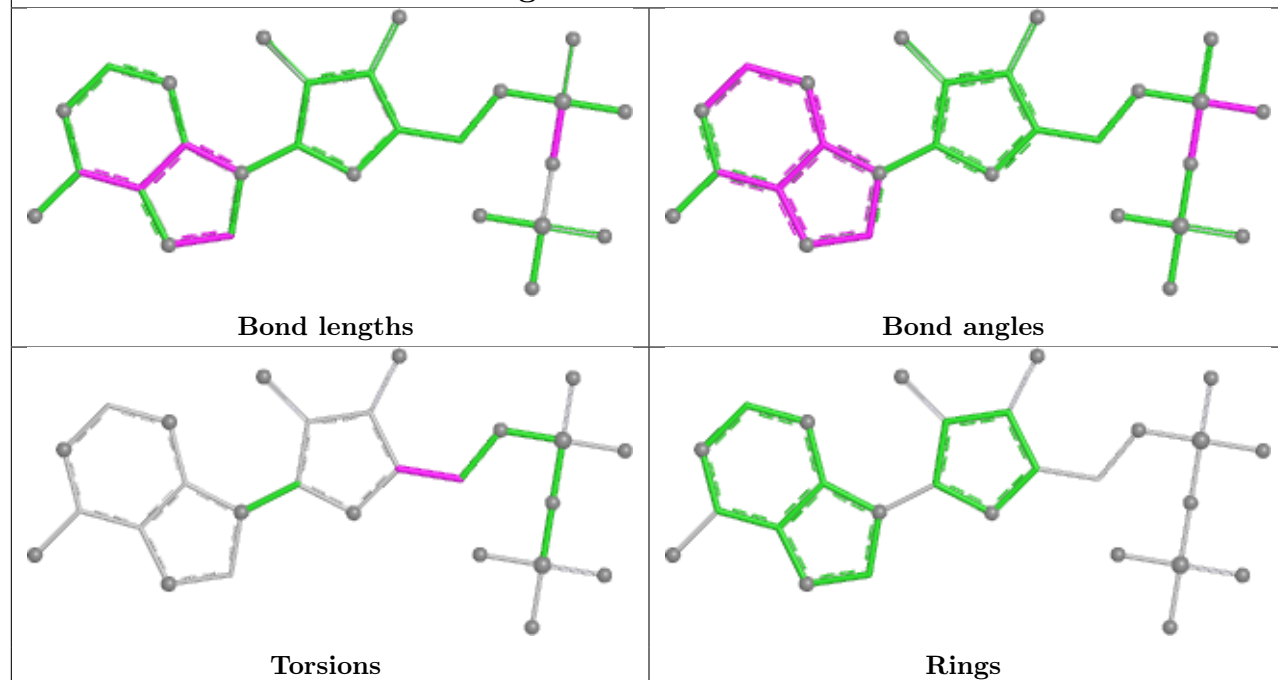


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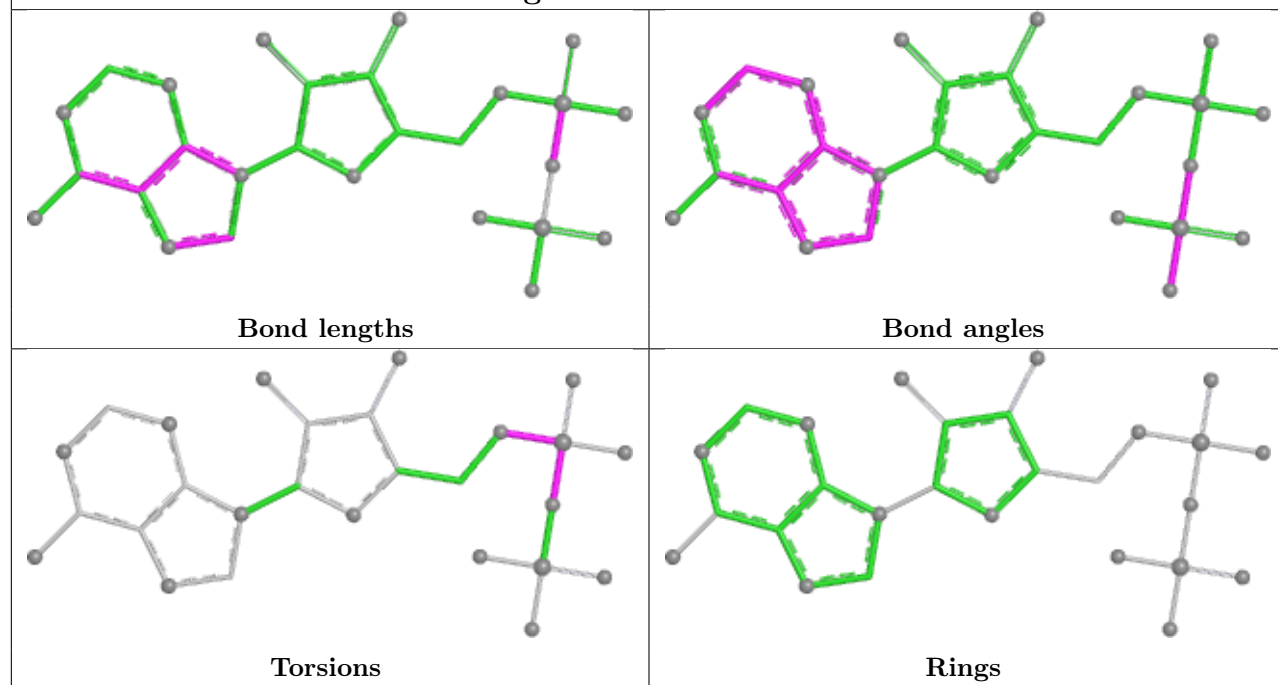


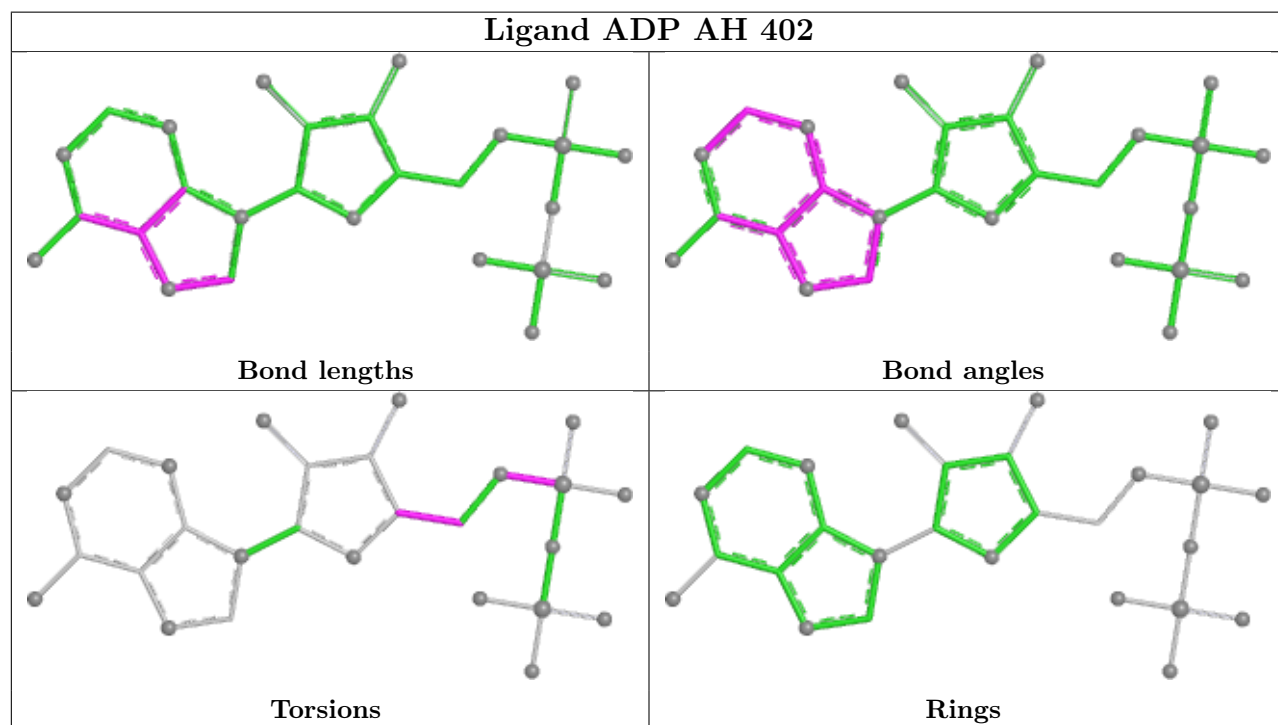
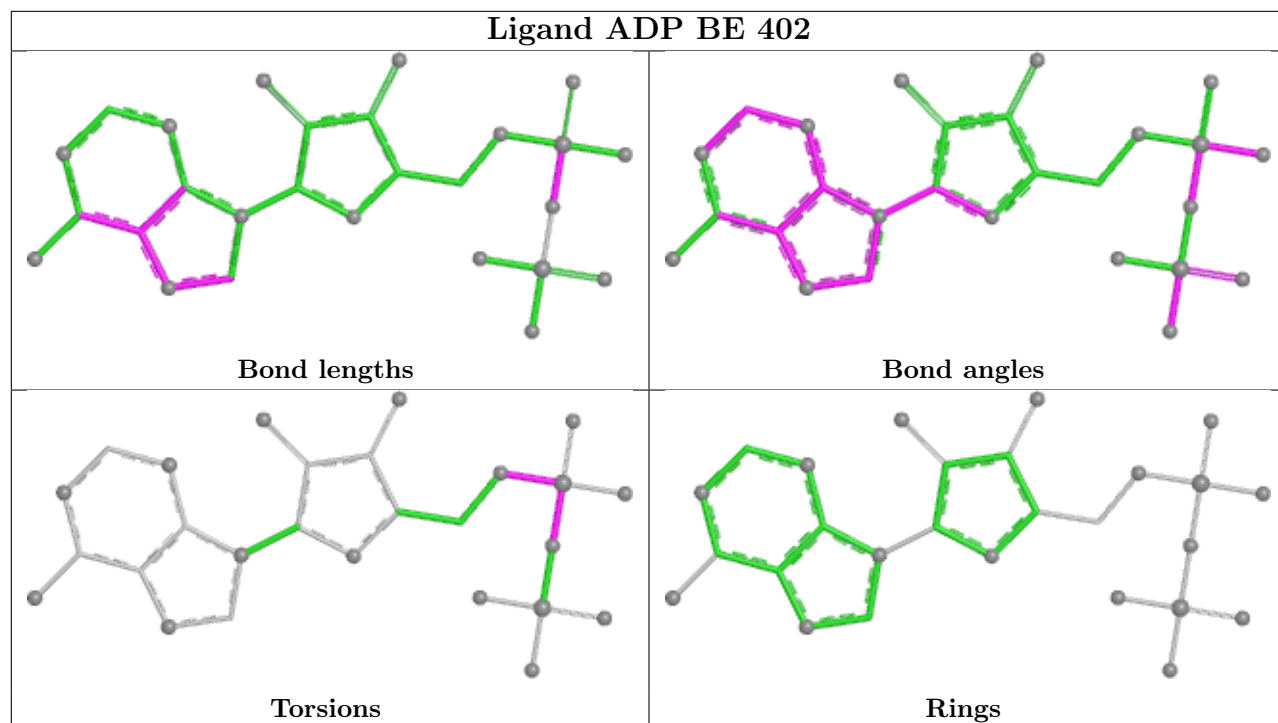


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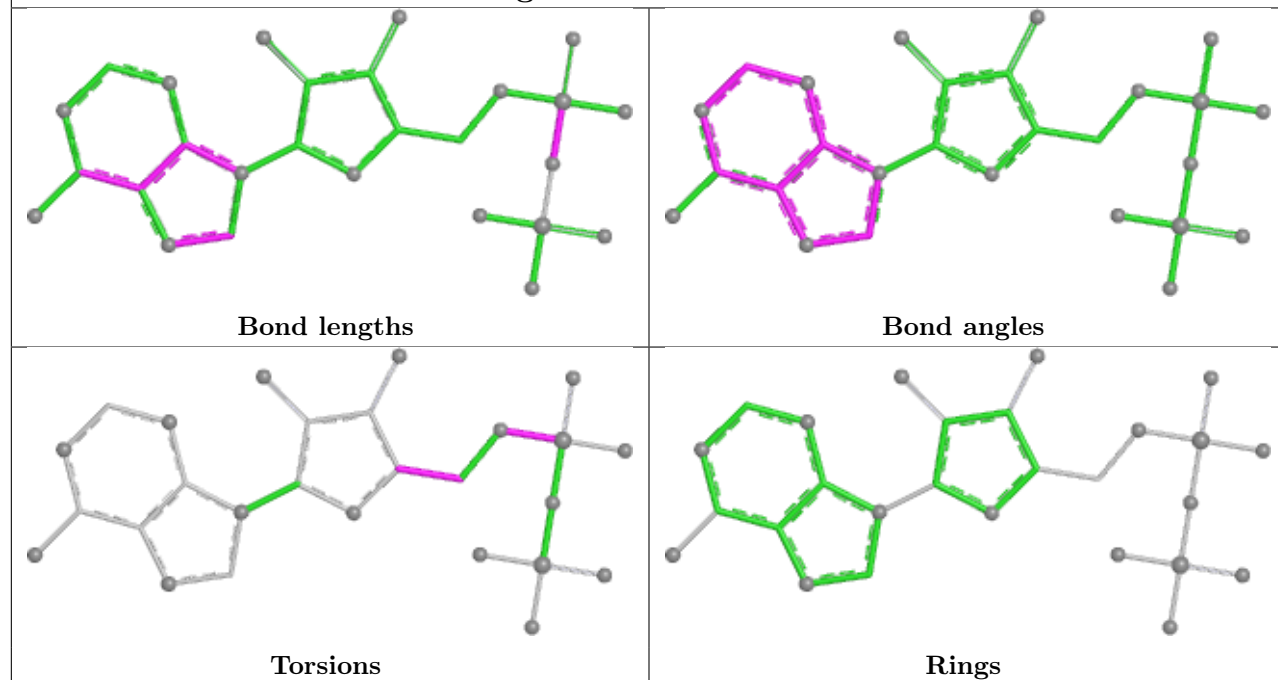


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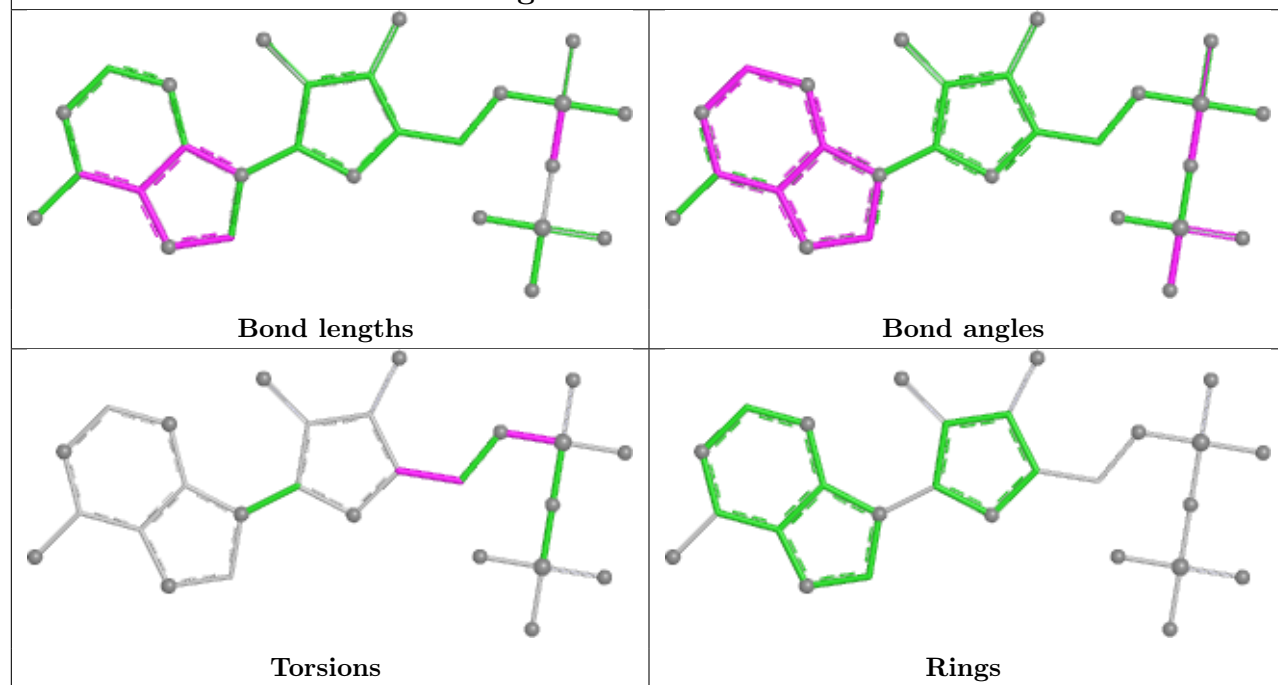




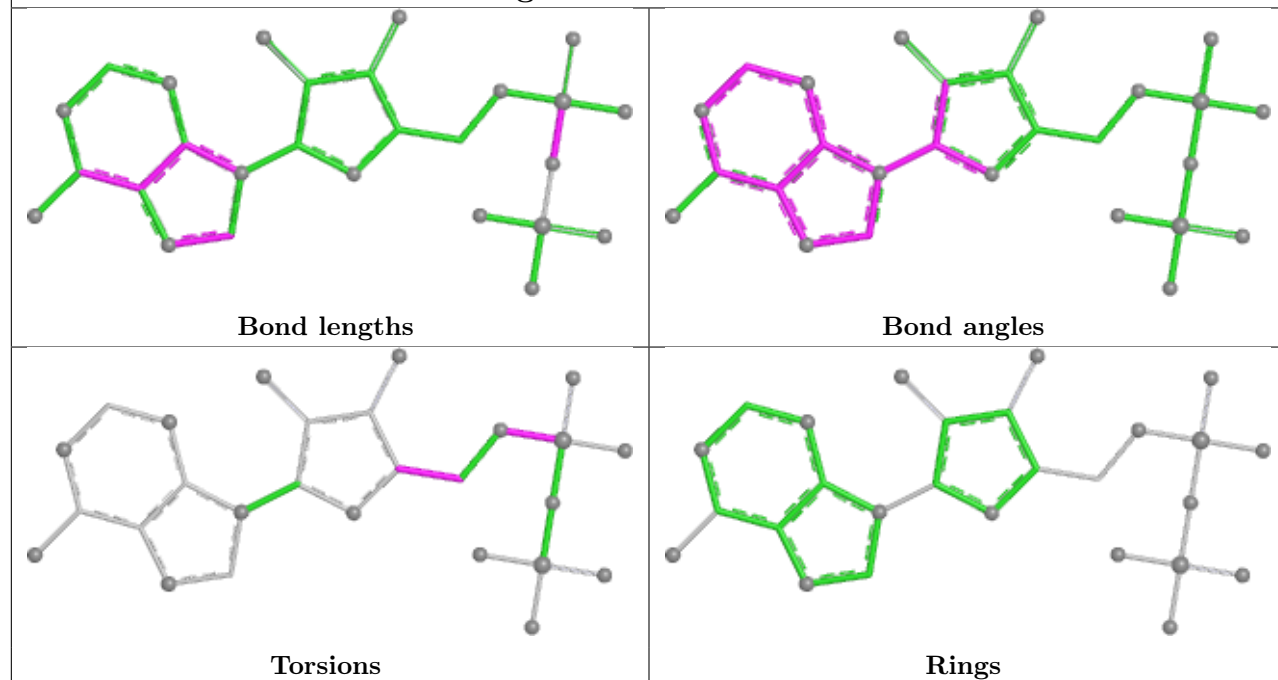
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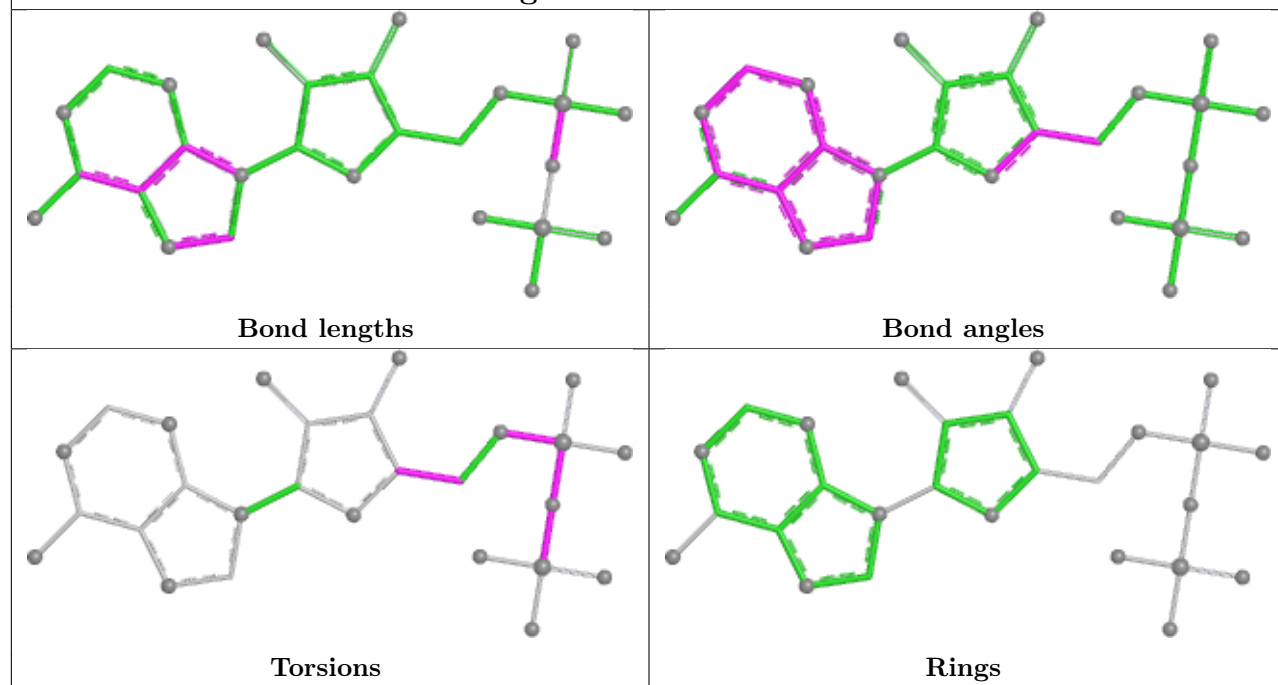
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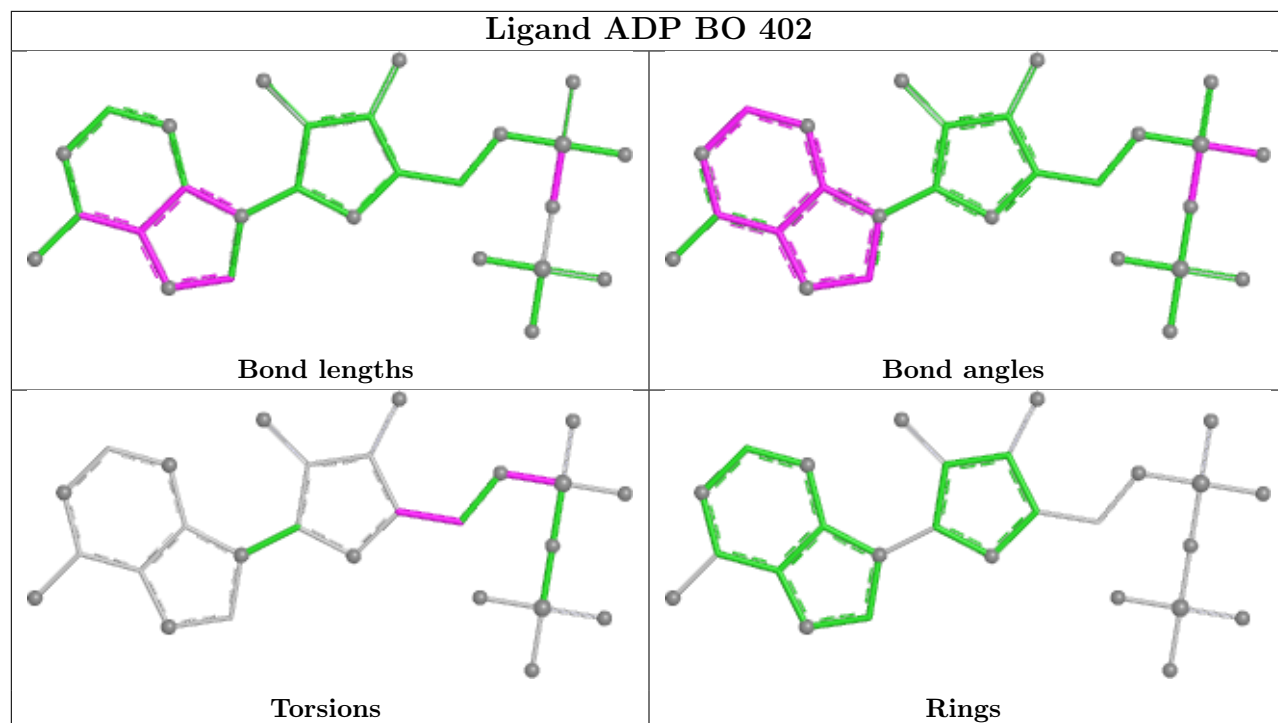
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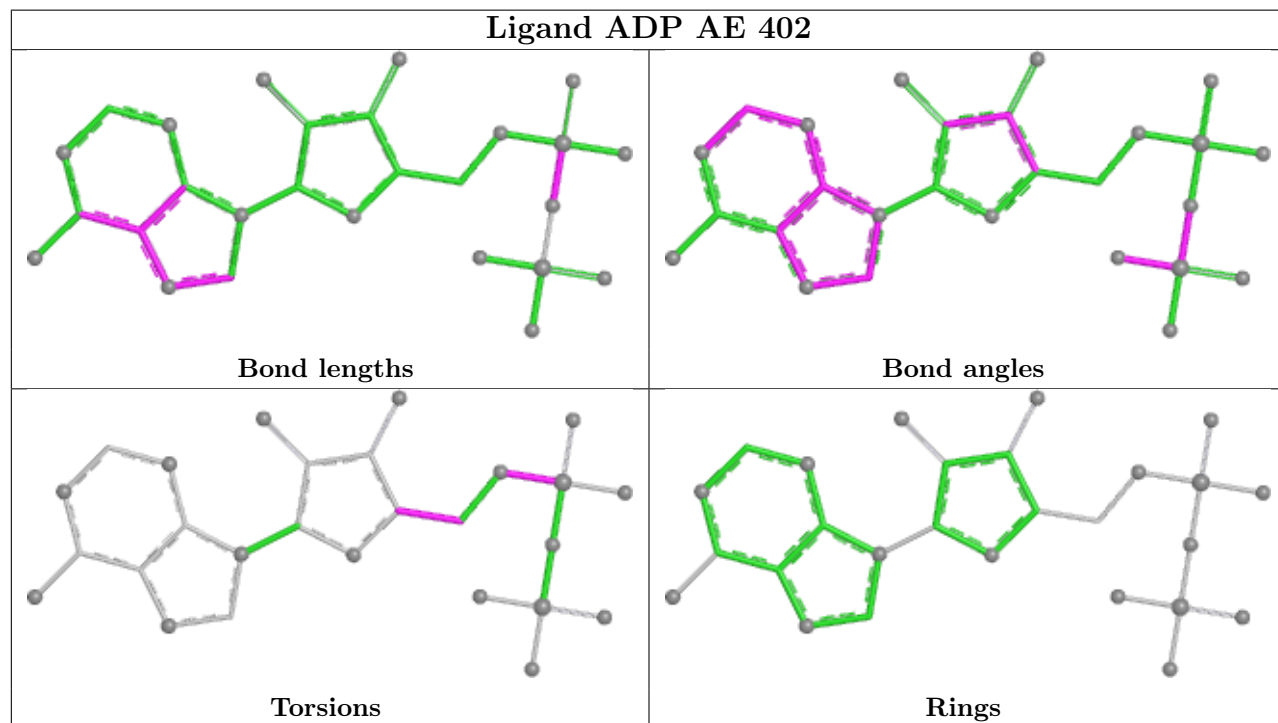
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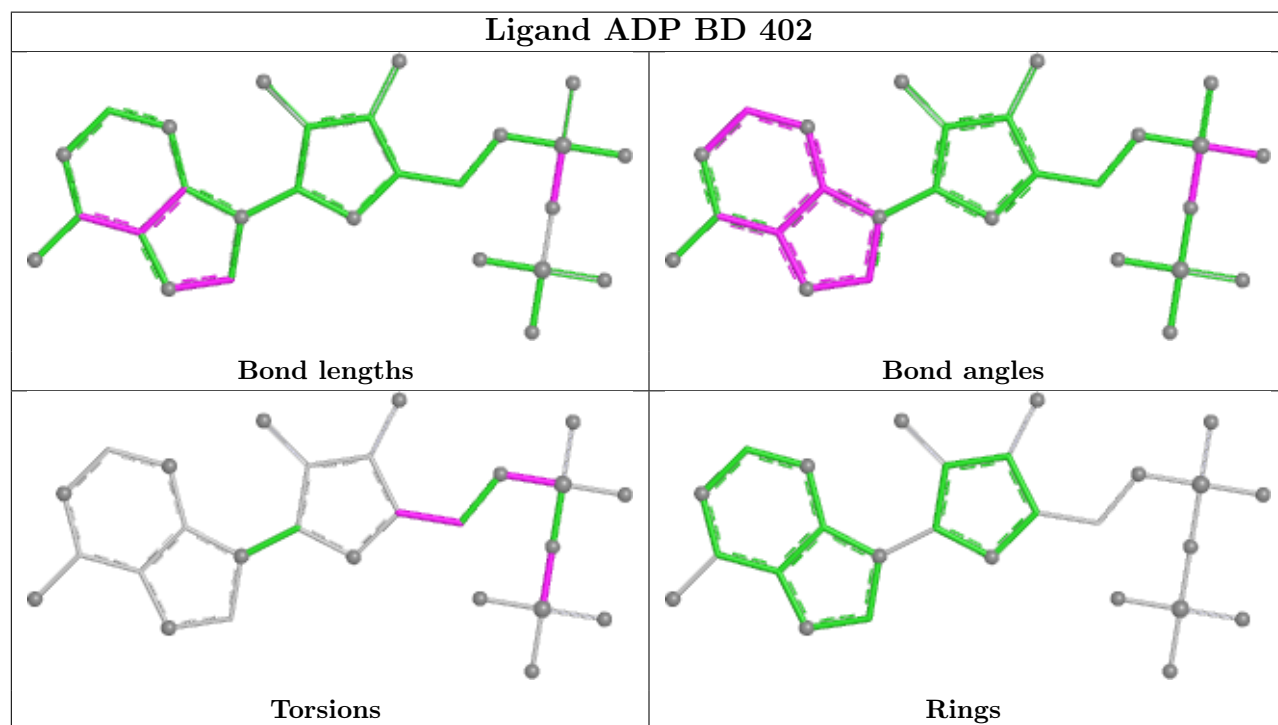
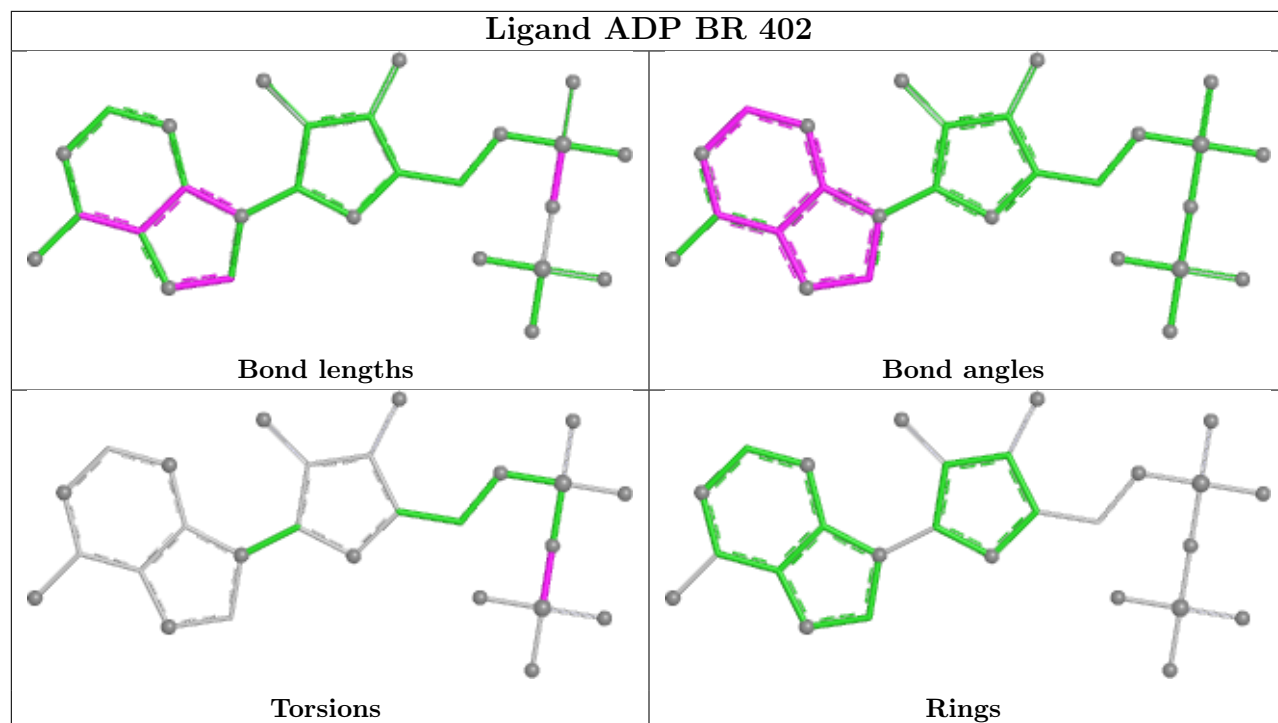


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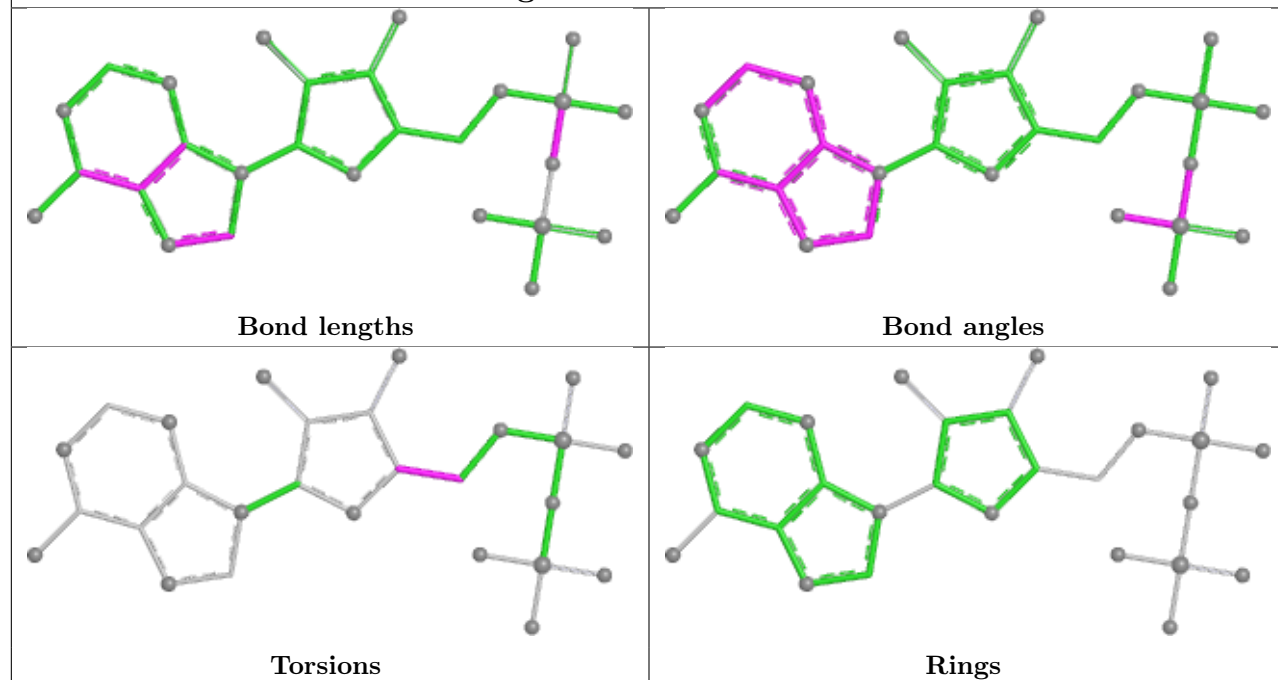


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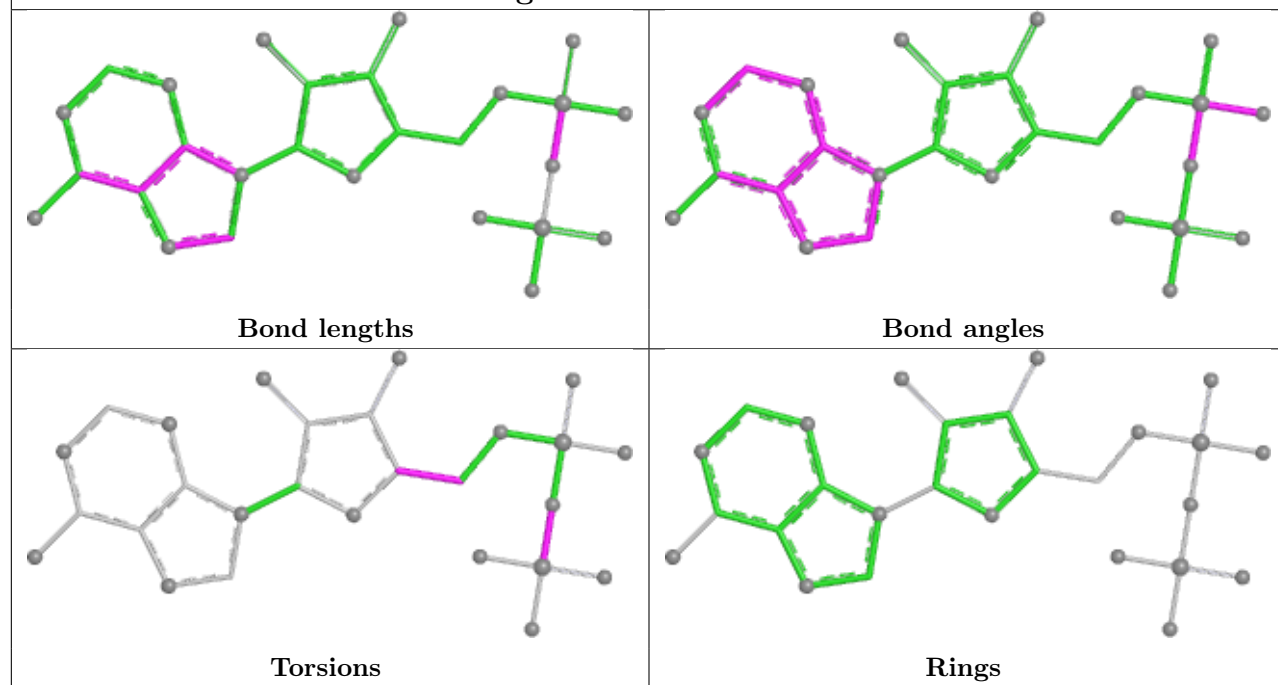


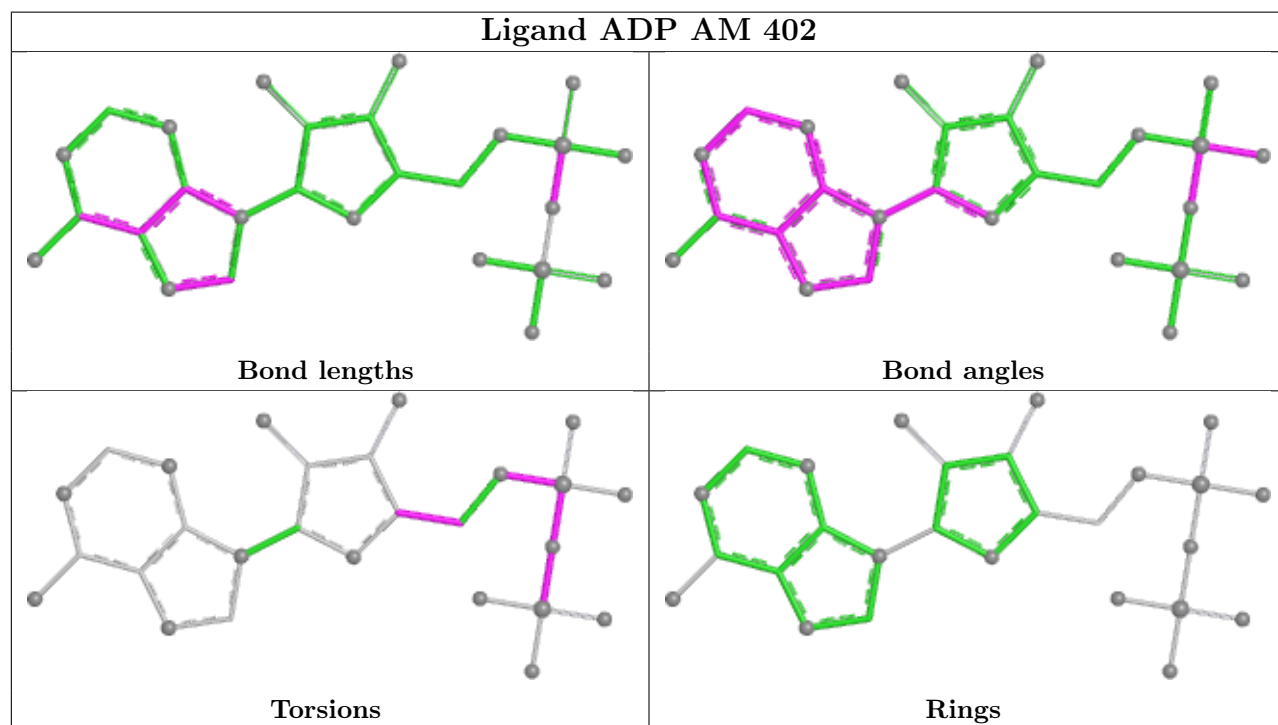
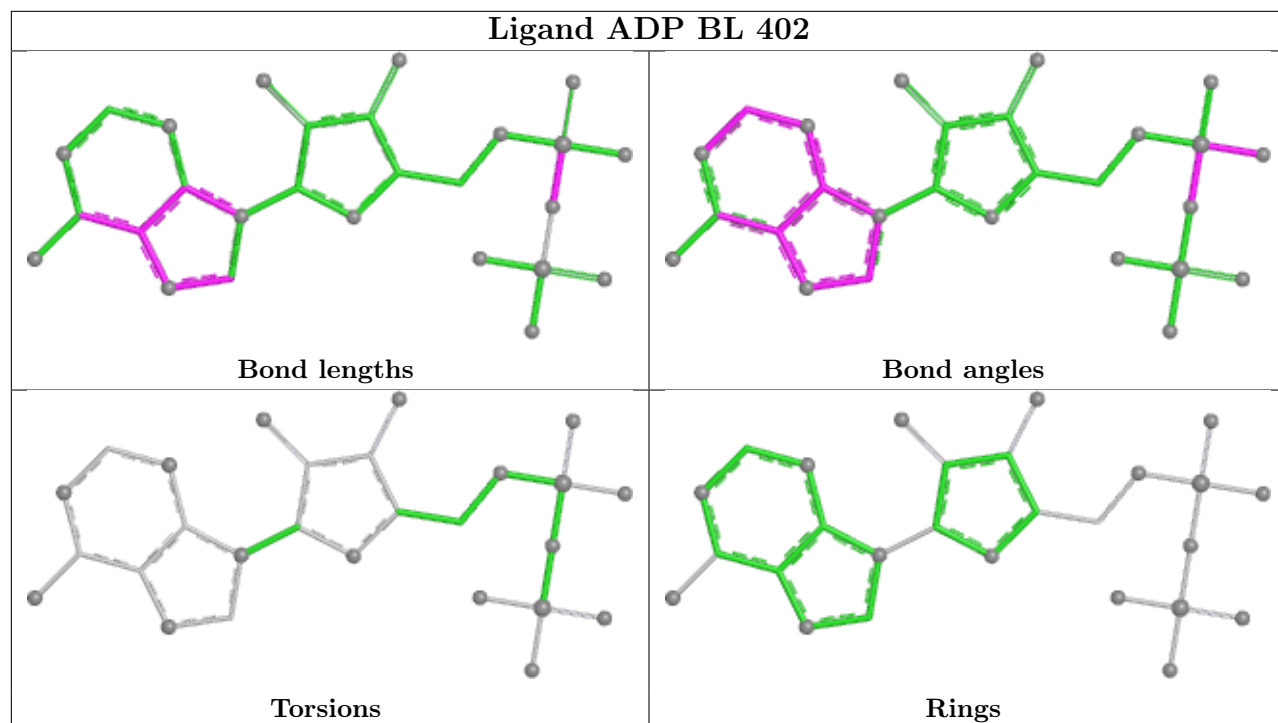


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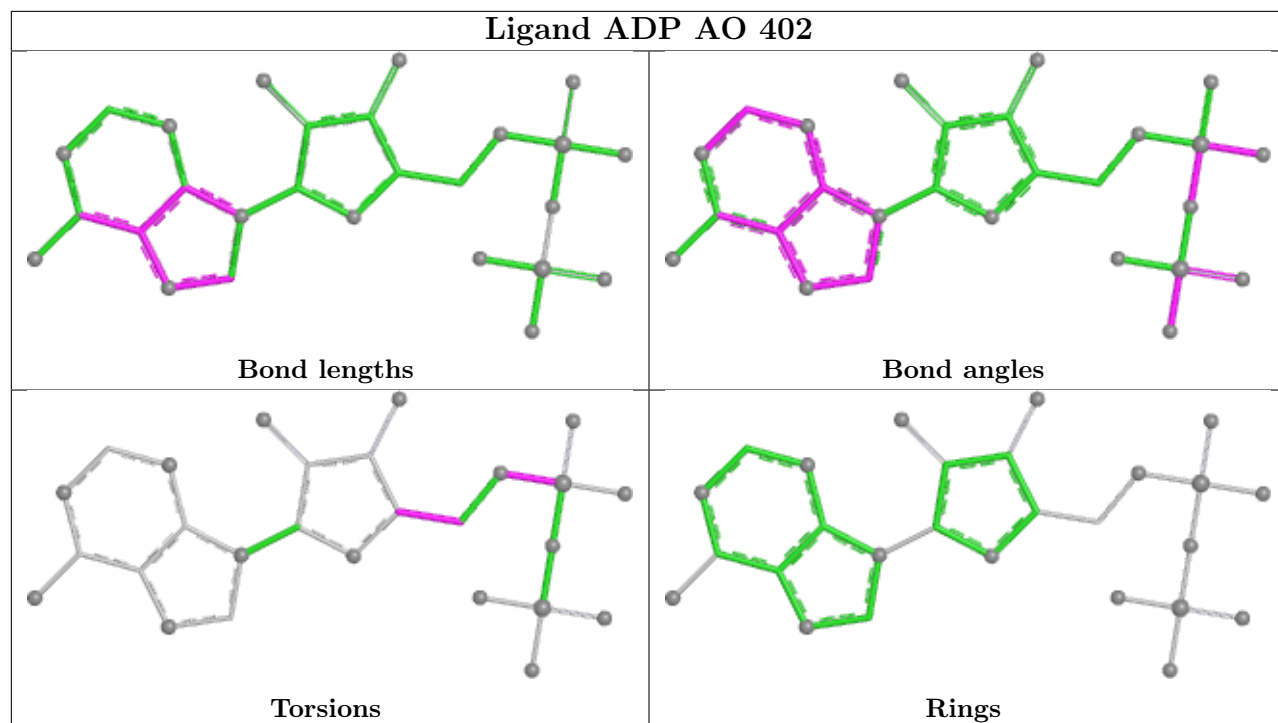


Ligand ADP BG 402

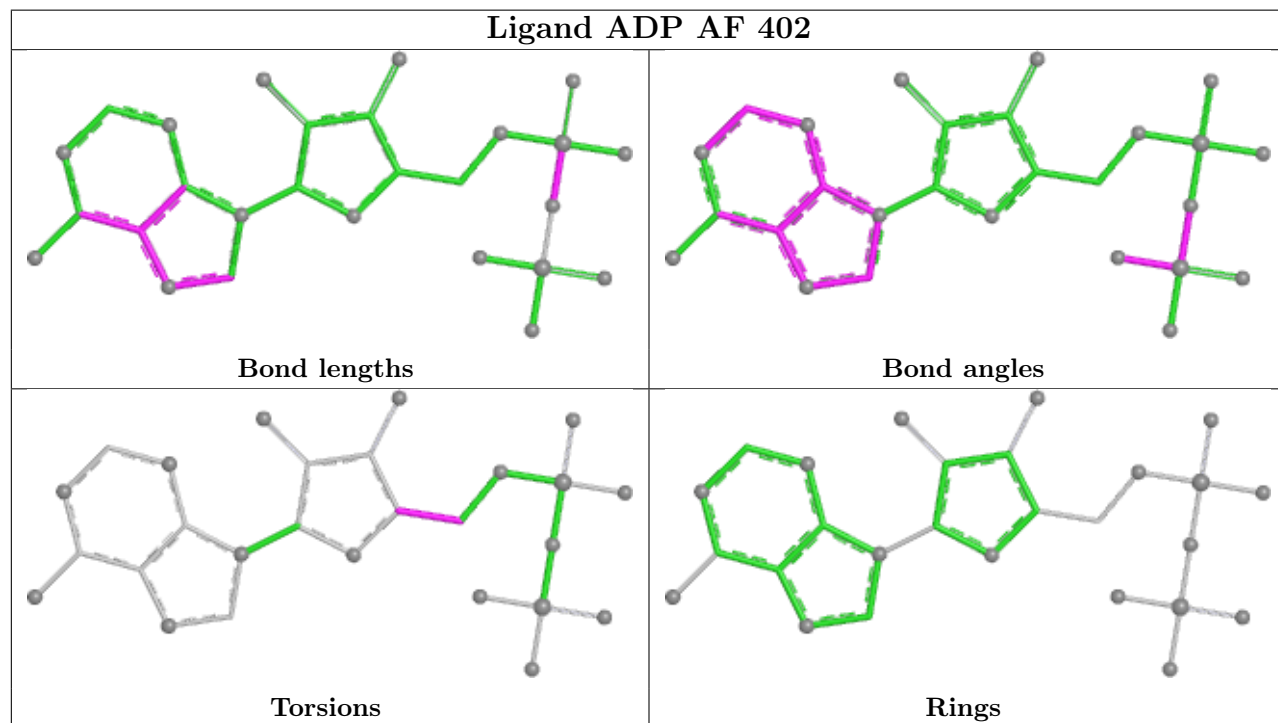


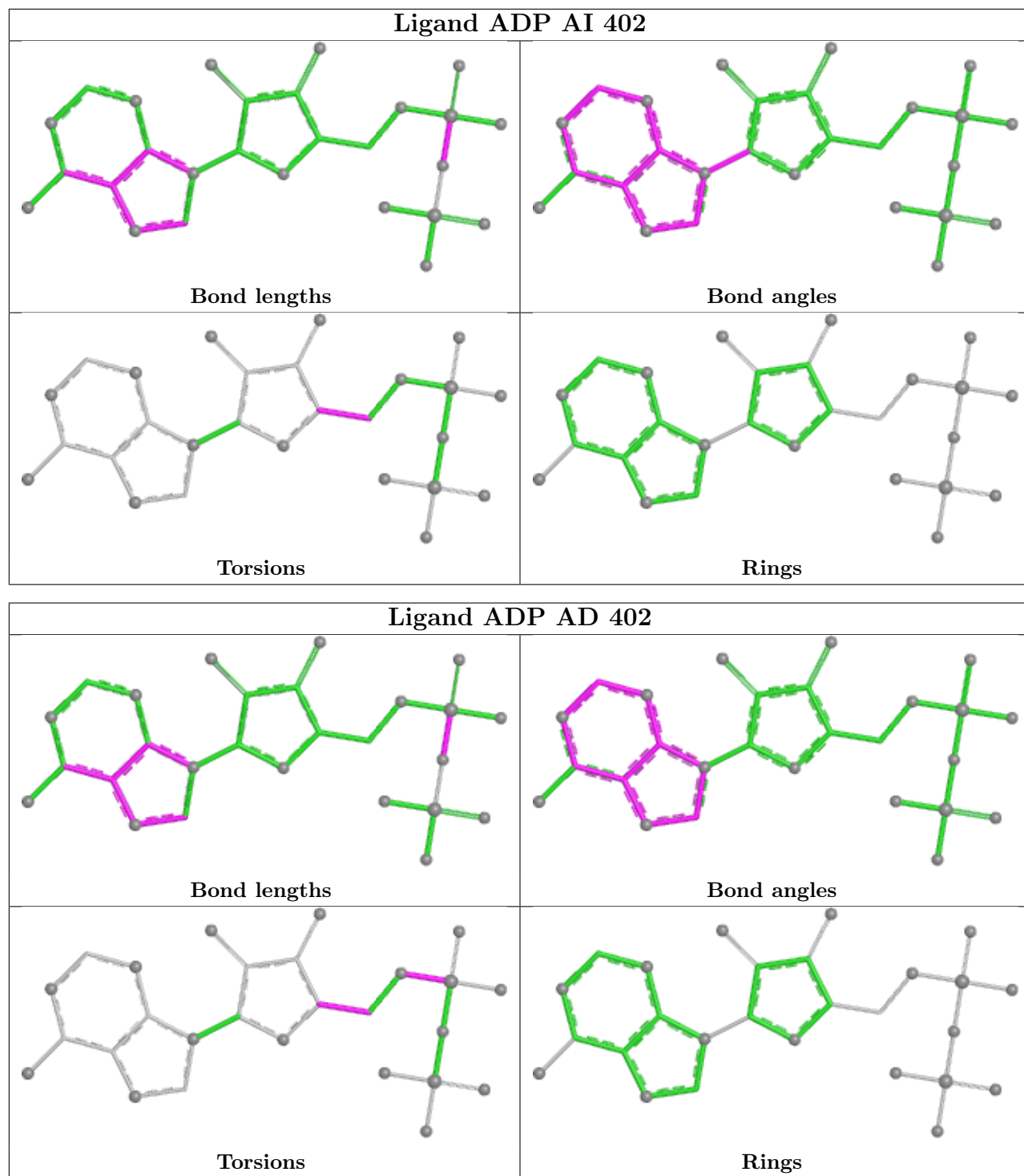


Ligand ADP AO 402



Ligand ADP AF 402





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	366/390 (93%)	-1.36	0 100 100	18, 30, 47, 54	0
1	AB	387/390 (99%)	-1.41	0 100 100	15, 25, 46, 57	0
1	AC	367/390 (94%)	-1.39	0 100 100	15, 29, 45, 54	0
1	AD	382/390 (97%)	-1.45	0 100 100	14, 25, 41, 58	0
1	AE	367/390 (94%)	-1.45	0 100 100	17, 25, 41, 55	0
1	AF	385/390 (98%)	-1.38	0 100 100	16, 27, 46, 59	0
1	AG	367/390 (94%)	-1.43	0 100 100	18, 27, 43, 54	0
1	AH	384/390 (98%)	-1.33	0 100 100	18, 30, 47, 61	0
1	AI	366/390 (93%)	-1.41	0 100 100	17, 28, 42, 51	0
1	AJ	385/390 (98%)	-1.41	0 100 100	16, 24, 43, 59	0
1	AK	367/390 (94%)	-1.43	0 100 100	17, 27, 43, 56	0
1	AL	384/390 (98%)	-1.46	0 100 100	14, 23, 41, 57	0
1	AM	367/390 (94%)	-1.42	0 100 100	17, 25, 40, 50	0
1	AN	382/390 (97%)	-1.40	0 100 100	16, 26, 43, 53	0
1	AO	366/390 (93%)	-1.37	0 100 100	18, 30, 45, 54	0
1	AP	381/390 (97%)	-1.43	0 100 100	15, 23, 39, 56	0
1	AQ	366/390 (93%)	-1.46	0 100 100	16, 25, 39, 51	0
1	AR	379/390 (97%)	-1.44	0 100 100	15, 23, 40, 50	0
1	BA	367/390 (94%)	-1.36	0 100 100	18, 30, 47, 54	0
1	BB	388/390 (99%)	-1.40	0 100 100	15, 25, 46, 58	0
1	BC	367/390 (94%)	-1.45	0 100 100	17, 26, 40, 52	0
1	BD	385/390 (98%)	-1.38	0 100 100	16, 27, 46, 59	0
1	BE	367/390 (94%)	-1.40	0 100 100	18, 29, 45, 53	0
1	BF	382/390 (97%)	-1.45	0 100 100	13, 24, 42, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
1	BG	367/390 (94%)	-1.41	0	100	100	16, 27, 42, 54	0
1	BH	382/390 (97%)	-1.44	0	100	100	15, 23, 41, 55	0
1	BI	367/390 (94%)	-1.41	0	100	100	17, 26, 41, 51	0
1	BJ	385/390 (98%)	-1.42	0	100	100	17, 25, 42, 61	0
1	BK	367/390 (94%)	-1.41	0	100	100	17, 26, 42, 50	0
1	BL	381/390 (97%)	-1.31	0	100	100	20, 31, 48, 59	0
1	BM	367/390 (94%)	-1.41	0	100	100	17, 26, 41, 51	0
1	BN	382/390 (97%)	-1.36	0	100	100	18, 27, 44, 52	0
1	BO	367/390 (94%)	-1.46	0	100	100	16, 25, 40, 51	0
1	BP	382/390 (97%)	-1.43	0	100	100	15, 24, 41, 50	0
1	BQ	366/390 (93%)	-1.36	0	100	100	19, 30, 44, 53	0
1	BR	381/390 (97%)	-1.43	0	100	100	15, 24, 40, 51	0
All	All	13498/14040 (96%)	-1.41	0	100	100	13, 26, 44, 61	0

There are no RSRZ outliers to report.

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
5	NO3	BF	404	4/4	0.97	0.08	18,21,22,25	0
2	NMG	AF	401	8/8	0.98	0.04	17,22,26,27	0
2	NMG	AP	401	8/8	0.98	0.06	19,22,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NMG	BH	401	8/8	0.98	0.04	18,22,24,24	0
2	NMG	BL	401	8/8	0.98	0.05	28,32,34,36	0
4	MG	AH	403	1/1	0.98	0.03	16,16,16,16	0
4	MG	AQ	403	1/1	0.98	0.05	15,15,15,15	0
4	MG	AR	403	1/1	0.98	0.04	11,11,11,11	0
4	MG	BF	403	1/1	0.98	0.04	11,11,11,11	0
5	NO3	AC	404	4/4	0.98	0.06	22,24,26,27	0
5	NO3	AJ	404	4/4	0.98	0.06	18,24,27,27	0
5	NO3	AK	404	4/4	0.98	0.05	24,25,27,28	0
5	NO3	AN	404	4/4	0.98	0.05	22,24,25,26	0
2	NMG	AA	501	8/8	0.98	0.05	20,23,25,25	0
5	NO3	BG	404	4/4	0.98	0.07	21,22,25,27	0
5	NO3	BQ	404	4/4	0.98	0.05	25,26,26,27	0
2	NMG	AQ	401	8/8	0.99	0.04	16,20,21,25	0
2	NMG	AR	401	8/8	0.99	0.03	18,21,24,24	0
2	NMG	BA	501	8/8	0.99	0.03	21,26,27,28	0
2	NMG	BB	401	8/8	0.99	0.05	14,20,22,23	0
2	NMG	BC	401	8/8	0.99	0.04	16,22,25,25	0
2	NMG	BD	401	8/8	0.99	0.04	20,23,24,24	0
2	NMG	BE	401	8/8	0.99	0.04	25,28,29,31	0
2	NMG	BF	401	8/8	0.99	0.03	16,19,24,24	0
2	NMG	BG	401	8/8	0.99	0.04	20,23,25,25	0
2	NMG	AD	401	8/8	0.99	0.04	18,24,26,26	0
2	NMG	BI	401	8/8	0.99	0.04	23,26,27,27	0
2	NMG	BJ	401	8/8	0.99	0.04	25,26,28,29	0
2	NMG	BK	401	8/8	0.99	0.03	21,25,26,29	0
2	NMG	AE	401	8/8	0.99	0.04	18,21,23,25	0
2	NMG	BM	401	8/8	0.99	0.05	22,24,25,26	0
2	NMG	BN	401	8/8	0.99	0.04	21,22,25,26	0
2	NMG	BO	401	8/8	0.99	0.04	21,26,28,29	0
2	NMG	BP	401	8/8	0.99	0.03	15,17,20,24	0
2	NMG	BQ	401	8/8	0.99	0.05	25,28,33,33	0
2	NMG	BR	401	8/8	0.99	0.03	15,17,22,23	0
3	ADP	AA	502	27/27	0.99	0.03	23,28,31,35	0
3	ADP	AC	402	27/27	0.99	0.03	24,27,32,33	0
3	ADP	AE	402	27/27	0.99	0.03	18,21,23,28	0
3	ADP	AF	402	27/27	0.99	0.03	21,27,30,35	0
3	ADP	AG	402	27/27	0.99	0.03	17,21,25,27	0
3	ADP	AH	402	27/27	0.99	0.04	20,26,30,37	0
3	ADP	AI	402	27/27	0.99	0.03	18,24,29,33	0
3	ADP	AJ	402	27/27	0.99	0.03	15,18,22,25	0
3	ADP	AK	402	27/27	0.99	0.03	17,22,24,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	AM	402	27/27	0.99	0.03	17,20,24,25	0
3	ADP	AO	402	27/27	0.99	0.03	19,24,28,31	0
3	ADP	AP	402	27/27	0.99	0.03	17,21,26,30	0
3	ADP	BA	502	27/27	0.99	0.03	21,25,29,32	0
3	ADP	BC	402	27/27	0.99	0.03	13,20,22,24	0
3	ADP	BD	402	27/27	0.99	0.03	19,25,28,31	0
3	ADP	BE	402	27/27	0.99	0.03	19,25,29,31	0
3	ADP	BL	402	27/27	0.99	0.04	23,29,34,38	0
3	ADP	BN	402	27/27	0.99	0.03	10,20,23,26	0
3	ADP	BQ	402	27/27	0.99	0.03	16,22,28,29	0
4	MG	AF	403	1/1	0.99	0.04	12,12,12,12	0
4	MG	AG	403	1/1	0.99	0.05	18,18,18,18	0
2	NMG	AB	401	8/8	0.99	0.03	16,23,28,28	0
4	MG	AI	403	1/1	0.99	0.05	15,15,15,15	0
4	MG	AJ	403	1/1	0.99	0.04	10,10,10,10	0
4	MG	AK	403	1/1	0.99	0.05	12,12,12,12	0
4	MG	AL	403	1/1	0.99	0.05	22,22,22,22	0
4	MG	AM	403	1/1	0.99	0.05	13,13,13,13	0
4	MG	AN	403	1/1	0.99	0.03	13,13,13,13	0
4	MG	AO	403	1/1	0.99	0.05	18,18,18,18	0
4	MG	AP	403	1/1	0.99	0.07	25,25,25,25	0
2	NMG	AG	401	8/8	0.99	0.04	16,21,22,25	0
2	NMG	AH	401	8/8	0.99	0.04	21,23,30,34	0
4	MG	BB	403	1/1	0.99	0.04	18,18,18,18	0
4	MG	BD	403	1/1	0.99	0.02	21,21,21,21	0
4	MG	BE	403	1/1	0.99	0.04	14,14,14,14	0
2	NMG	AI	401	8/8	0.99	0.03	18,22,24,27	0
4	MG	BG	403	1/1	0.99	0.05	20,20,20,20	0
4	MG	BH	403	1/1	0.99	0.05	19,19,19,19	0
4	MG	BI	403	1/1	0.99	0.06	10,10,10,10	0
4	MG	BL	403	1/1	0.99	0.04	18,18,18,18	0
4	MG	BM	403	1/1	0.99	0.04	9,9,9,9	0
4	MG	BP	403	1/1	0.99	0.05	8,8,8,8	0
4	MG	BQ	403	1/1	0.99	0.05	12,12,12,12	0
5	NO3	AA	504	4/4	0.99	0.04	25,26,27,28	0
5	NO3	AB	404	4/4	0.99	0.05	16,17,23,23	0
2	NMG	AJ	401	8/8	0.99	0.03	19,24,26,30	0
5	NO3	AD	404	4/4	0.99	0.04	24,29,29,30	0
5	NO3	AE	404	4/4	0.99	0.04	21,23,23,25	0
5	NO3	AF	404	4/4	0.99	0.06	21,22,25,26	0
5	NO3	AG	404	4/4	0.99	0.03	19,21,25,27	0
5	NO3	AH	404	4/4	0.99	0.04	21,23,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NO3	AI	404	4/4	0.99	0.03	22,25,28,28	0
2	NMG	AK	401	8/8	0.99	0.04	20,24,25,29	0
2	NMG	AL	401	8/8	0.99	0.04	17,19,21,22	0
5	NO3	AL	404	4/4	0.99	0.07	20,21,22,22	0
5	NO3	AM	404	4/4	0.99	0.04	22,25,26,28	0
2	NMG	AM	401	8/8	0.99	0.04	17,20,21,24	0
5	NO3	AO	404	4/4	0.99	0.05	23,25,28,36	0
5	NO3	AP	404	4/4	0.99	0.04	20,21,24,27	0
5	NO3	AQ	404	4/4	0.99	0.06	18,22,22,22	0
5	NO3	AR	404	4/4	0.99	0.04	21,22,27,29	0
5	NO3	BA	504	4/4	0.99	0.05	25,27,28,31	0
5	NO3	BB	404	4/4	0.99	0.04	20,21,24,24	0
5	NO3	BC	404	4/4	0.99	0.05	16,21,24,24	0
5	NO3	BD	404	4/4	0.99	0.04	21,23,23,27	0
5	NO3	BE	404	4/4	0.99	0.04	24,25,26,29	0
2	NMG	AN	401	8/8	0.99	0.04	21,24,31,31	0
2	NMG	AO	401	8/8	0.99	0.04	22,27,32,32	0
5	NO3	BH	404	4/4	0.99	0.05	20,21,22,23	0
5	NO3	BI	404	4/4	0.99	0.03	19,20,25,25	0
5	NO3	BJ	404	4/4	0.99	0.07	22,24,25,29	0
5	NO3	BK	404	4/4	0.99	0.03	21,21,22,24	0
5	NO3	BL	404	4/4	0.99	0.06	25,31,33,33	0
5	NO3	BM	404	4/4	0.99	0.04	21,22,24,24	0
5	NO3	BN	404	4/4	0.99	0.04	23,24,24,26	0
5	NO3	BO	404	4/4	0.99	0.04	23,23,23,28	0
5	NO3	BP	404	4/4	0.99	0.03	18,20,22,24	0
2	NMG	AC	401	8/8	0.99	0.03	22,24,26,27	0
5	NO3	BR	404	4/4	0.99	0.04	14,19,22,22	0
3	ADP	BK	402	27/27	1.00	0.03	12,19,23,25	0
3	ADP	AQ	402	27/27	1.00	0.03	14,18,22,23	0
3	ADP	BM	402	27/27	1.00	0.02	13,20,23,26	0
3	ADP	AR	402	27/27	1.00	0.02	11,19,21,24	0
4	MG	BA	503	1/1	1.00	0.03	13,13,13,13	0
3	ADP	BO	402	27/27	1.00	0.03	12,18,21,25	0
4	MG	BC	403	1/1	1.00	0.04	11,11,11,11	0
3	ADP	BP	402	27/27	1.00	0.02	14,18,21,21	0
3	ADP	AD	402	27/27	1.00	0.03	16,21,24,27	0
3	ADP	BR	402	27/27	1.00	0.02	13,17,21,23	0
4	MG	AA	503	1/1	1.00	0.04	16,16,16,16	0
4	MG	AB	403	1/1	1.00	0.06	11,11,11,11	0
4	MG	AC	403	1/1	1.00	0.04	16,16,16,16	0
4	MG	BJ	403	1/1	1.00	0.03	12,12,12,12	0

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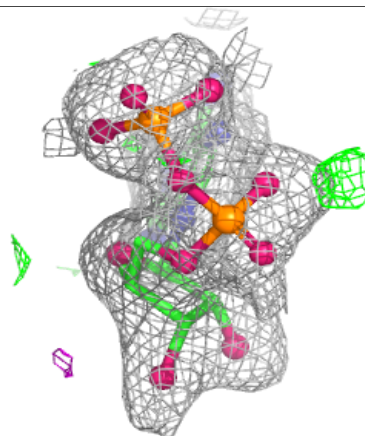
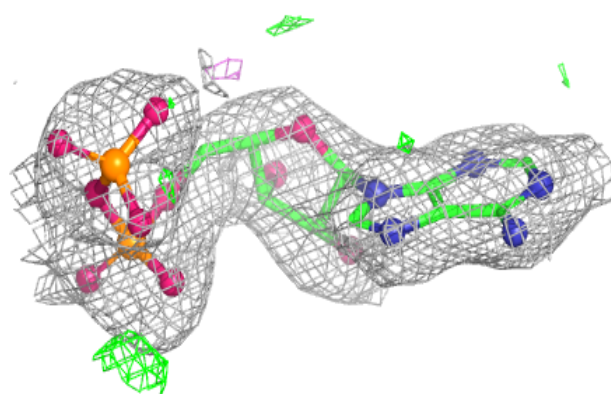
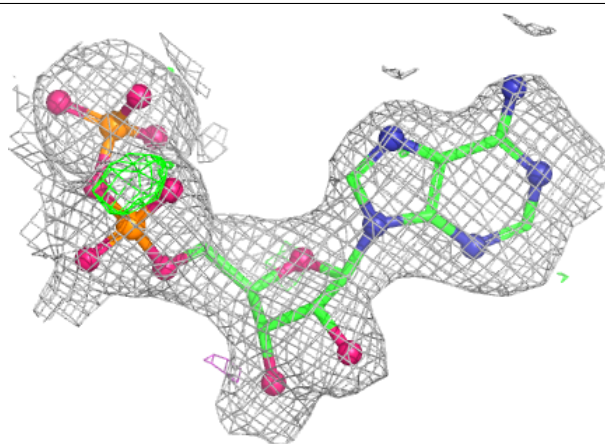
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	BK	403	1/1	1.00	0.03	11,11,11,11	0
4	MG	AD	403	1/1	1.00	0.03	13,13,13,13	0
4	MG	AE	403	1/1	1.00	0.08	15,15,15,15	0
4	MG	BN	403	1/1	1.00	0.05	22,22,22,22	0
4	MG	BO	403	1/1	1.00	0.06	10,10,10,10	0
3	ADP	BB	402	27/27	1.00	0.03	18,21,23,26	0
3	ADP	AN	402	27/27	1.00	0.03	13,20,23,23	0
4	MG	BR	403	1/1	1.00	0.05	37,37,37,37	0
3	ADP	AB	402	27/27	1.00	0.02	14,18,21,22	0
3	ADP	AL	402	27/27	1.00	0.03	14,18,21,23	0
3	ADP	BF	402	27/27	1.00	0.02	13,18,22,24	0
3	ADP	BG	402	27/27	1.00	0.03	21,27,29,30	0
3	ADP	BH	402	27/27	1.00	0.02	14,17,21,23	0
3	ADP	BI	402	27/27	1.00	0.03	16,21,25,27	0
3	ADP	BJ	402	27/27	1.00	0.03	12,18,20,21	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.

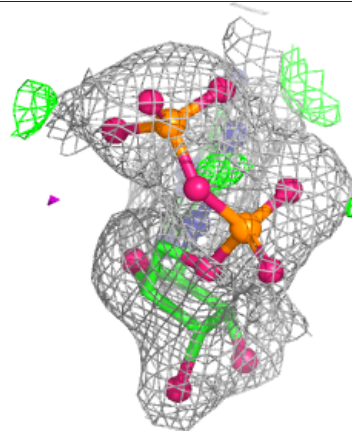
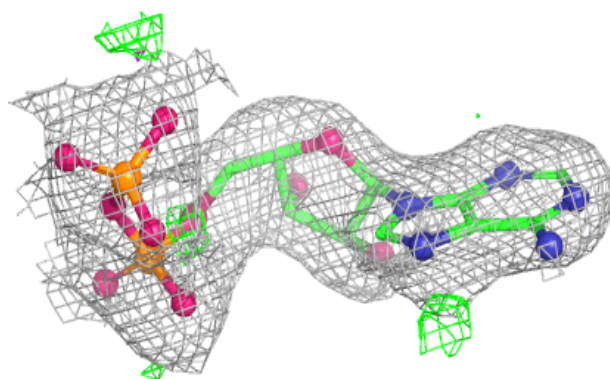
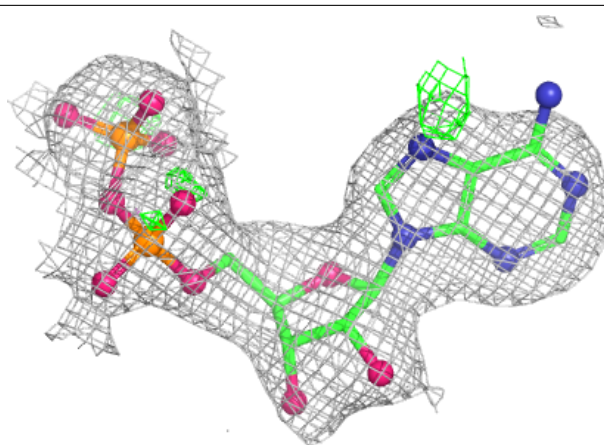
Electron density around ADP AA 502:

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



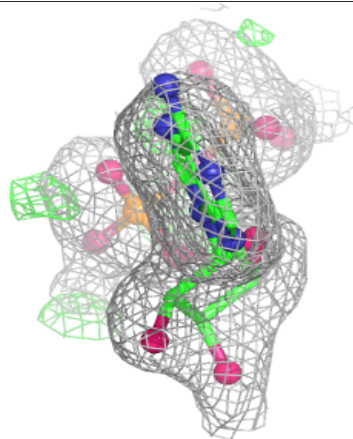
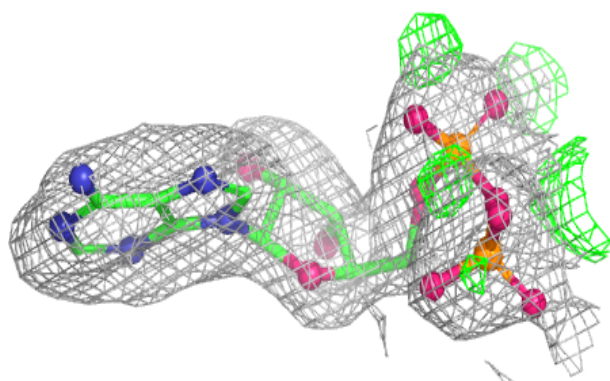
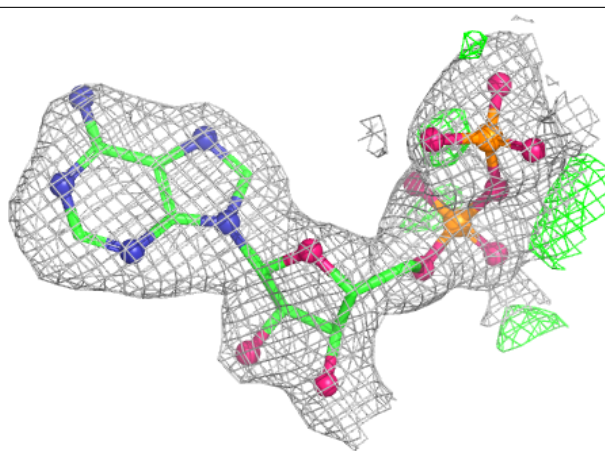
Electron density around ADP AC 402:

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



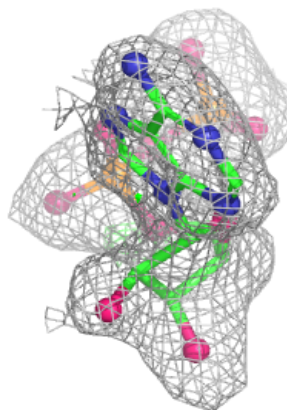
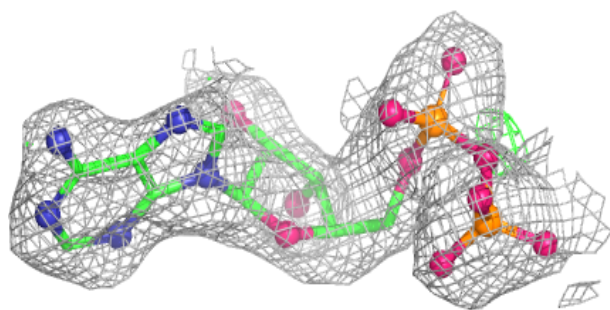
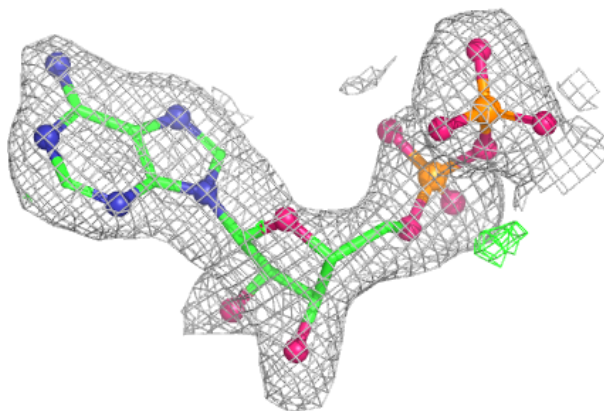
Electron density around ADP AE 402:

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



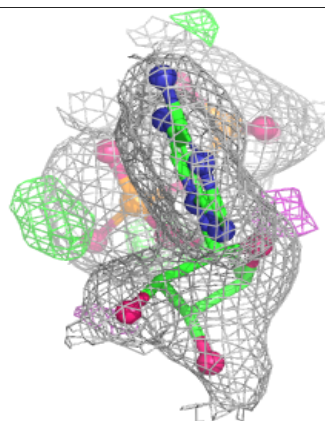
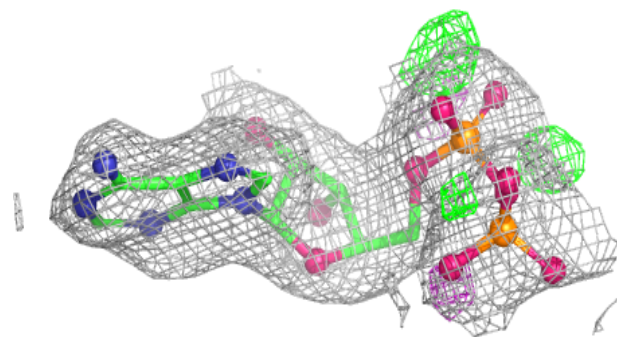
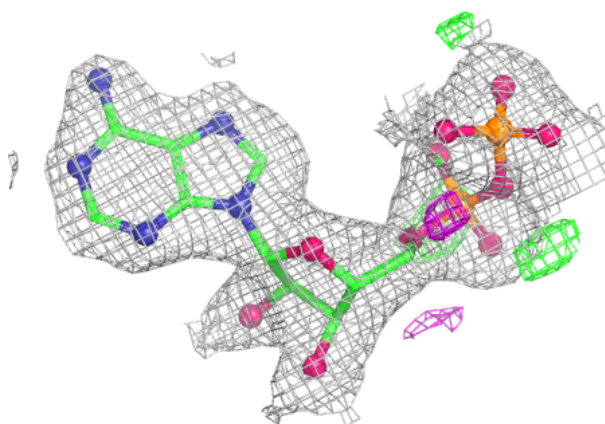
Electron density around ADP AF 402:

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



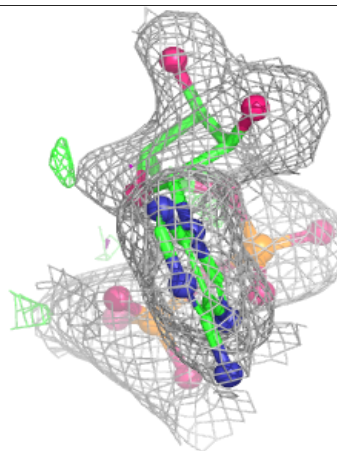
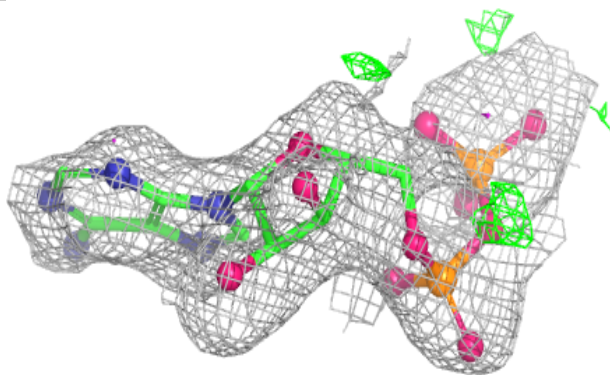
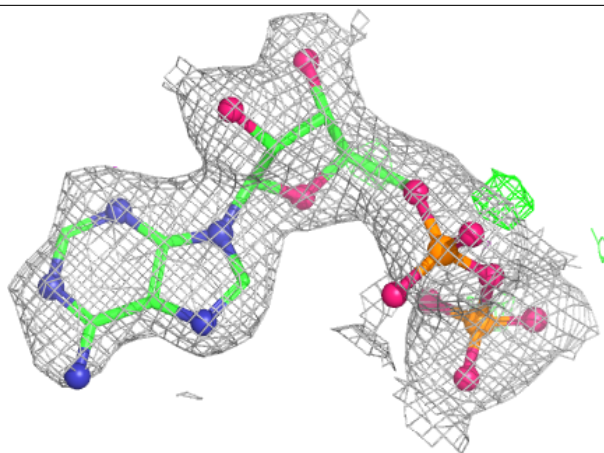
Electron density around ADP AG 402:

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



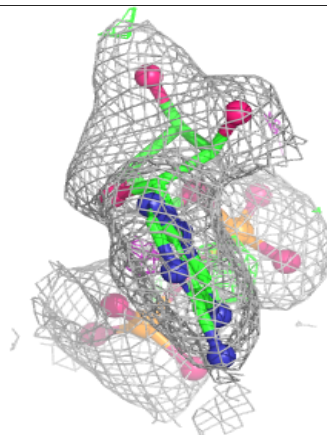
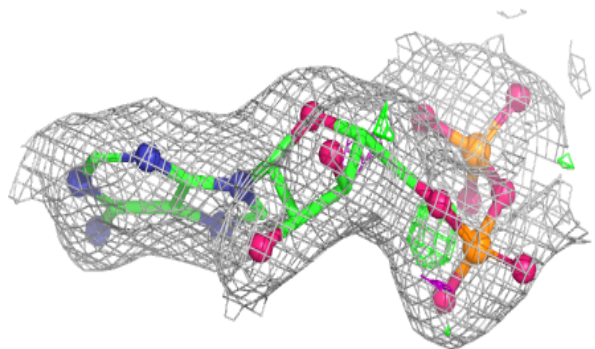
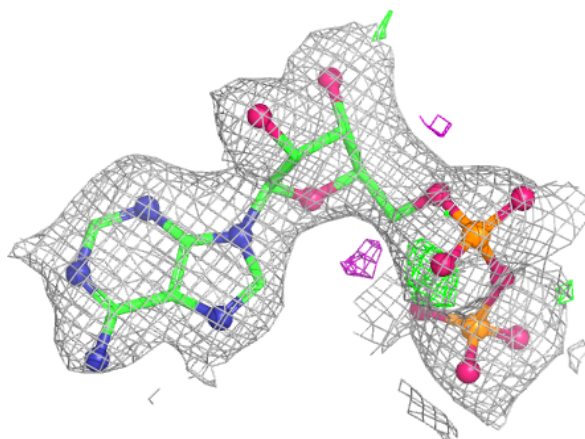
Electron density around ADP AH 402:

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



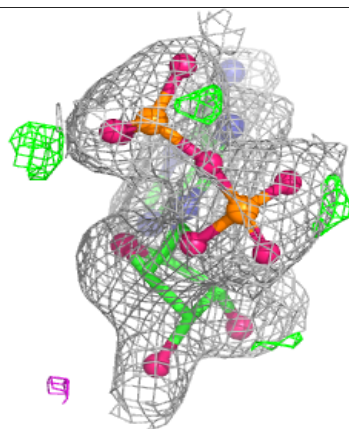
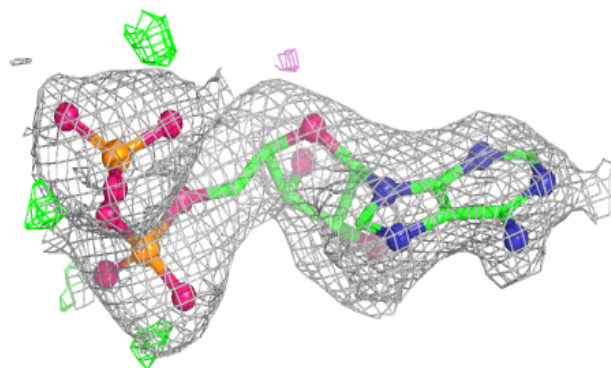
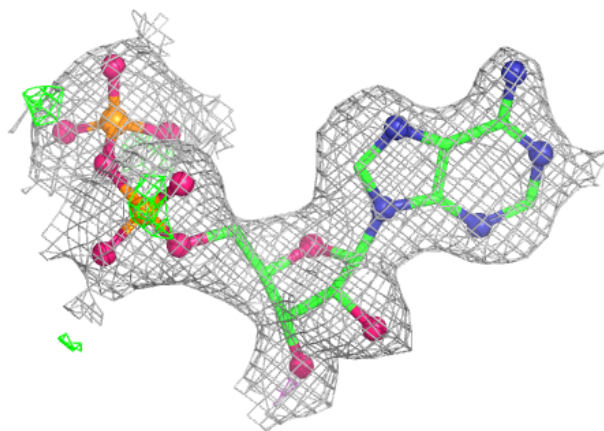
Electron density around ADP AI 402:

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



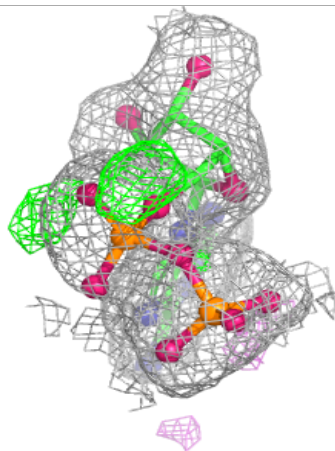
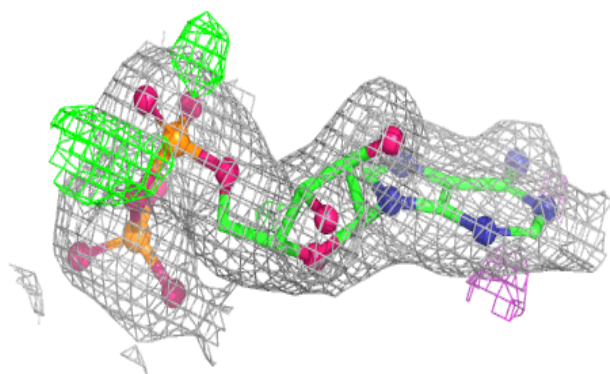
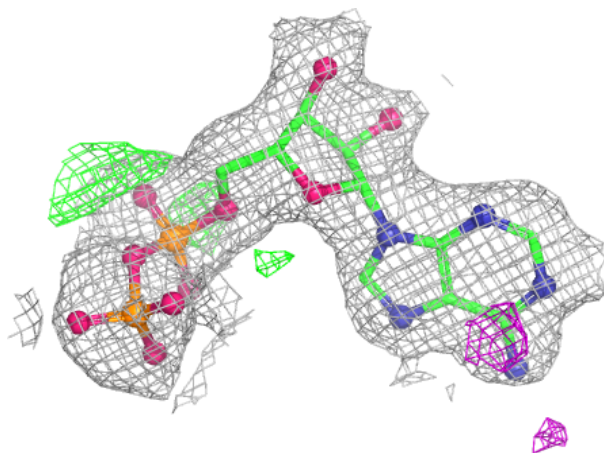
Electron density around ADP AJ 402:

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



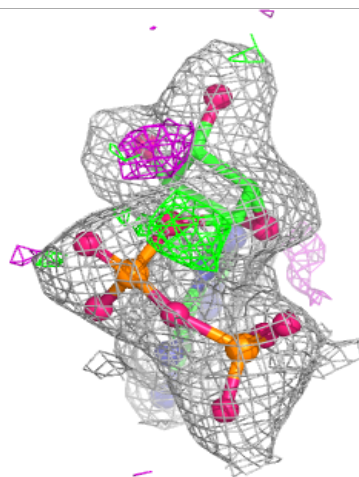
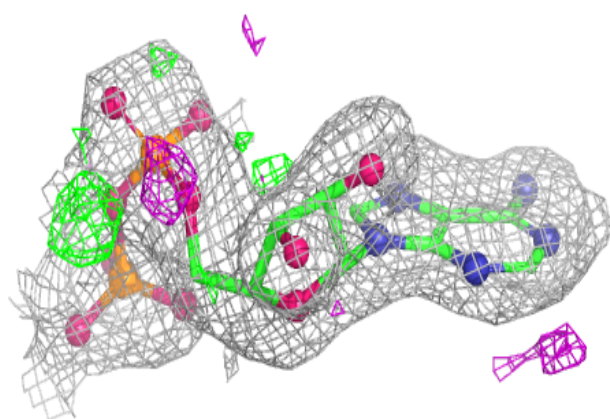
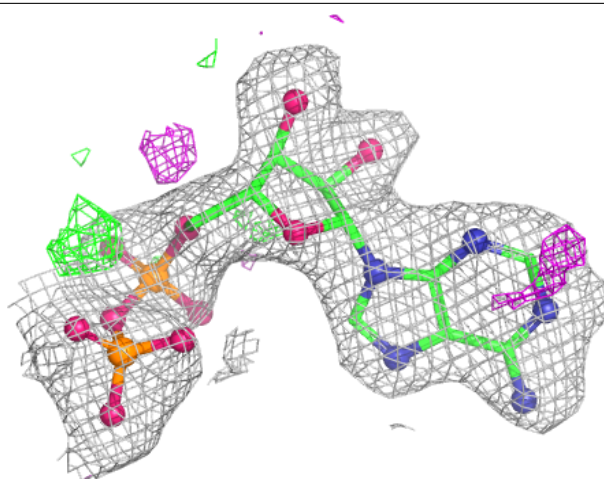
Electron density around ADP AK 402:

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



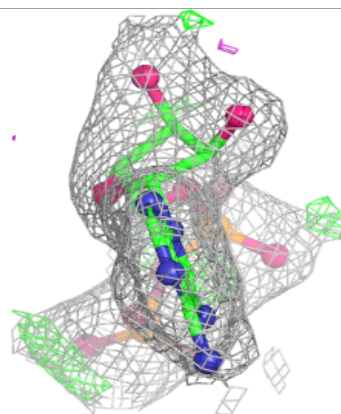
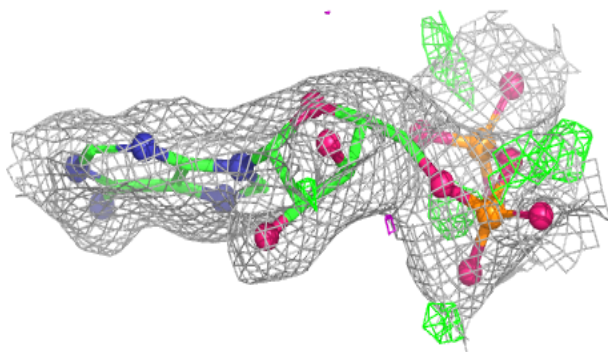
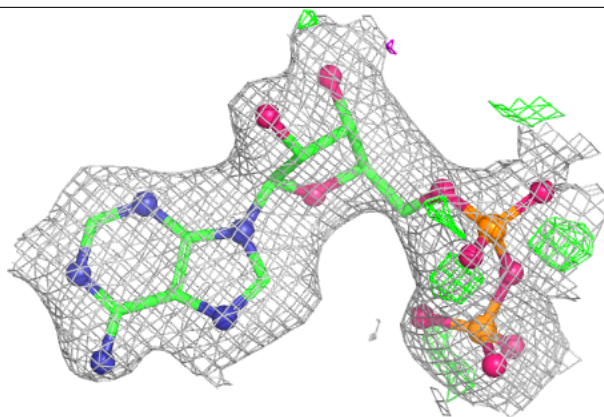
Electron density around ADP AM 402:

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

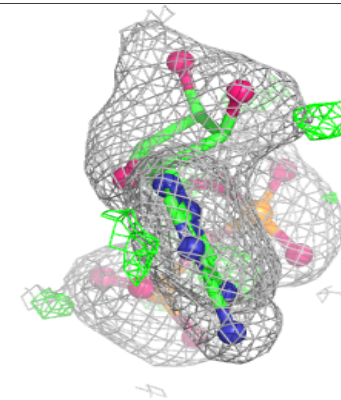
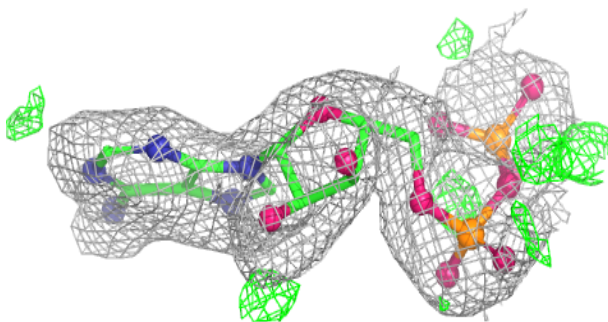
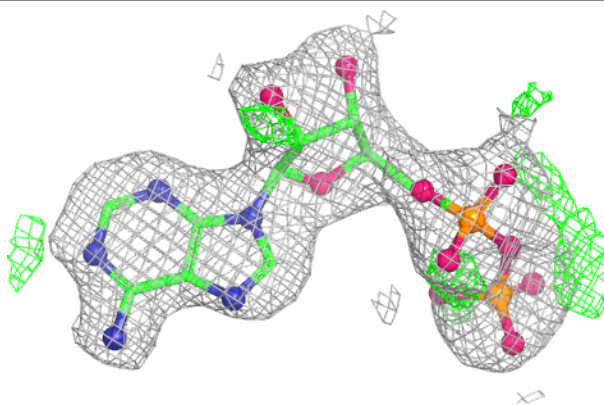


Electron density around ADP AO 402:

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

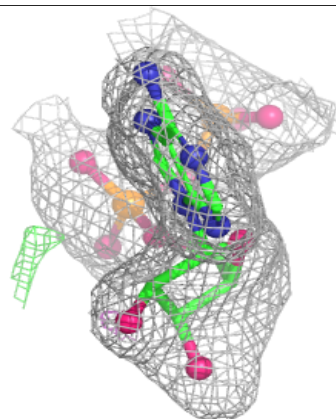
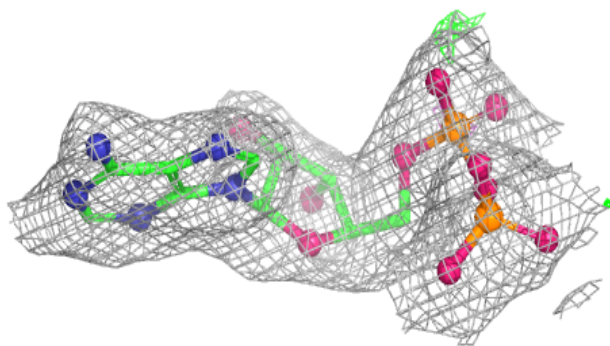
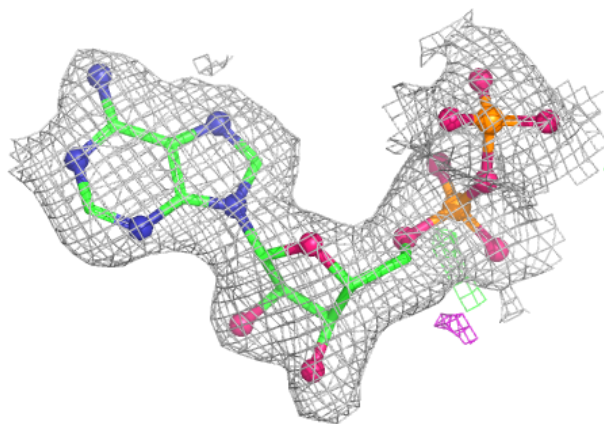
**Electron density around ADP AP 402:**

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



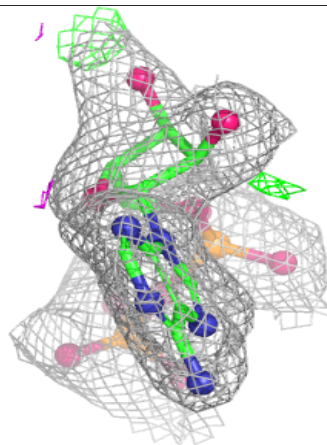
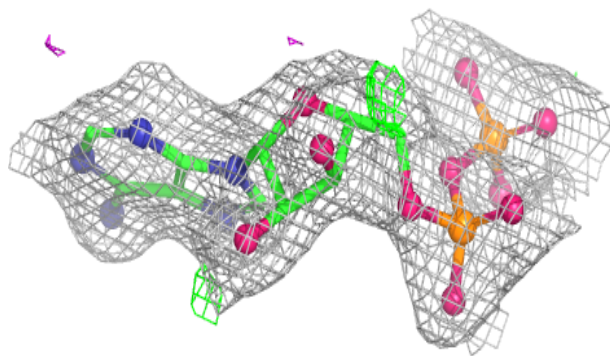
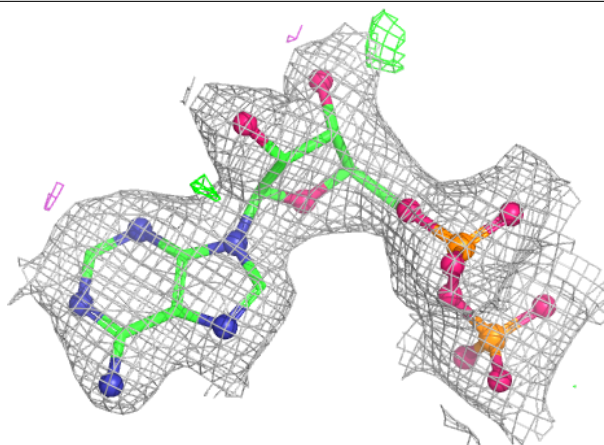
Electron density around ADP BA 502:

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



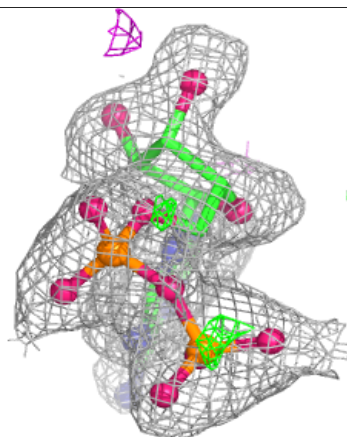
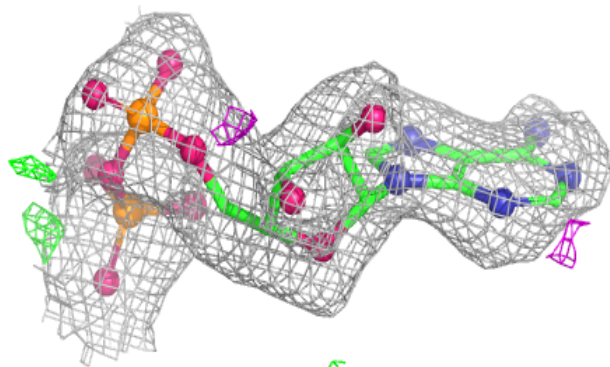
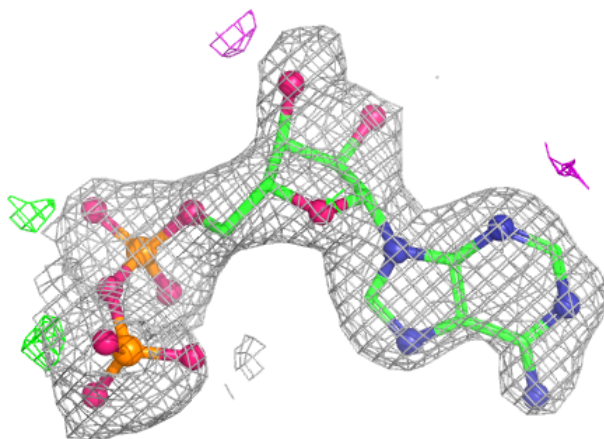
Electron density around ADP BC 402:

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



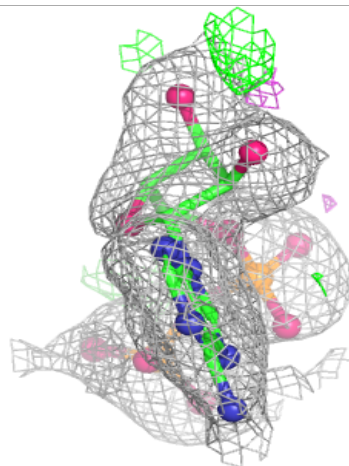
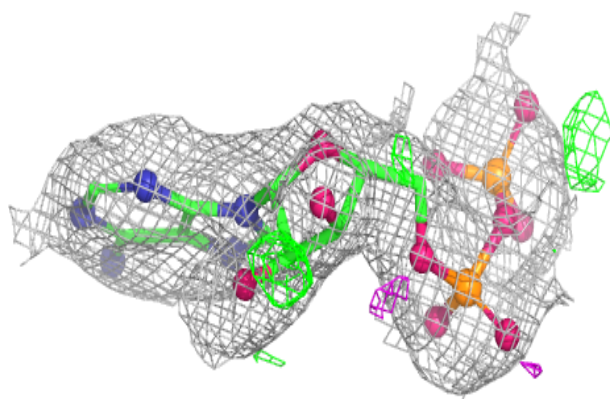
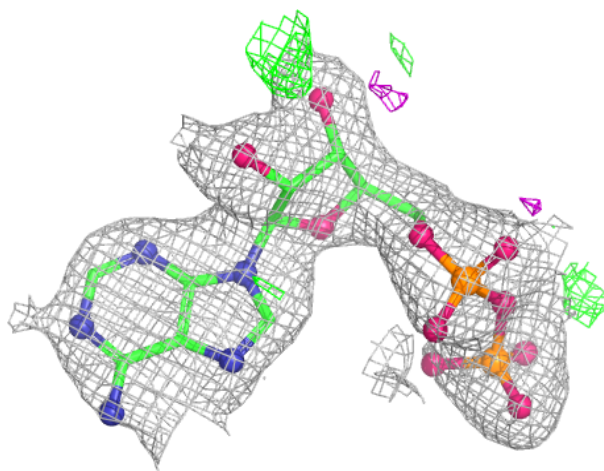
Electron density around ADP BD 402:

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



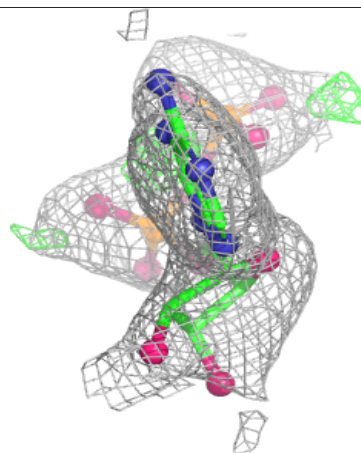
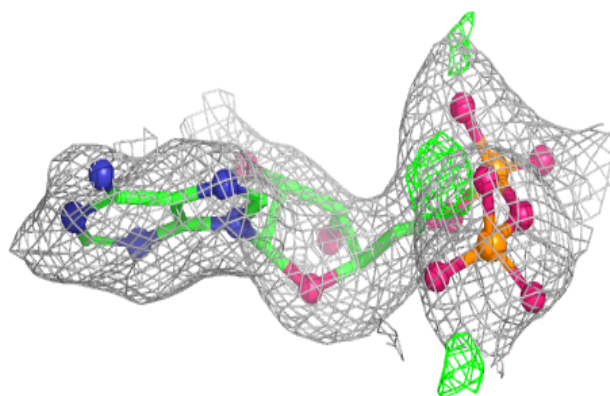
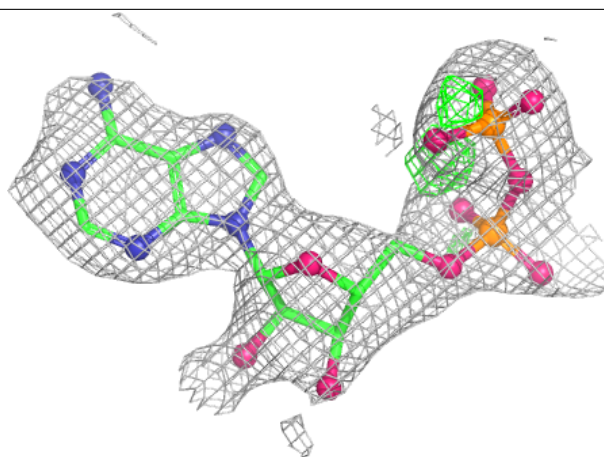
Electron density around ADP BE 402:

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



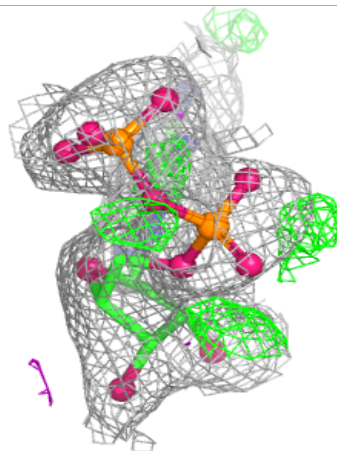
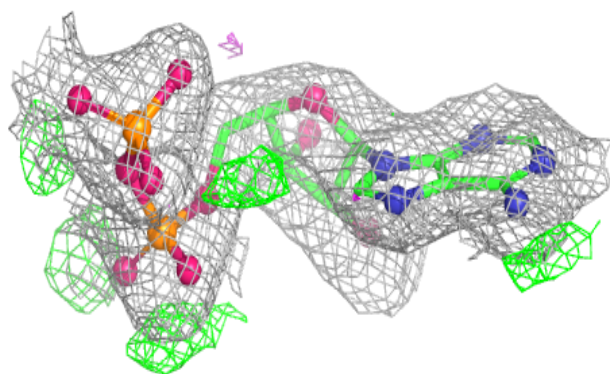
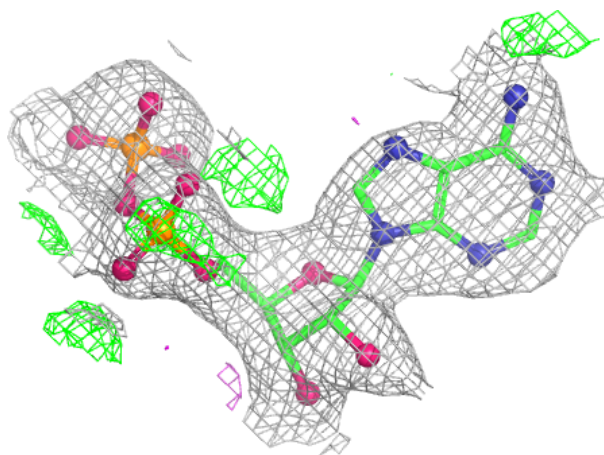
Electron density around ADP BL 402:

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



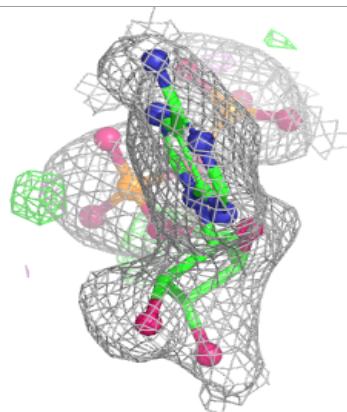
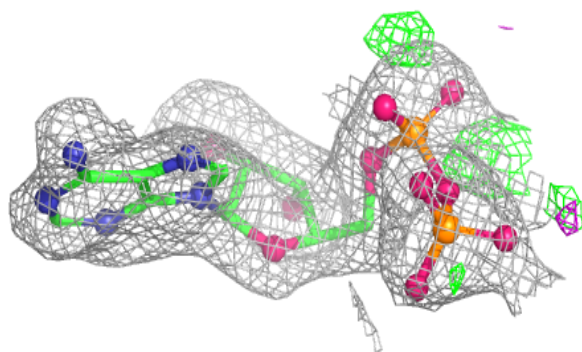
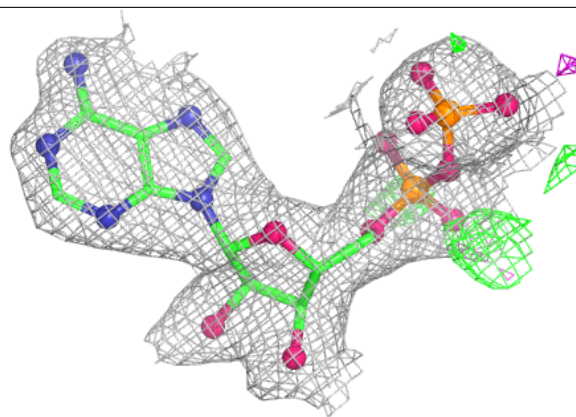
Electron density around ADP BN 402:

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

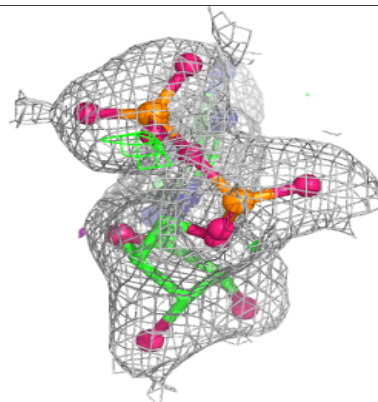
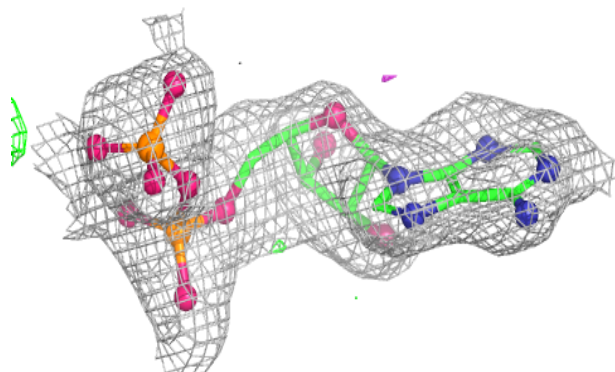
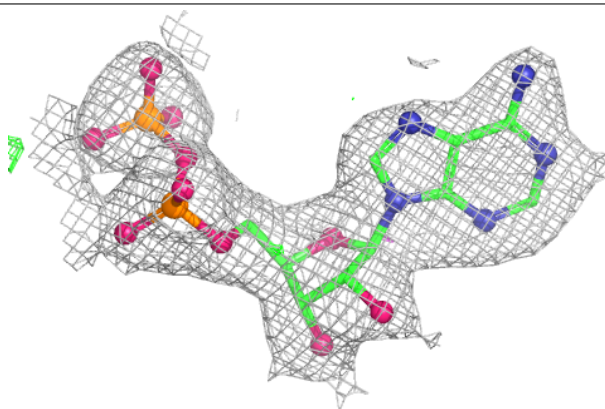


Electron density around ADP BQ 402:

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

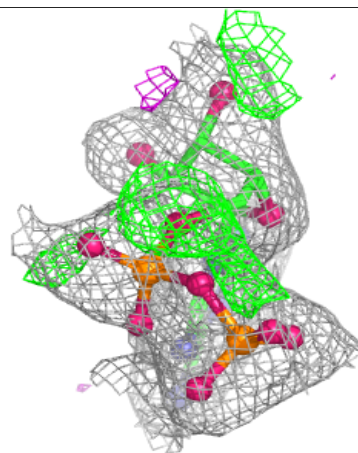
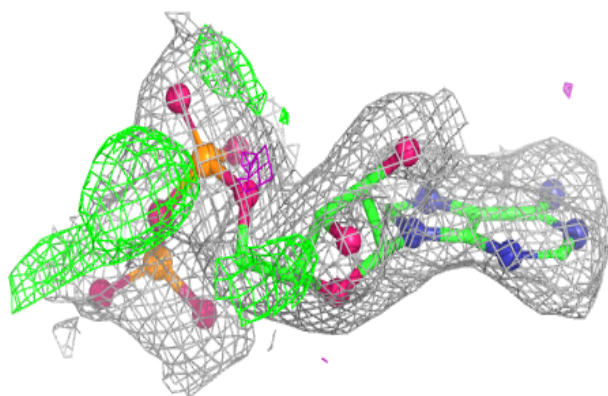
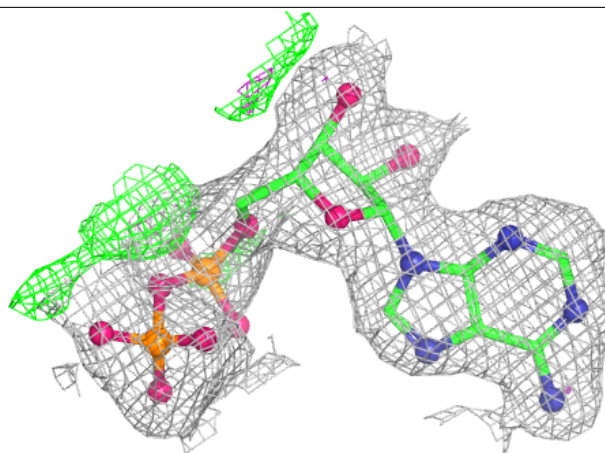
**Electron density around ADP BK 402:**

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

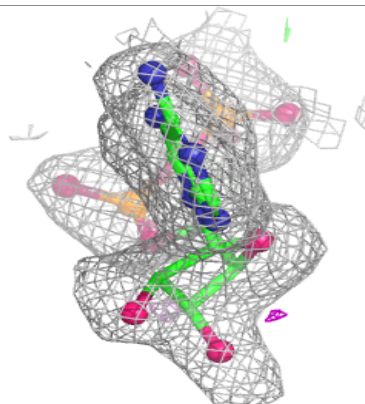
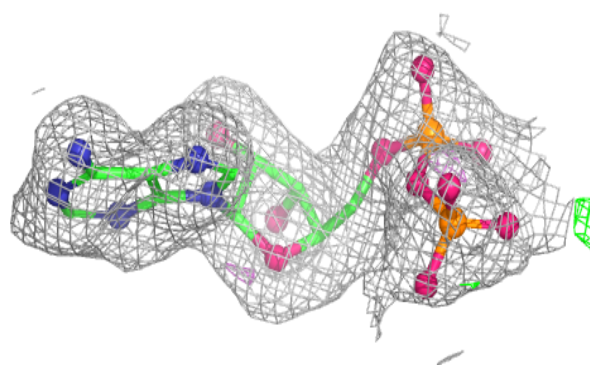
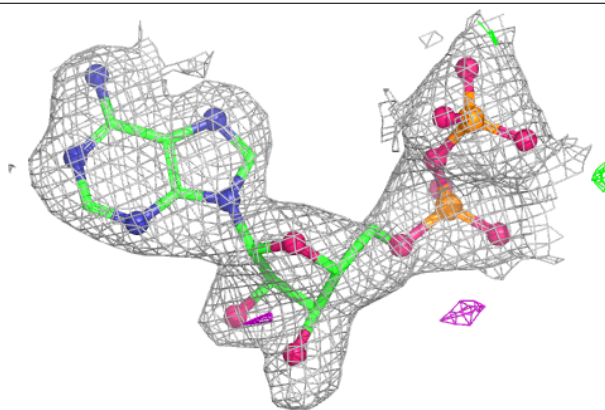


Electron density around ADP AQ 402:

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

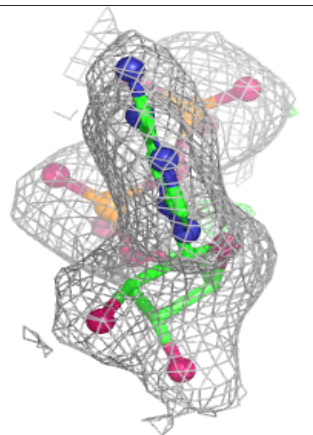
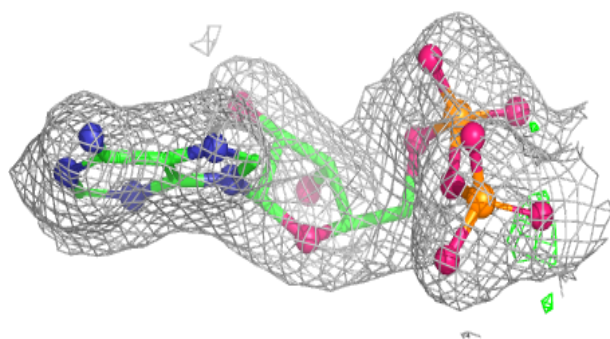
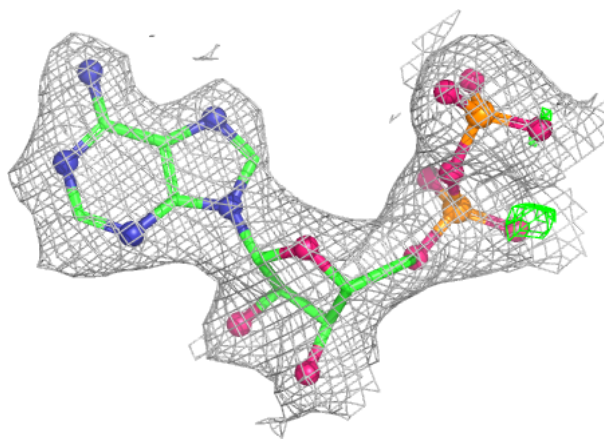
**Electron density around ADP BM 402:**

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



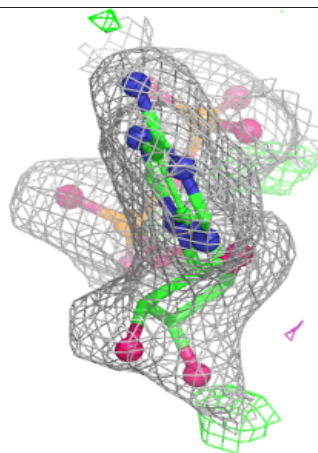
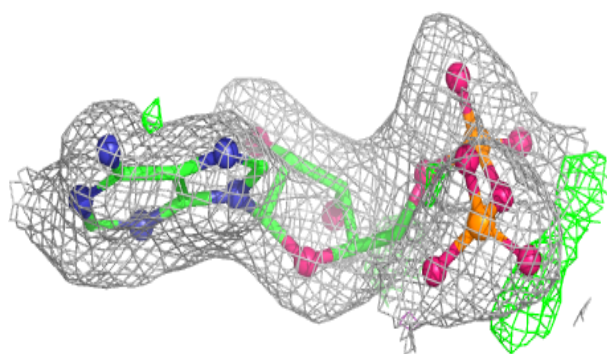
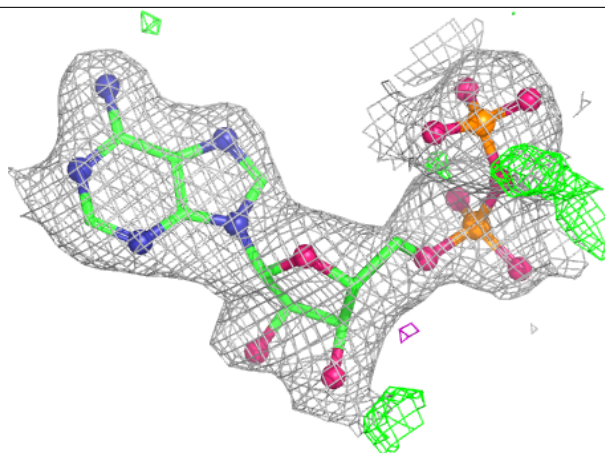
Electron density around ADP AR 402:

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



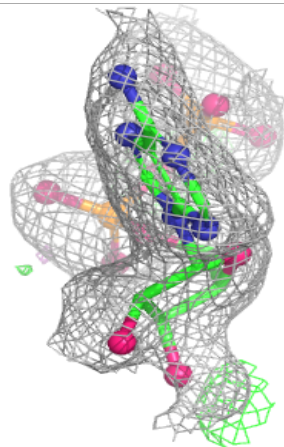
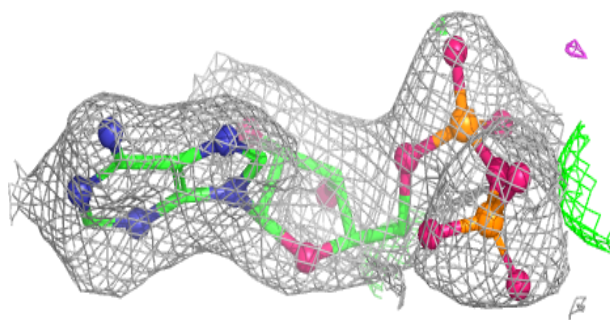
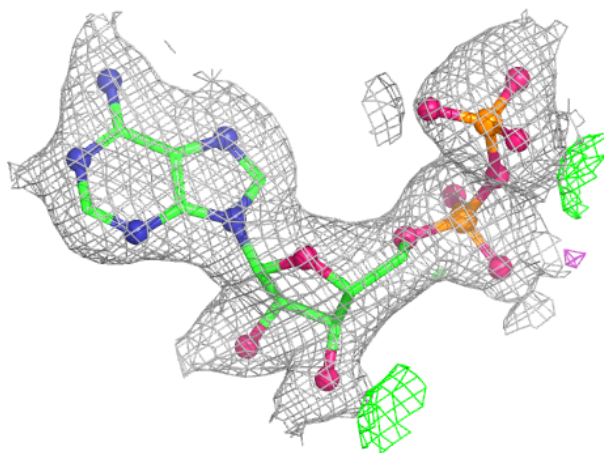
Electron density around ADP BO 402:

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



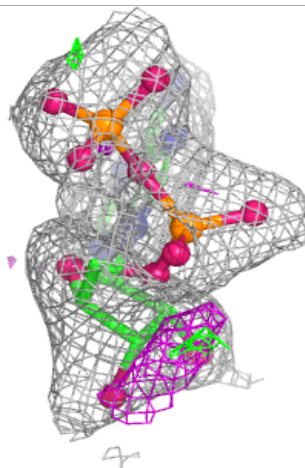
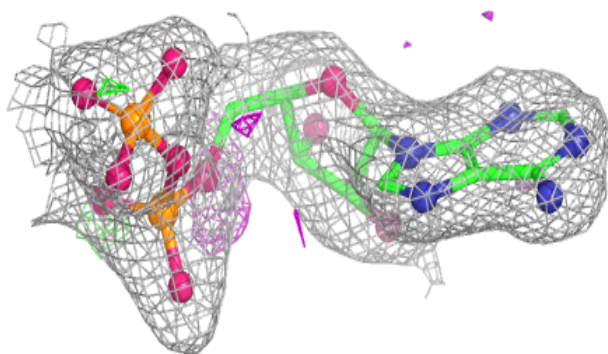
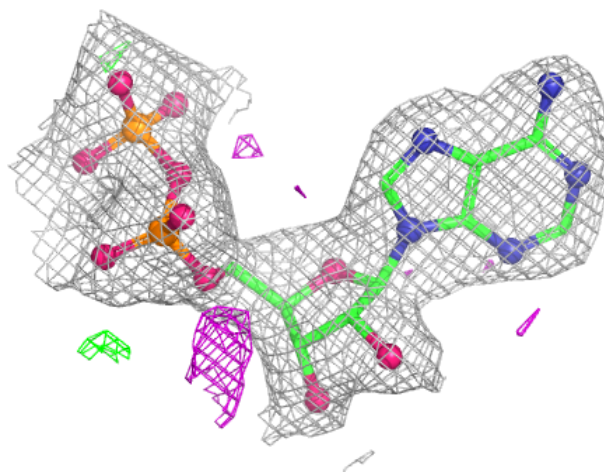
Electron density around ADP BP 402:

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



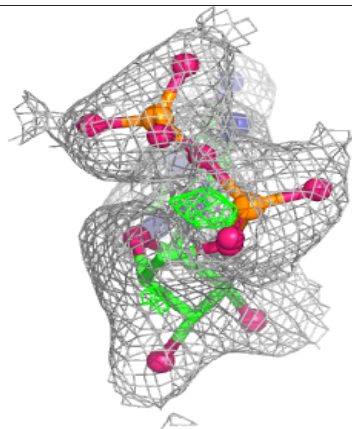
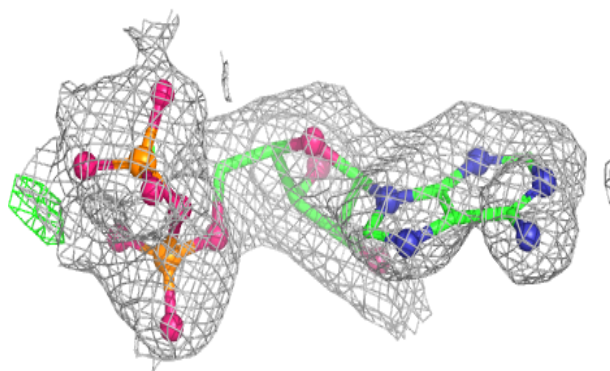
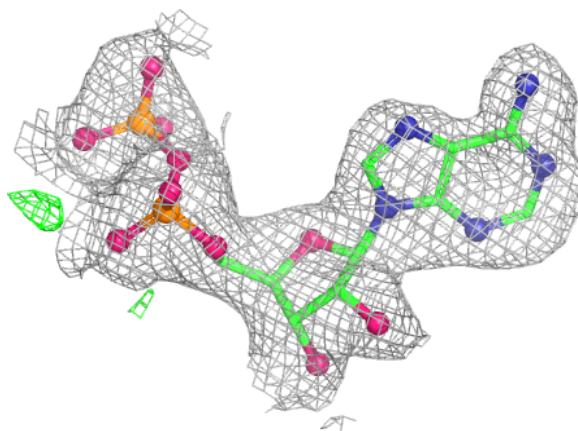
Electron density around ADP AD 402:

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



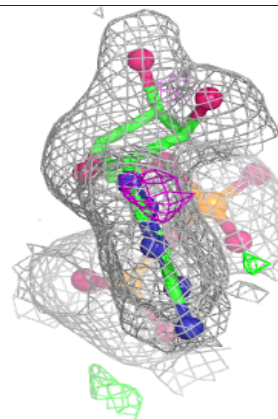
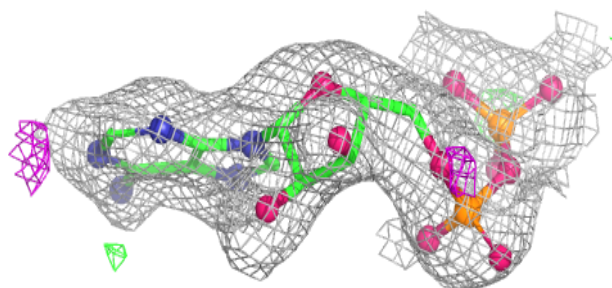
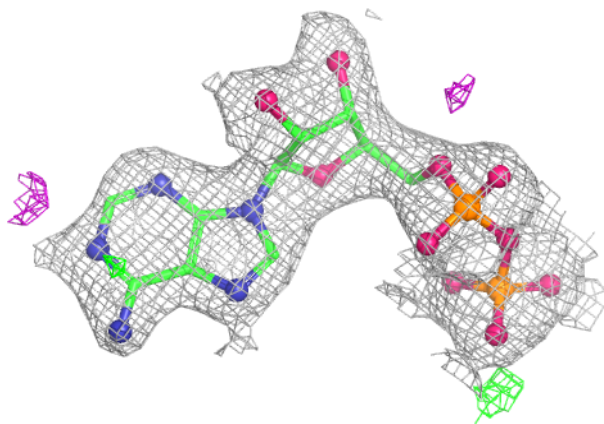
Electron density around ADP BR 402:

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



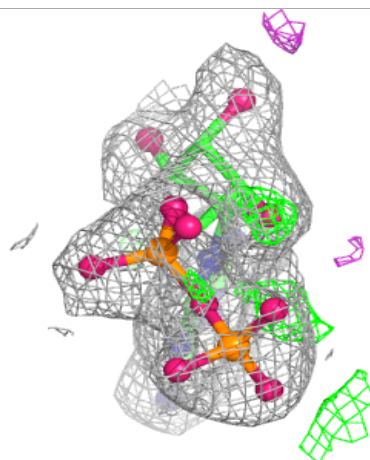
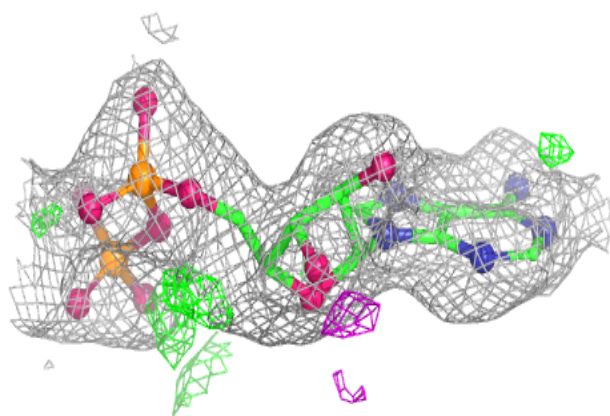
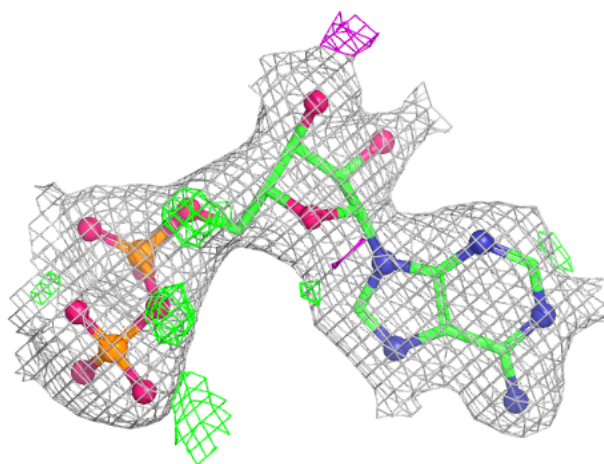
Electron density around ADP BB 402:

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



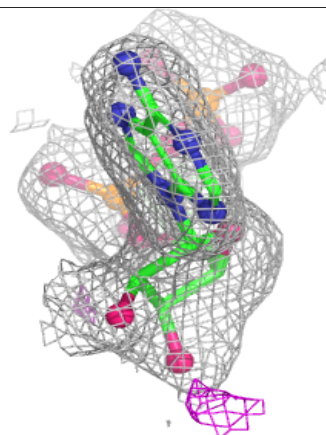
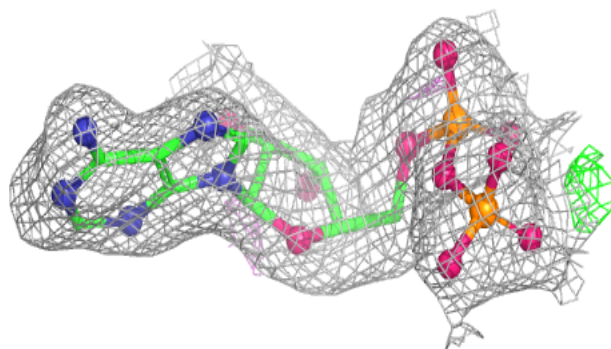
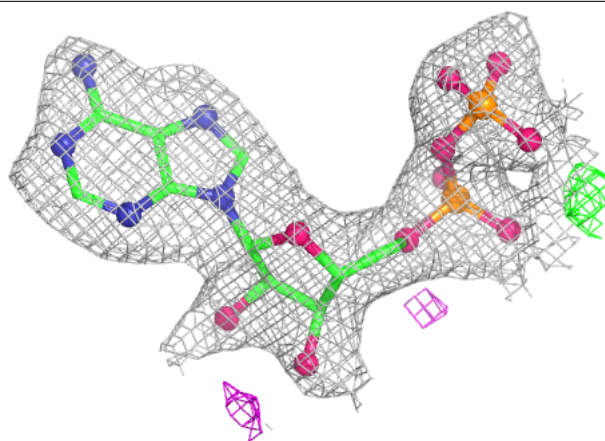
Electron density around ADP AN 402:

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

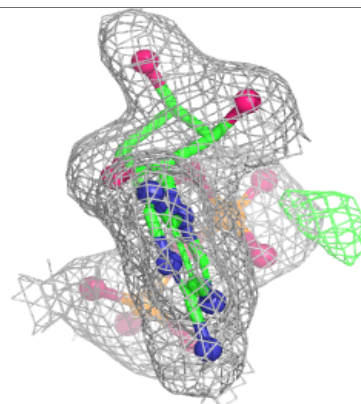
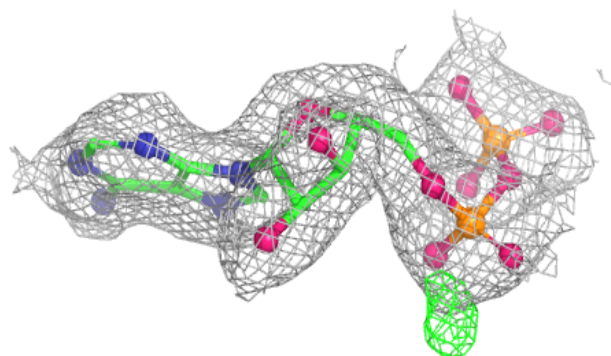
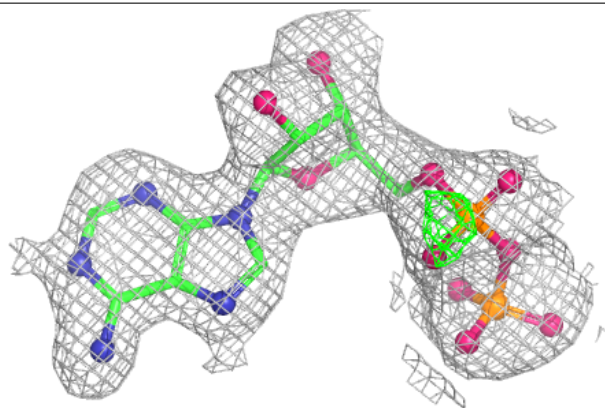


Electron density around ADP AB 402:

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

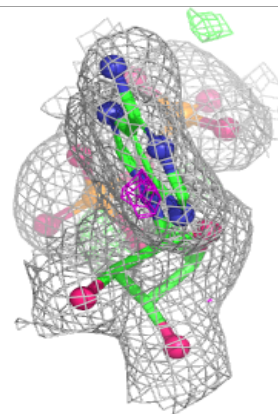
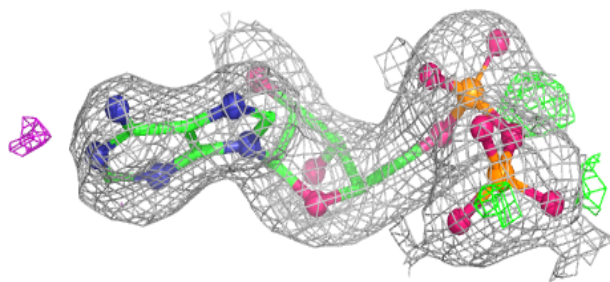
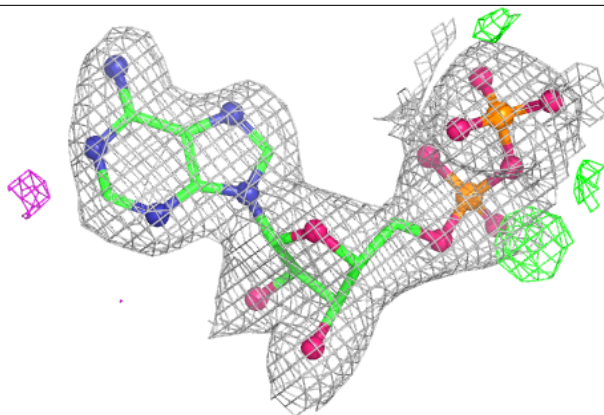
**Electron density around ADP AL 402:**

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



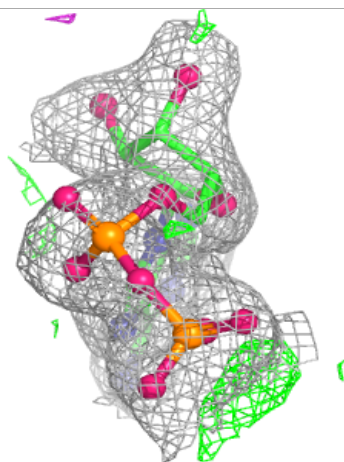
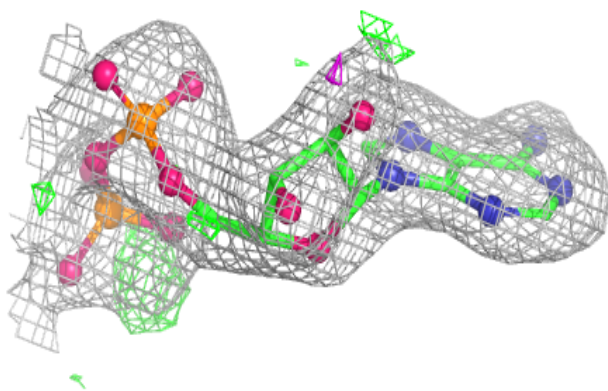
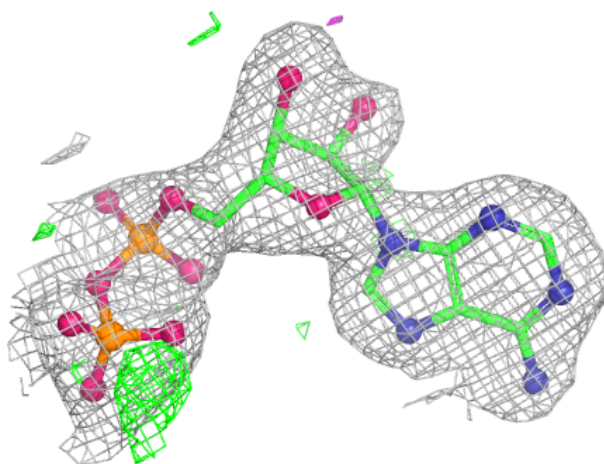
Electron density around ADP BF 402:

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



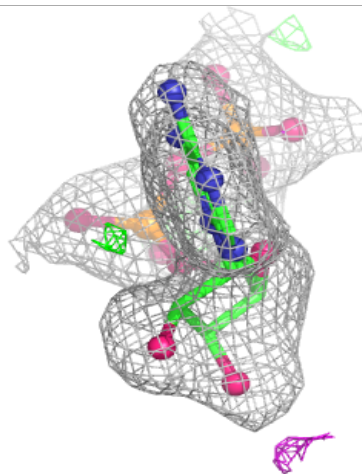
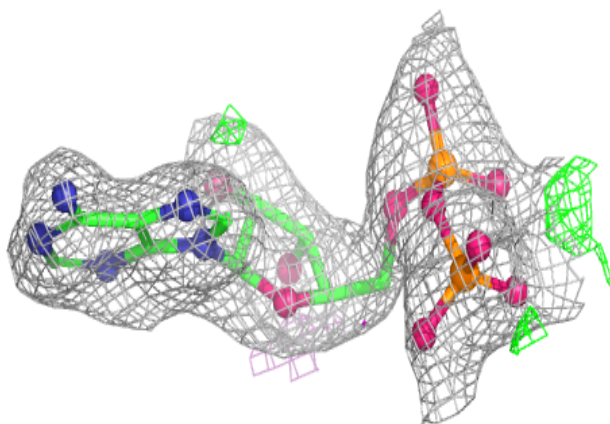
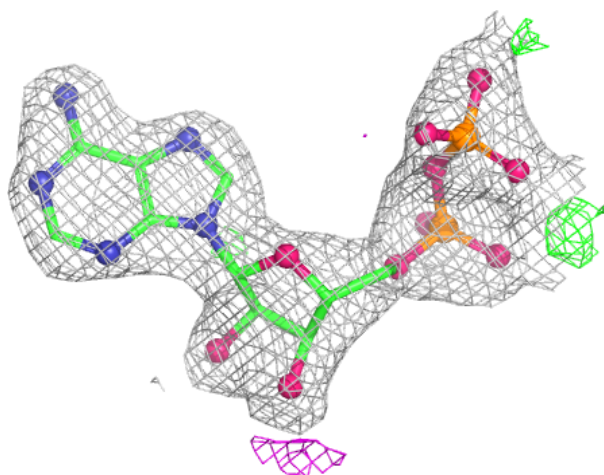
Electron density around ADP BG 402:

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



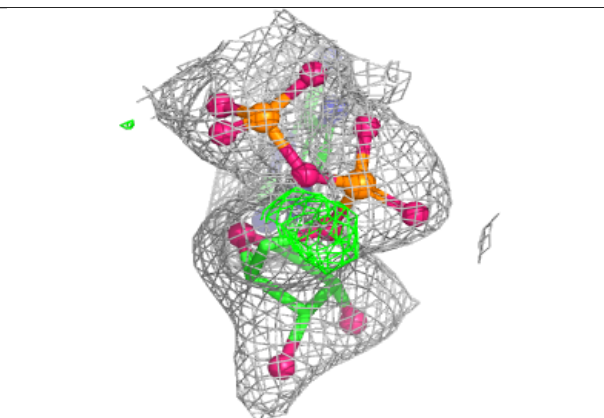
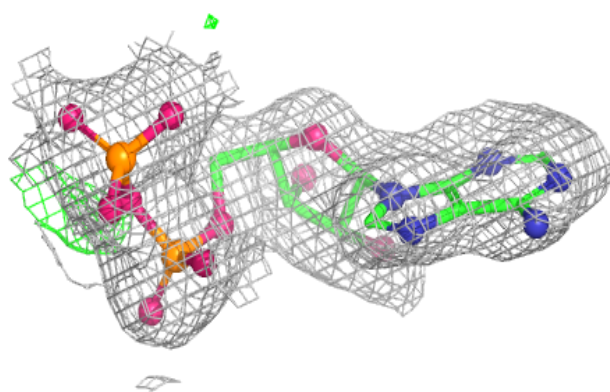
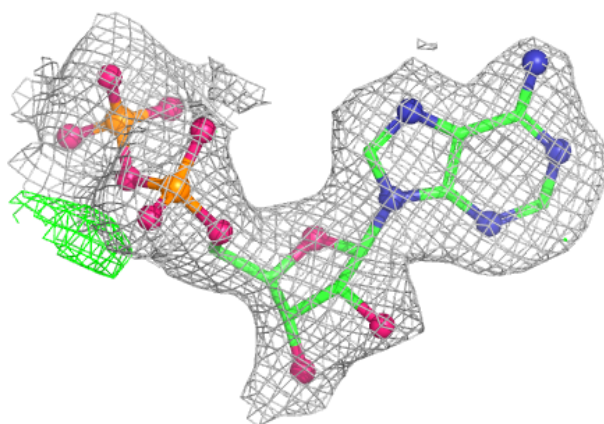
Electron density around ADP BH 402:

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

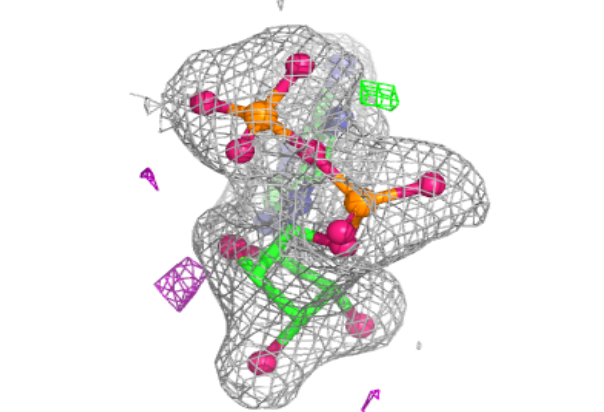
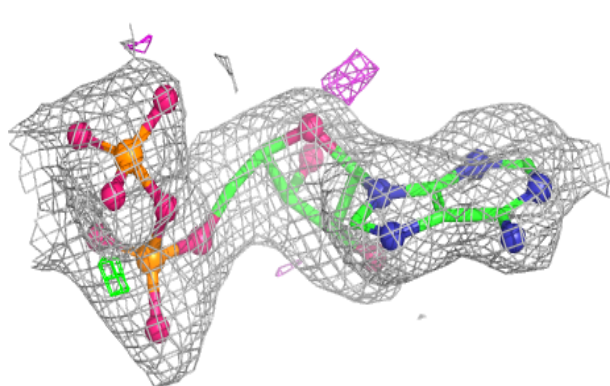
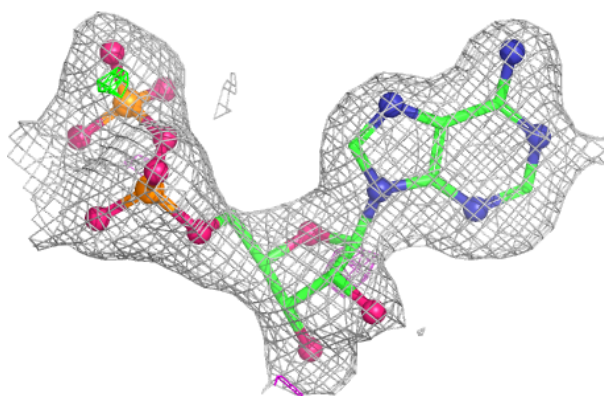


Electron density around ADP BI 402:

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

**Electron density around ADP BJ 402:**

$2mF_o-DF_c$ (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.