



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 01:30 pm BST

PDB ID : 4V8R / pdb_00004v8r
Title : The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning
Authors : Kalisman, N.; Schroder, G.F.; Levitt, M.
Deposited on : 2012-03-28
Resolution : 3.80 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

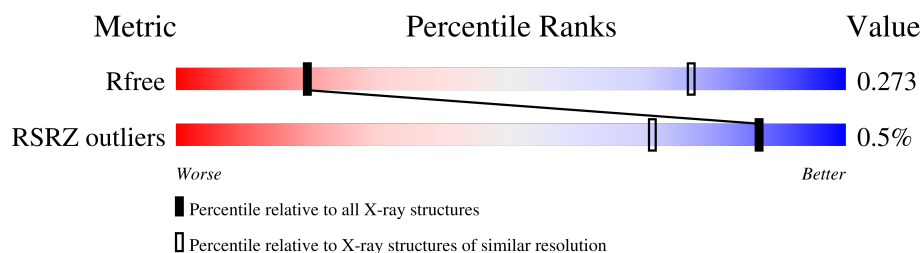
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 128780 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 T-COMPLEX PROTEIN 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Aa	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	BA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Ba	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			

- Molecule 2 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Ab	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	BB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Bb	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			

- Molecule 3 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Ad	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	BD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Bd	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AD	345	ASP	GLY	engineered mutation	UNP P39078
Ad	1345	ASP	GLY	engineered mutation	UNP P39078
BD	3345	ASP	GLY	engineered mutation	UNP P39078
Bd	4345	ASP	GLY	engineered mutation	UNP P39078

- Molecule 4 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Ae	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	BE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Be	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			

- Molecule 5 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Ag	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	BG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Bg	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	901	GLY	-	insertion	UNP P39077
AG	902	SER	-	insertion	UNP P39077
AG	903	GLY	-	insertion	UNP P39077
AG	904	SER	-	insertion	UNP P39077
AG	905	GLY	-	insertion	UNP P39077
AG	906	TRP	-	insertion	UNP P39077
AG	907	SER	-	insertion	UNP P39077
AG	908	HIS	-	insertion	UNP P39077
AG	909	PRO	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	910	GLN	-	insertion	UNP P39077
AG	911	PHE	-	insertion	UNP P39077
AG	912	GLU	-	insertion	UNP P39077
AG	913	LYS	-	insertion	UNP P39077
AG	914	GLY	-	insertion	UNP P39077
AG	915	SER	-	insertion	UNP P39077
AG	916	GLY	-	insertion	UNP P39077
AG	917	LYS	-	insertion	UNP P39077
AG	918	ARG	-	insertion	UNP P39077
AG	919	ARG	-	insertion	UNP P39077
AG	920	TRP	-	insertion	UNP P39077
AG	921	LYS	-	insertion	UNP P39077
AG	922	LYS	-	insertion	UNP P39077
AG	923	ASN	-	insertion	UNP P39077
AG	924	PHE	-	insertion	UNP P39077
AG	925	ILE	-	insertion	UNP P39077
AG	926	ALA	-	insertion	UNP P39077
AG	927	VAL	-	insertion	UNP P39077
AG	928	SER	-	insertion	UNP P39077
AG	929	ALA	-	insertion	UNP P39077
AG	930	ALA	-	insertion	UNP P39077
AG	931	ASN	-	insertion	UNP P39077
AG	932	ARG	-	insertion	UNP P39077
AG	933	PHE	-	insertion	UNP P39077
AG	934	LYS	-	insertion	UNP P39077
AG	935	LYS	-	insertion	UNP P39077
AG	936	ILE	-	insertion	UNP P39077
AG	937	SER	-	insertion	UNP P39077
AG	938	SER	-	insertion	UNP P39077
AG	939	SER	-	insertion	UNP P39077
AG	940	GLY	-	insertion	UNP P39077
AG	941	ALA	-	insertion	UNP P39077
AG	942	LEU	-	insertion	UNP P39077
AG	943	GLY	-	insertion	UNP P39077
AG	944	SER	-	insertion	UNP P39077
AG	945	GLY	-	insertion	UNP P39077
AG	946	HIS	-	insertion	UNP P39077
AG	947	HIS	-	insertion	UNP P39077
AG	948	HIS	-	insertion	UNP P39077
AG	949	HIS	-	insertion	UNP P39077
AG	950	HIS	-	insertion	UNP P39077
AG	951	HIS	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	952	HIS	-	insertion	UNP P39077
AG	953	HIS	-	insertion	UNP P39077
AG	954	GLY	-	insertion	UNP P39077
AG	955	SER	-	insertion	UNP P39077
AG	956	GLY	-	insertion	UNP P39077
Ag	1901	GLY	-	insertion	UNP P39077
Ag	1902	SER	-	insertion	UNP P39077
Ag	1903	GLY	-	insertion	UNP P39077
Ag	1904	SER	-	insertion	UNP P39077
Ag	1905	GLY	-	insertion	UNP P39077
Ag	1906	TRP	-	insertion	UNP P39077
Ag	1907	SER	-	insertion	UNP P39077
Ag	1908	HIS	-	insertion	UNP P39077
Ag	1909	PRO	-	insertion	UNP P39077
Ag	1910	GLN	-	insertion	UNP P39077
Ag	1911	PHE	-	insertion	UNP P39077
Ag	1912	GLU	-	insertion	UNP P39077
Ag	1913	LYS	-	insertion	UNP P39077
Ag	1914	GLY	-	insertion	UNP P39077
Ag	1915	SER	-	insertion	UNP P39077
Ag	1916	GLY	-	insertion	UNP P39077
Ag	1917	LYS	-	insertion	UNP P39077
Ag	1918	ARG	-	insertion	UNP P39077
Ag	1919	ARG	-	insertion	UNP P39077
Ag	1920	TRP	-	insertion	UNP P39077
Ag	1921	LYS	-	insertion	UNP P39077
Ag	1922	LYS	-	insertion	UNP P39077
Ag	1923	ASN	-	insertion	UNP P39077
Ag	1924	PHE	-	insertion	UNP P39077
Ag	1925	ILE	-	insertion	UNP P39077
Ag	1926	ALA	-	insertion	UNP P39077
Ag	1927	VAL	-	insertion	UNP P39077
Ag	1928	SER	-	insertion	UNP P39077
Ag	1929	ALA	-	insertion	UNP P39077
Ag	1930	ALA	-	insertion	UNP P39077
Ag	1931	ASN	-	insertion	UNP P39077
Ag	1932	ARG	-	insertion	UNP P39077
Ag	1933	PHE	-	insertion	UNP P39077
Ag	1934	LYS	-	insertion	UNP P39077
Ag	1935	LYS	-	insertion	UNP P39077
Ag	1936	ILE	-	insertion	UNP P39077
Ag	1937	SER	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Ag	1938	SER	-	insertion	UNP P39077
Ag	1939	SER	-	insertion	UNP P39077
Ag	1940	GLY	-	insertion	UNP P39077
Ag	1941	ALA	-	insertion	UNP P39077
Ag	1942	LEU	-	insertion	UNP P39077
Ag	1943	GLY	-	insertion	UNP P39077
Ag	1944	SER	-	insertion	UNP P39077
Ag	1945	GLY	-	insertion	UNP P39077
Ag	1946	HIS	-	insertion	UNP P39077
Ag	1947	HIS	-	insertion	UNP P39077
Ag	1948	HIS	-	insertion	UNP P39077
Ag	1949	HIS	-	insertion	UNP P39077
Ag	1950	HIS	-	insertion	UNP P39077
Ag	1951	HIS	-	insertion	UNP P39077
Ag	1952	HIS	-	insertion	UNP P39077
Ag	1953	HIS	-	insertion	UNP P39077
Ag	1954	GLY	-	insertion	UNP P39077
Ag	1955	SER	-	insertion	UNP P39077
Ag	1956	GLY	-	insertion	UNP P39077
BG	3901	GLY	-	insertion	UNP P39077
BG	3902	SER	-	insertion	UNP P39077
BG	3903	GLY	-	insertion	UNP P39077
BG	3904	SER	-	insertion	UNP P39077
BG	3905	GLY	-	insertion	UNP P39077
BG	3906	TRP	-	insertion	UNP P39077
BG	3907	SER	-	insertion	UNP P39077
BG	3908	HIS	-	insertion	UNP P39077
BG	3909	PRO	-	insertion	UNP P39077
BG	3910	GLN	-	insertion	UNP P39077
BG	3911	PHE	-	insertion	UNP P39077
BG	3912	GLU	-	insertion	UNP P39077
BG	3913	LYS	-	insertion	UNP P39077
BG	3914	GLY	-	insertion	UNP P39077
BG	3915	SER	-	insertion	UNP P39077
BG	3916	GLY	-	insertion	UNP P39077
BG	3917	LYS	-	insertion	UNP P39077
BG	3918	ARG	-	insertion	UNP P39077
BG	3919	ARG	-	insertion	UNP P39077
BG	3920	TRP	-	insertion	UNP P39077
BG	3921	LYS	-	insertion	UNP P39077
BG	3922	LYS	-	insertion	UNP P39077
BG	3923	ASN	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
BG	3924	PHE	-	insertion	UNP P39077
BG	3925	ILE	-	insertion	UNP P39077
BG	3926	ALA	-	insertion	UNP P39077
BG	3927	VAL	-	insertion	UNP P39077
BG	3928	SER	-	insertion	UNP P39077
BG	3929	ALA	-	insertion	UNP P39077
BG	3930	ALA	-	insertion	UNP P39077
BG	3931	ASN	-	insertion	UNP P39077
BG	3932	ARG	-	insertion	UNP P39077
BG	3933	PHE	-	insertion	UNP P39077
BG	3934	LYS	-	insertion	UNP P39077
BG	3935	LYS	-	insertion	UNP P39077
BG	3936	ILE	-	insertion	UNP P39077
BG	3937	SER	-	insertion	UNP P39077
BG	3938	SER	-	insertion	UNP P39077
BG	3939	SER	-	insertion	UNP P39077
BG	3940	GLY	-	insertion	UNP P39077
BG	3941	ALA	-	insertion	UNP P39077
BG	3942	LEU	-	insertion	UNP P39077
BG	3943	GLY	-	insertion	UNP P39077
BG	3944	SER	-	insertion	UNP P39077
BG	3945	GLY	-	insertion	UNP P39077
BG	3946	HIS	-	insertion	UNP P39077
BG	3947	HIS	-	insertion	UNP P39077
BG	3948	HIS	-	insertion	UNP P39077
BG	3949	HIS	-	insertion	UNP P39077
BG	3950	HIS	-	insertion	UNP P39077
BG	3951	HIS	-	insertion	UNP P39077
BG	3952	HIS	-	insertion	UNP P39077
BG	3953	HIS	-	insertion	UNP P39077
BG	3954	GLY	-	insertion	UNP P39077
BG	3955	SER	-	insertion	UNP P39077
BG	3956	GLY	-	insertion	UNP P39077
Bg	4901	GLY	-	insertion	UNP P39077
Bg	4902	SER	-	insertion	UNP P39077
Bg	4903	GLY	-	insertion	UNP P39077
Bg	4904	SER	-	insertion	UNP P39077
Bg	4905	GLY	-	insertion	UNP P39077
Bg	4906	TRP	-	insertion	UNP P39077
Bg	4907	SER	-	insertion	UNP P39077
Bg	4908	HIS	-	insertion	UNP P39077
Bg	4909	PRO	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4910	GLN	-	insertion	UNP P39077
Bg	4911	PHE	-	insertion	UNP P39077
Bg	4912	GLU	-	insertion	UNP P39077
Bg	4913	LYS	-	insertion	UNP P39077
Bg	4914	GLY	-	insertion	UNP P39077
Bg	4915	SER	-	insertion	UNP P39077
Bg	4916	GLY	-	insertion	UNP P39077
Bg	4917	LYS	-	insertion	UNP P39077
Bg	4918	ARG	-	insertion	UNP P39077
Bg	4919	ARG	-	insertion	UNP P39077
Bg	4920	TRP	-	insertion	UNP P39077
Bg	4921	LYS	-	insertion	UNP P39077
Bg	4922	LYS	-	insertion	UNP P39077
Bg	4923	ASN	-	insertion	UNP P39077
Bg	4924	PHE	-	insertion	UNP P39077
Bg	4925	ILE	-	insertion	UNP P39077
Bg	4926	ALA	-	insertion	UNP P39077
Bg	4927	VAL	-	insertion	UNP P39077
Bg	4928	SER	-	insertion	UNP P39077
Bg	4929	ALA	-	insertion	UNP P39077
Bg	4930	ALA	-	insertion	UNP P39077
Bg	4931	ASN	-	insertion	UNP P39077
Bg	4932	ARG	-	insertion	UNP P39077
Bg	4933	PHE	-	insertion	UNP P39077
Bg	4934	LYS	-	insertion	UNP P39077
Bg	4935	LYS	-	insertion	UNP P39077
Bg	4936	ILE	-	insertion	UNP P39077
Bg	4937	SER	-	insertion	UNP P39077
Bg	4938	SER	-	insertion	UNP P39077
Bg	4939	SER	-	insertion	UNP P39077
Bg	4940	GLY	-	insertion	UNP P39077
Bg	4941	ALA	-	insertion	UNP P39077
Bg	4942	LEU	-	insertion	UNP P39077
Bg	4943	GLY	-	insertion	UNP P39077
Bg	4944	SER	-	insertion	UNP P39077
Bg	4945	GLY	-	insertion	UNP P39077
Bg	4946	HIS	-	insertion	UNP P39077
Bg	4947	HIS	-	insertion	UNP P39077
Bg	4948	HIS	-	insertion	UNP P39077
Bg	4949	HIS	-	insertion	UNP P39077
Bg	4950	HIS	-	insertion	UNP P39077
Bg	4951	HIS	-	insertion	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4952	HIS	-	insertion	UNP P39077
Bg	4953	HIS	-	insertion	UNP P39077
Bg	4954	GLY	-	insertion	UNP P39077
Bg	4955	SER	-	insertion	UNP P39077
Bg	4956	GLY	-	insertion	UNP P39077

- Molecule 6 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Ah	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	BH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Bh	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			

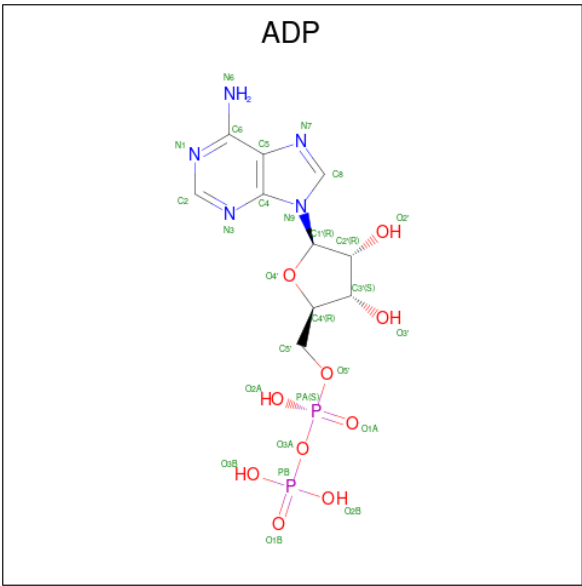
- Molecule 7 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Aq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	BQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Bq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			

- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Az	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	BZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Bz	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



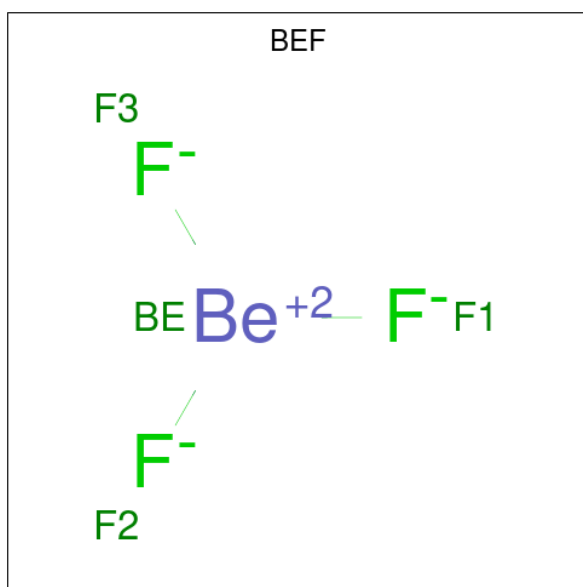
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AZ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Aa	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ab	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ad	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ae	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ag	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Ah	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Aq	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Az	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BZ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ba	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bb	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bd	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Be	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bg	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bh	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bq	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bz	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AA	1	Total	Be	F	0	0
			4	1	3		
10	AB	1	Total	Be	F	0	0
			4	1	3		
10	AD	1	Total	Be	F	0	0
			4	1	3		
10	AE	1	Total	Be	F	0	0
			4	1	3		
10	AG	1	Total	Be	F	0	0
			4	1	3		
10	AH	1	Total	Be	F	0	0
			4	1	3		
10	AQ	1	Total	Be	F	0	0
			4	1	3		
10	AZ	1	Total	Be	F	0	0
			4	1	3		
10	Aa	1	Total	Be	F	0	0
			4	1	3		
10	Ab	1	Total	Be	F	0	0
			4	1	3		
10	Ad	1	Total	Be	F	0	0
			4	1	3		
10	Ae	1	Total	Be	F	0	0
			4	1	3		
10	Ag	1	Total	Be	F	0	0
			4	1	3		
10	Ah	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	Aq	1	Total 4	Be 1	F 3	0	0
10	Az	1	Total 4	Be 1	F 3	0	0
10	BA	1	Total 4	Be 1	F 3	0	0
10	BB	1	Total 4	Be 1	F 3	0	0
10	BD	1	Total 4	Be 1	F 3	0	0
10	BE	1	Total 4	Be 1	F 3	0	0
10	BG	1	Total 4	Be 1	F 3	0	0
10	BH	1	Total 4	Be 1	F 3	0	0
10	BQ	1	Total 4	Be 1	F 3	0	0
10	BZ	1	Total 4	Be 1	F 3	0	0
10	Ba	1	Total 4	Be 1	F 3	0	0
10	Bb	1	Total 4	Be 1	F 3	0	0
10	Bd	1	Total 4	Be 1	F 3	0	0
10	Be	1	Total 4	Be 1	F 3	0	0
10	Bg	1	Total 4	Be 1	F 3	0	0
10	Bh	1	Total 4	Be 1	F 3	0	0
10	Bq	1	Total 4	Be 1	F 3	0	0
10	Bz	1	Total 4	Be 1	F 3	0	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AA	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AB	1	Total 1	Mg 1	0	0
11	AD	1	Total 1	Mg 1	0	0
11	AE	1	Total 1	Mg 1	0	0
11	AG	1	Total 1	Mg 1	0	0
11	AH	1	Total 1	Mg 1	0	0
11	AQ	1	Total 1	Mg 1	0	0
11	AZ	1	Total 1	Mg 1	0	0
11	Aa	1	Total 1	Mg 1	0	0
11	Ab	1	Total 1	Mg 1	0	0
11	Ad	1	Total 1	Mg 1	0	0
11	Ae	1	Total 1	Mg 1	0	0
11	Ag	1	Total 1	Mg 1	0	0
11	Ah	1	Total 1	Mg 1	0	0
11	Aq	1	Total 1	Mg 1	0	0
11	Az	1	Total 1	Mg 1	0	0
11	BA	1	Total 1	Mg 1	0	0
11	BB	1	Total 1	Mg 1	0	0
11	BD	1	Total 1	Mg 1	0	0
11	BE	1	Total 1	Mg 1	0	0
11	BG	1	Total 1	Mg 1	0	0
11	BH	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	BQ	1	Total	Mg	0	0
			1	1		
11	BZ	1	Total	Mg	0	0
			1	1		
11	Ba	1	Total	Mg	0	0
			1	1		
11	Bb	1	Total	Mg	0	0
			1	1		
11	Bd	1	Total	Mg	0	0
			1	1		
11	Be	1	Total	Mg	0	0
			1	1		
11	Bg	1	Total	Mg	0	0
			1	1		
11	Bh	1	Total	Mg	0	0
			1	1		
11	Bq	1	Total	Mg	0	0
			1	1		
11	Bz	1	Total	Mg	0	0
			1	1		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	89.95 – 3.80 89.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (89.95-3.80) 91.5 (89.95-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.78Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.248 , 0.284 0.237 , 0.273	Depositor DCC
R_{free} test set	10483 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 129.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	128780	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 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
9	ADP	Aq	1601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.66	15 (35%)
9	ADP	AD	601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.74	13 (30%)
9	ADP	Ad	1601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.74	13 (30%)
10	BEF	Ag	2002	9	0,3,3	-	-	-	-	-
9	ADP	AQ	601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.67	15 (35%)
10	BEF	BA	3602	9	0,3,3	-	-	-	-	-
10	BEF	Bg	5002	9	0,3,3	-	-	-	-	-
10	BEF	Ba	4602	9	0,3,3	-	-	-	-	-
10	BEF	AQ	602	9	0,3,3	-	-	-	-	-
10	BEF	AD	602	9	0,3,3	-	-	-	-	-
9	ADP	Bz	4601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.64	13 (30%)
9	ADP	Az	1601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.63	13 (30%)
9	ADP	Bd	4601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.74	13 (30%)
9	ADP	BH	3601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.66	12 (28%)
10	BEF	Ah	1602	9	0,3,3	-	-	-	-	-
10	BEF	Bh	4602	9	0,3,3	-	-	-	-	-
9	ADP	AE	601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.64	12 (28%)
9	ADP	Bb	4601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.64	13 (30%)
9	ADP	BA	3601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.71	13 (30%)
9	ADP	Ag	2001	11,10	27,29,29	2.57	7 (25%)	42,45,45	2.61	11 (26%)
9	ADP	BZ	3601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.63	13 (30%)
10	BEF	Aa	1602	9	0,3,3	-	-	-	-	-
10	BEF	AH	602	9	0,3,3	-	-	-	-	-
10	BEF	BH	3602	9	0,3,3	-	-	-	-	-
10	BEF	Ab	1602	9	0,3,3	-	-	-	-	-
10	BEF	Bz	4602	9	0,3,3	-	-	-	-	-
10	BEF	AA	602	9	0,3,3	-	-	-	-	-
9	ADP	AA	601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.71	13 (30%)
10	BEF	Bq	4602	9	0,3,3	-	-	-	-	-
9	ADP	Ae	1601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.64	12 (28%)
9	ADP	Ab	1601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.64	13 (30%)
9	ADP	BD	3601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.74	13 (30%)
9	ADP	AZ	601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.63	13 (30%)
9	ADP	Bq	4601	11,10	27,29,29	2.53	7 (25%)	42,45,45	2.59	12 (28%)
10	BEF	Ad	1602	9	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BEF	Aq	1602	9	0,3,3	-	-	-		
10	BEF	AE	602	9	0,3,3	-	-	-		
10	BEF	BD	3602	9	0,3,3	-	-	-		
10	BEF	Bb	4602	9	0,3,3	-	-	-		
10	BEF	Ae	1602	9	0,3,3	-	-	-		
10	BEF	BG	4002	9	0,3,3	-	-	-		
10	BEF	Bd	4602	9	0,3,3	-	-	-		
10	BEF	BB	3602	9	0,3,3	-	-	-		
9	ADP	AB	601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.64	13 (30%)
10	BEF	AG	1002	9	0,3,3	-	-	-		
10	BEF	AZ	602	9	0,3,3	-	-	-		
9	ADP	Aa	1601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.70	13 (30%)
10	BEF	Az	1602	9	0,3,3	-	-	-		
9	ADP	BE	3601	11,10	27,29,29	2.56	7 (25%)	42,45,45	2.64	12 (28%)
9	ADP	Bg	5001	11,10	27,29,29	2.58	7 (25%)	42,45,45	2.63	11 (26%)
10	BEF	Be	4602	9	0,3,3	-	-	-		
9	ADP	Ah	1601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.66	12 (28%)
10	BEF	BQ	3602	9	0,3,3	-	-	-		
10	BEF	BZ	3602	9	0,3,3	-	-	-		
9	ADP	Be	4601	11,10	27,29,29	2.57	7 (25%)	42,45,45	2.65	12 (28%)
10	BEF	BE	3602	9	0,3,3	-	-	-		
9	ADP	BB	3601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.65	13 (30%)
9	ADP	BG	4001	11,10	27,29,29	2.58	7 (25%)	42,45,45	2.62	11 (26%)
9	ADP	AG	1001	11,10	27,29,29	2.58	7 (25%)	42,45,45	2.63	11 (26%)
9	ADP	Bh	4601	11,10	27,29,29	2.54	7 (25%)	42,45,45	2.66	12 (28%)
9	ADP	BQ	3601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.67	15 (35%)
9	ADP	AH	601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.65	12 (28%)
10	BEF	AB	602	9	0,3,3	-	-	-		
9	ADP	Ba	4601	11,10	27,29,29	2.55	7 (25%)	42,45,45	2.71	13 (30%)

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
9	ADP	Aq	1601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AD	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Ad	1601	11,10	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	AQ	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Bz	4601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Az	1601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Bd	4601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	BH	3601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AE	601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	Bb	4601	11,10	-	4/16/32/32	0/3/3/3
9	ADP	BA	3601	11,10	-	3/16/32/32	0/3/3/3
9	ADP	Ag	2001	11,10	-	2/16/32/32	0/3/3/3
9	ADP	BZ	3601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AA	601	11,10	-	3/16/32/32	0/3/3/3
9	ADP	Ae	1601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	Ab	1601	11,10	-	4/16/32/32	0/3/3/3
9	ADP	BD	3601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AZ	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Bq	4601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AB	601	11,10	-	4/16/32/32	0/3/3/3
9	ADP	Aa	1601	11,10	-	3/16/32/32	0/3/3/3
9	ADP	BE	3601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	Bg	5001	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Ah	1601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Be	4601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	BB	3601	11,10	-	4/16/32/32	0/3/3/3
9	ADP	BG	4001	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AG	1001	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Bh	4601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	BQ	3601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	AH	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	Ba	4601	11,10	-	3/16/32/32	0/3/3/3

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Bg	5001	ADP	C8-N7	8.88	1.48	1.31
9	AG	1001	ADP	C8-N7	8.87	1.48	1.31
9	BG	4001	ADP	C8-N7	8.87	1.48	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BD	3601	ADP	C8-N7	8.86	1.48	1.31
9	Bz	4601	ADP	C8-N7	8.85	1.48	1.31

The worst 5 of 405 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Bz	4601	ADP	N9-C8-N7	-10.06	100.16	113.91
9	AZ	601	ADP	N9-C8-N7	-10.04	100.18	113.91
9	Az	1601	ADP	N9-C8-N7	-10.03	100.19	113.91
9	BZ	3601	ADP	N9-C8-N7	-10.03	100.19	113.91
9	BD	3601	ADP	N9-C8-N7	-9.69	100.66	113.91

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

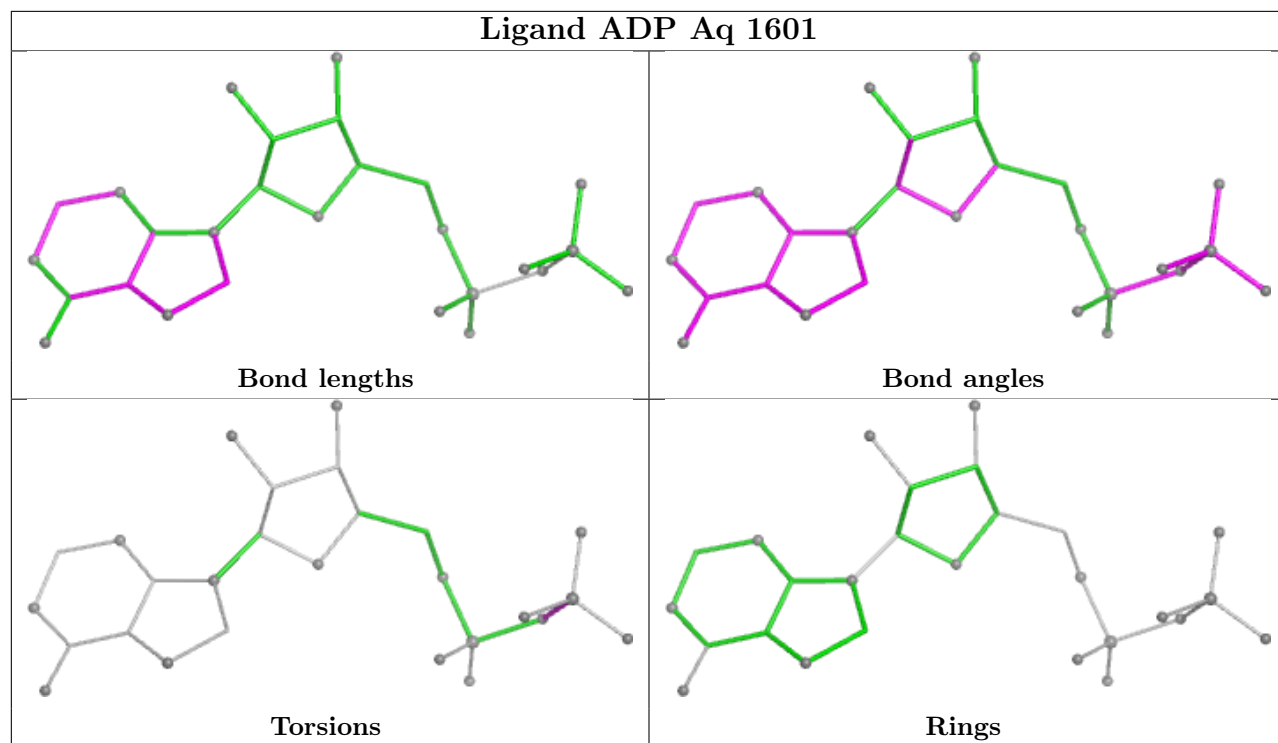
Mol	Chain	Res	Type	Atoms
9	AA	601	ADP	C5'-O5'-PA-O3A
9	AB	601	ADP	PA-O3A-PB-O2B
9	AB	601	ADP	PA-O3A-PB-O3B
9	AD	601	ADP	PA-O3A-PB-O2B
9	AE	601	ADP	PA-O3A-PB-O2B

There are no ring outliers.

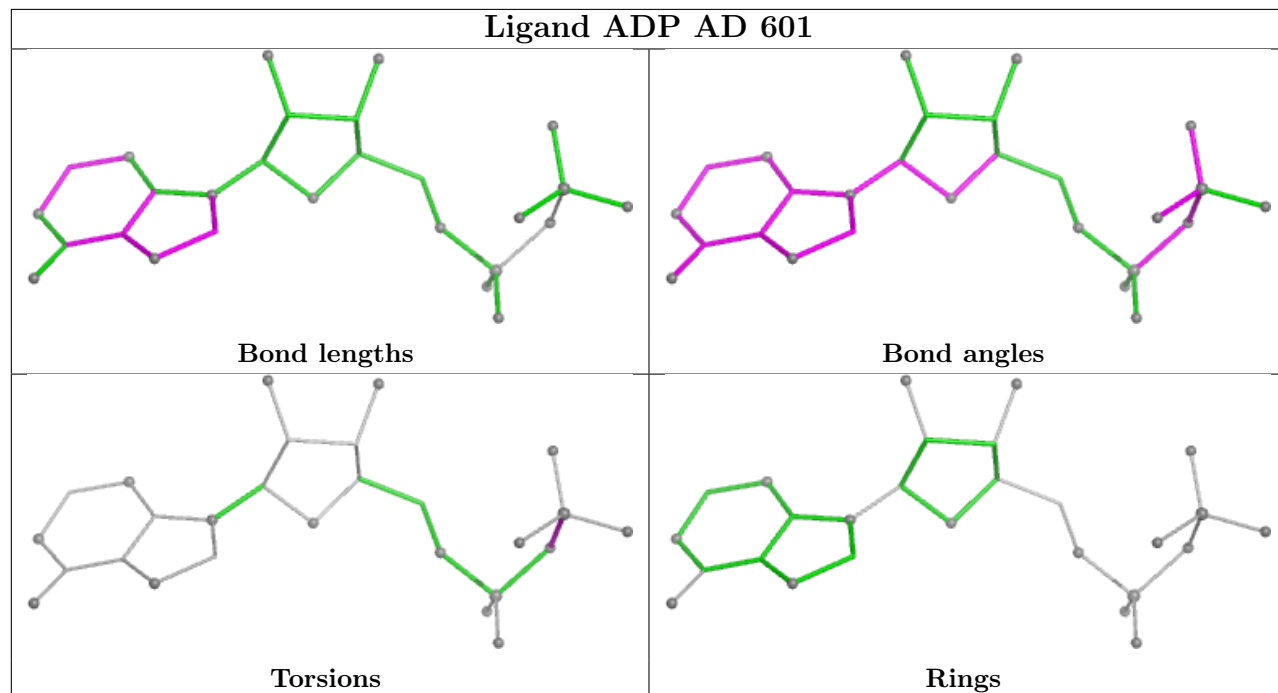
No monomer is involved in short contacts.

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

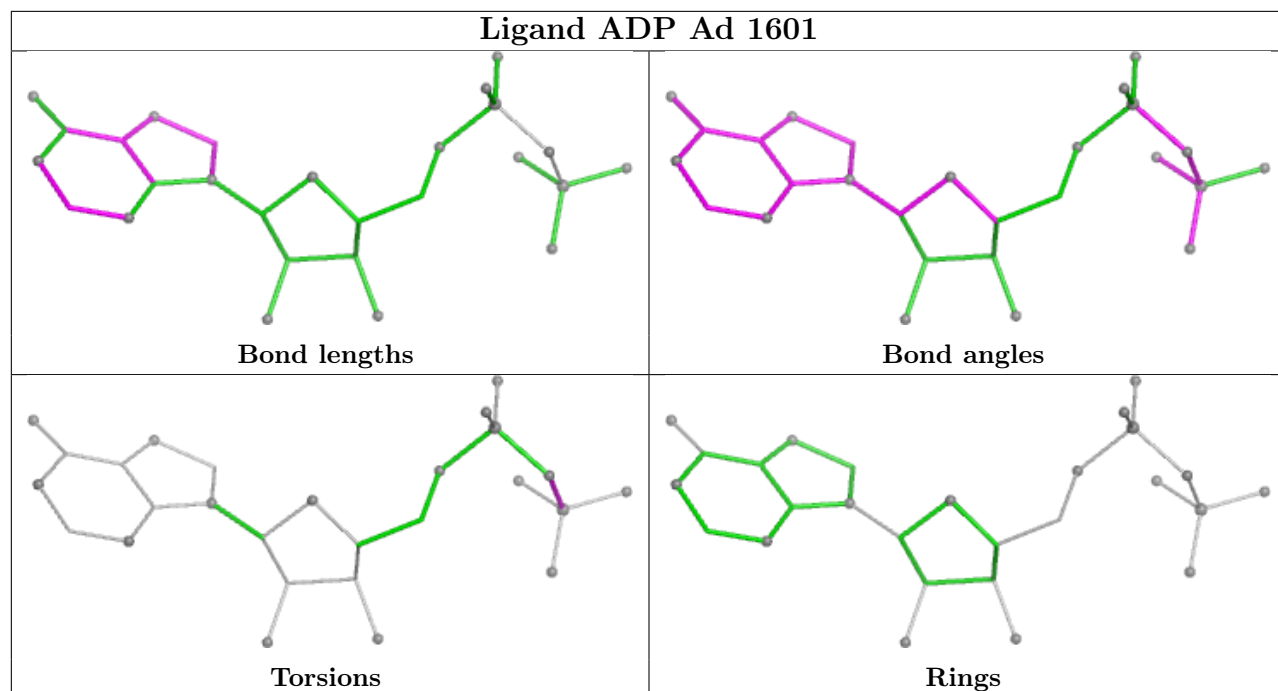
Ligand ADP Aq 1601



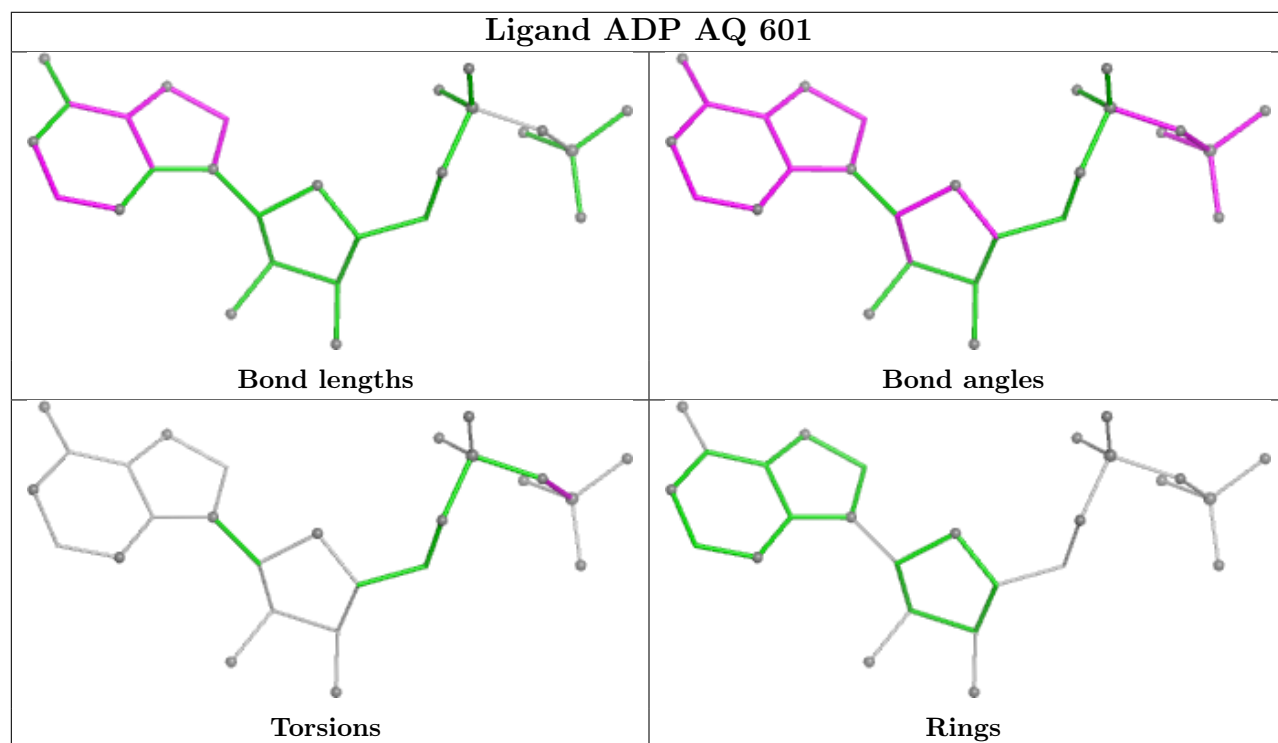
Ligand ADP AD 601



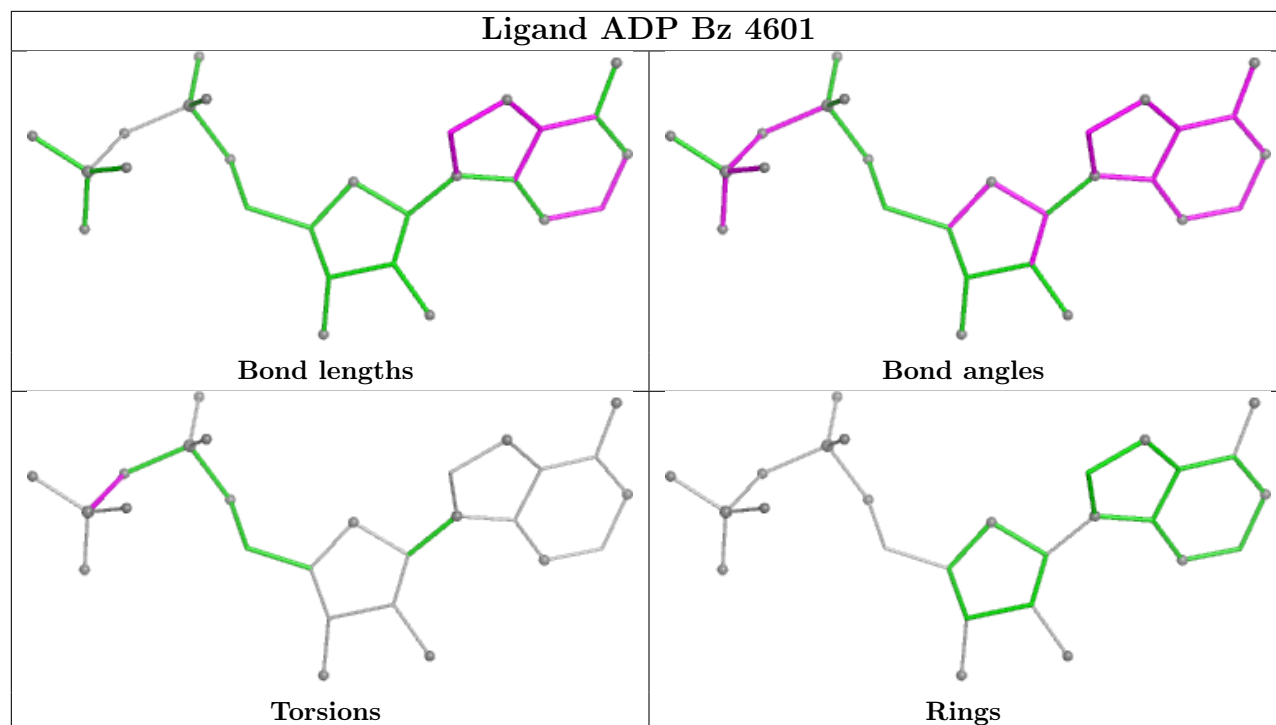
Ligand ADP Ad 1601



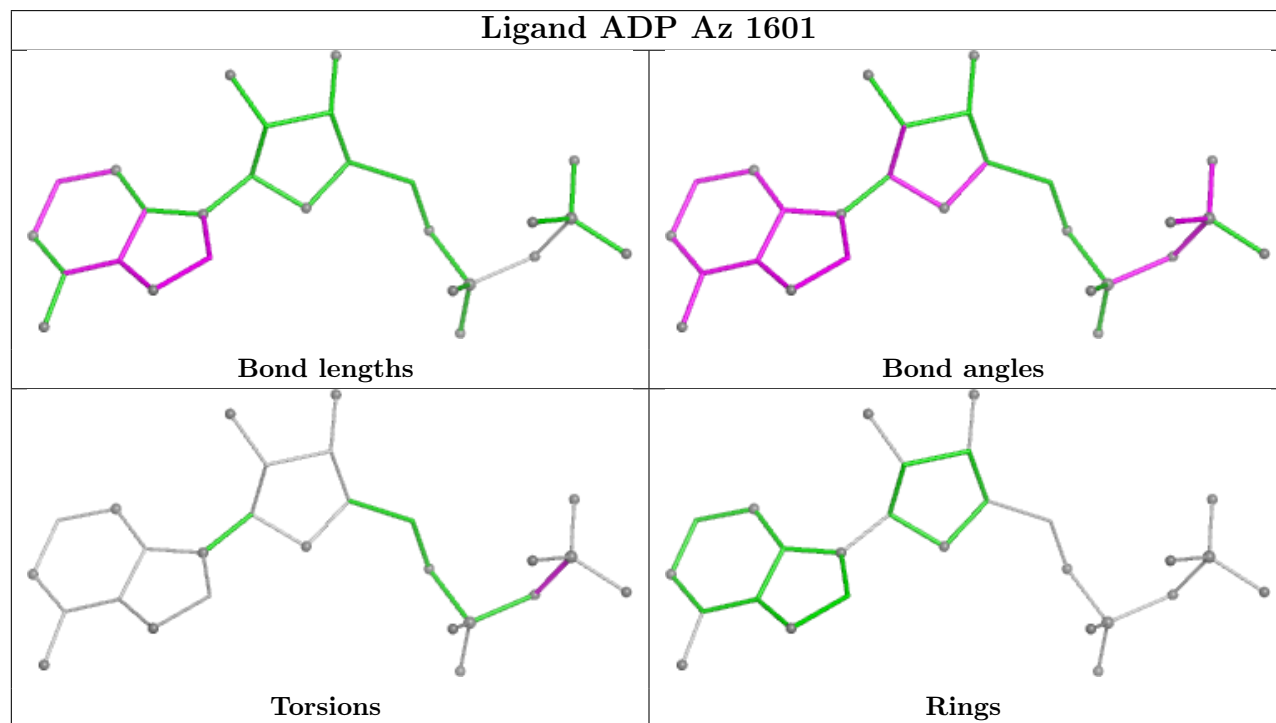
Ligand ADP AQ 601



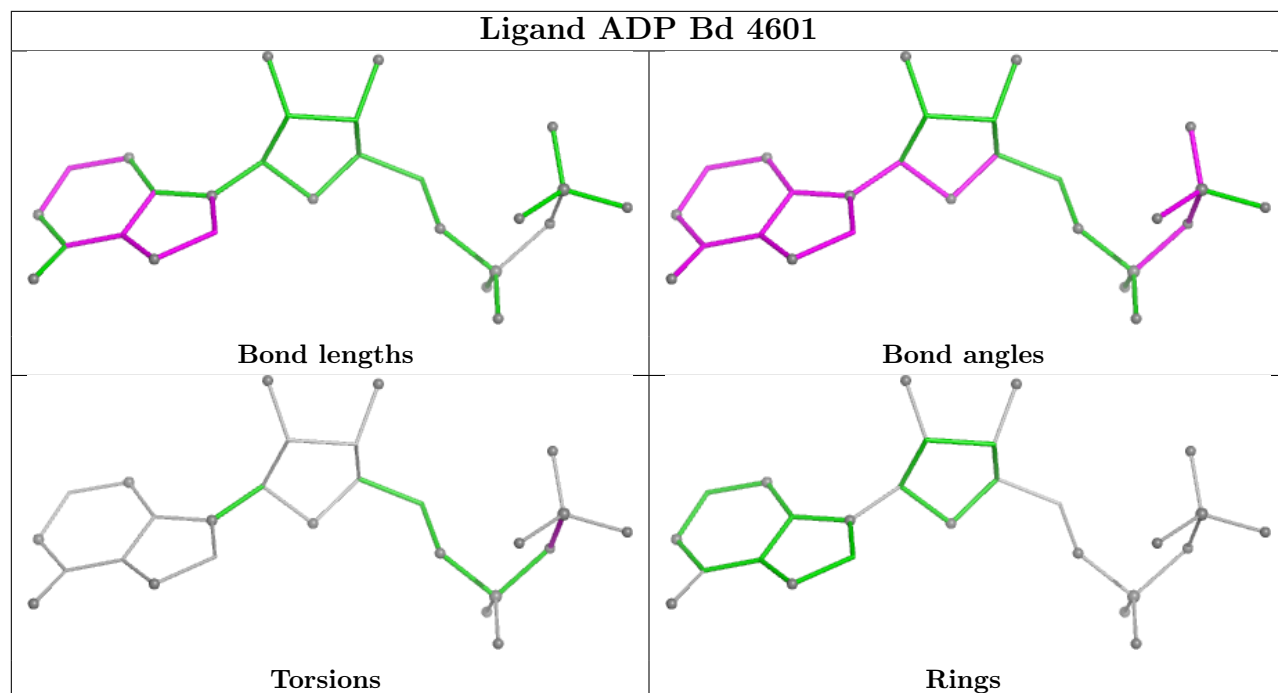
Ligand ADP Bz 4601



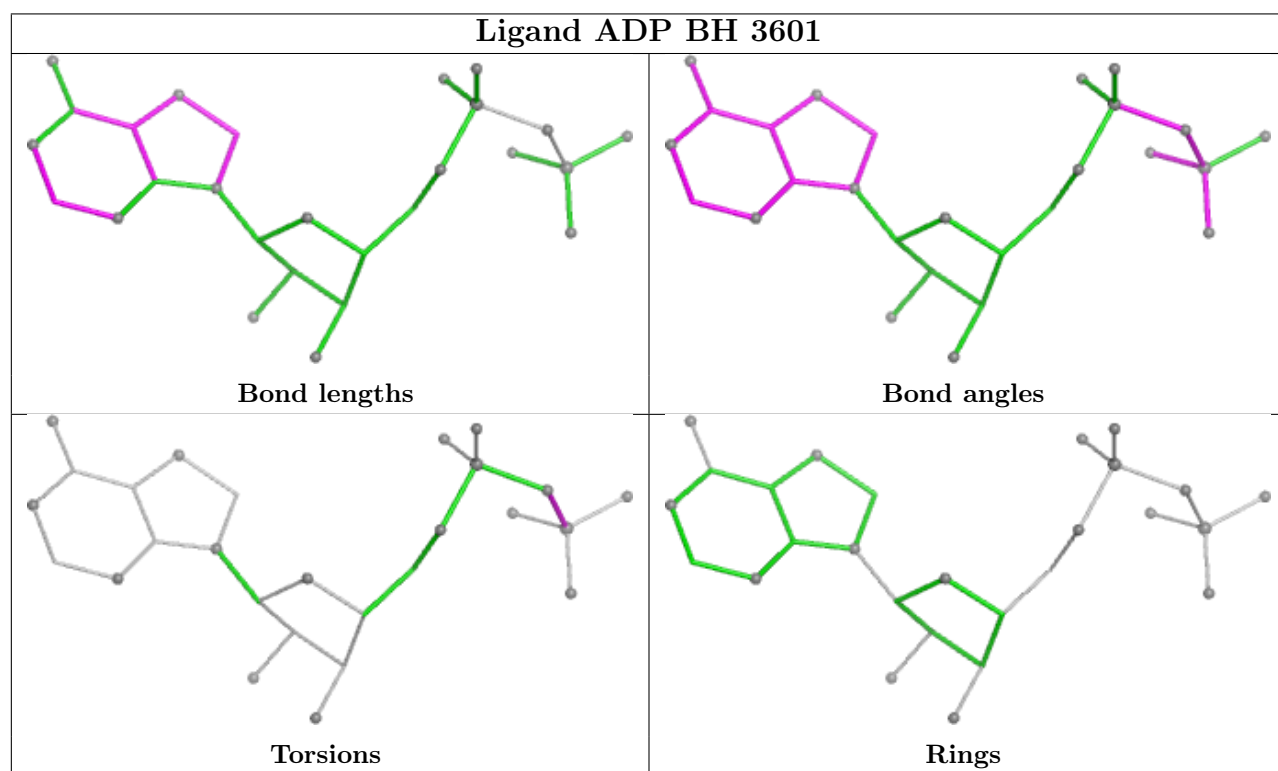
Ligand ADP Az 1601



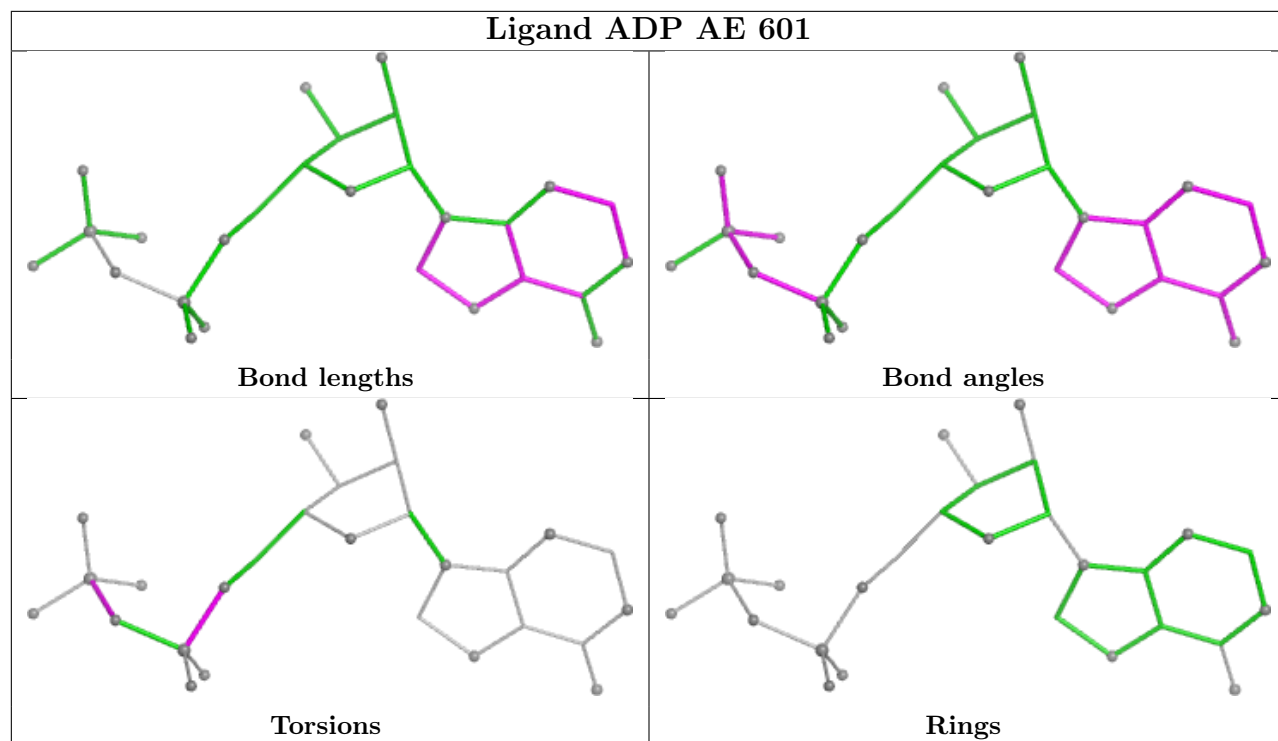
Ligand ADP Bd 4601



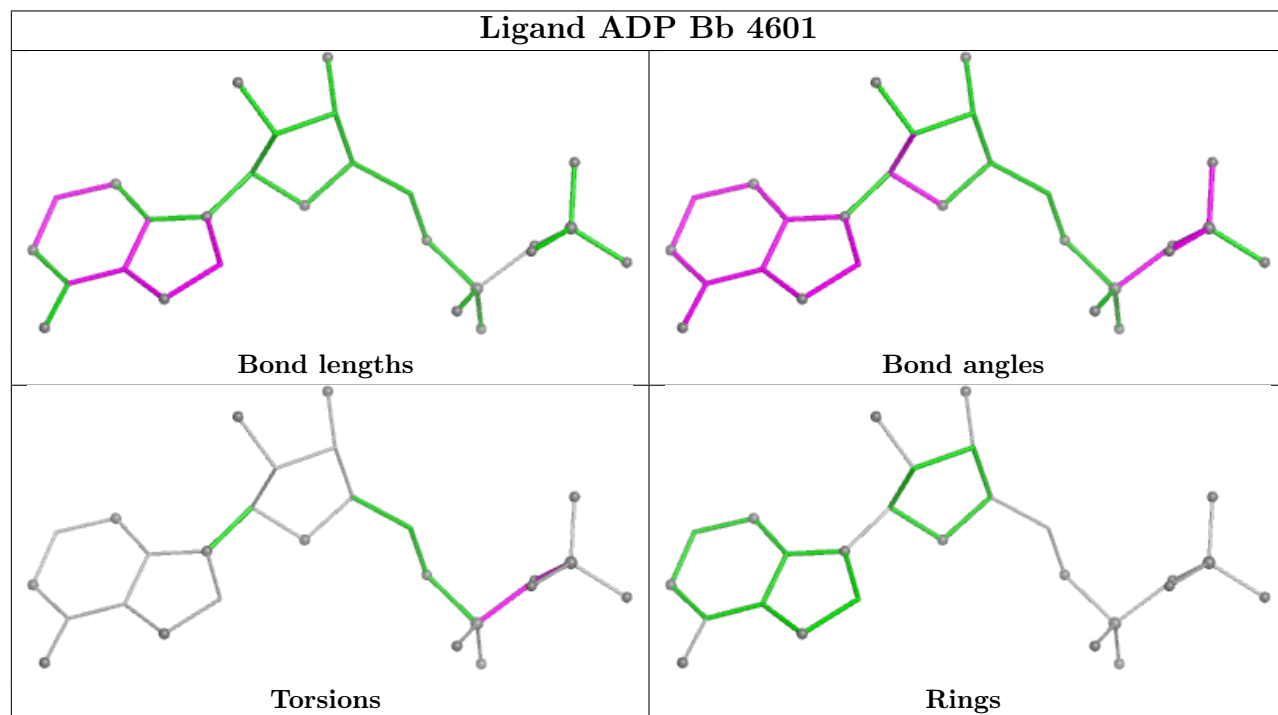
Ligand ADP BH 3601



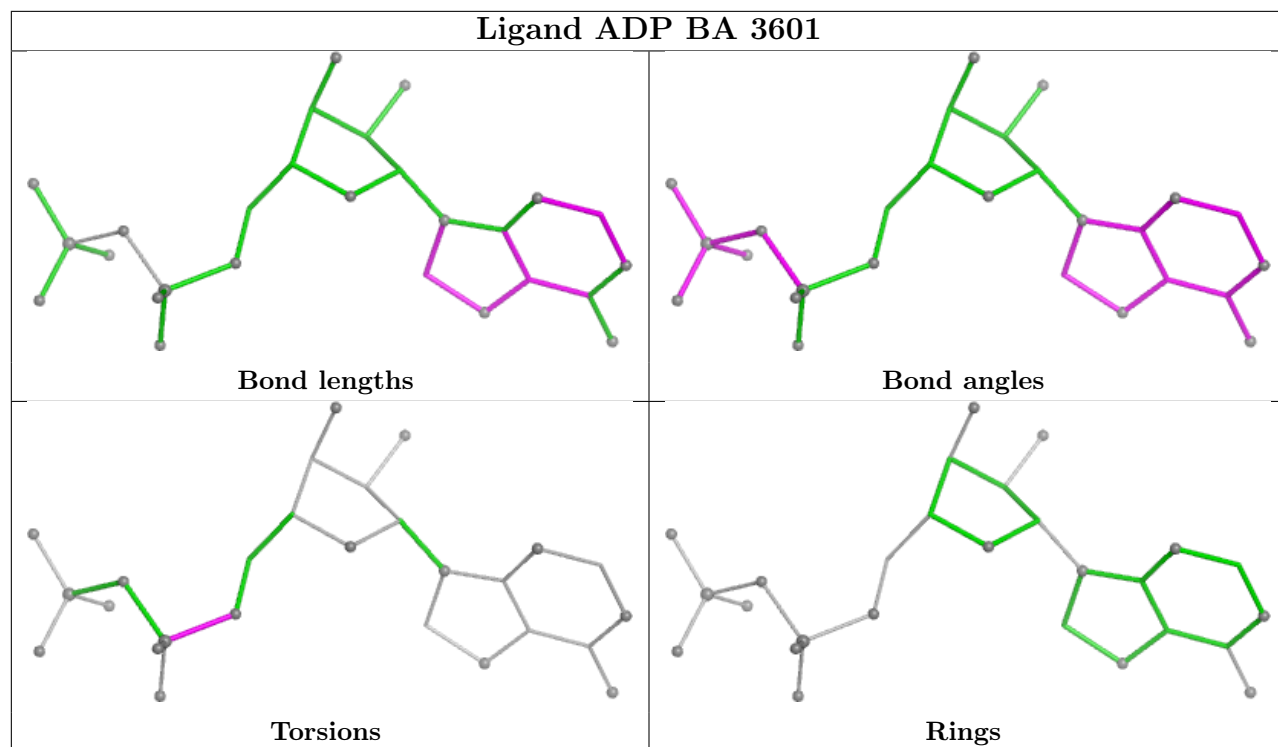
Ligand ADP AE 601



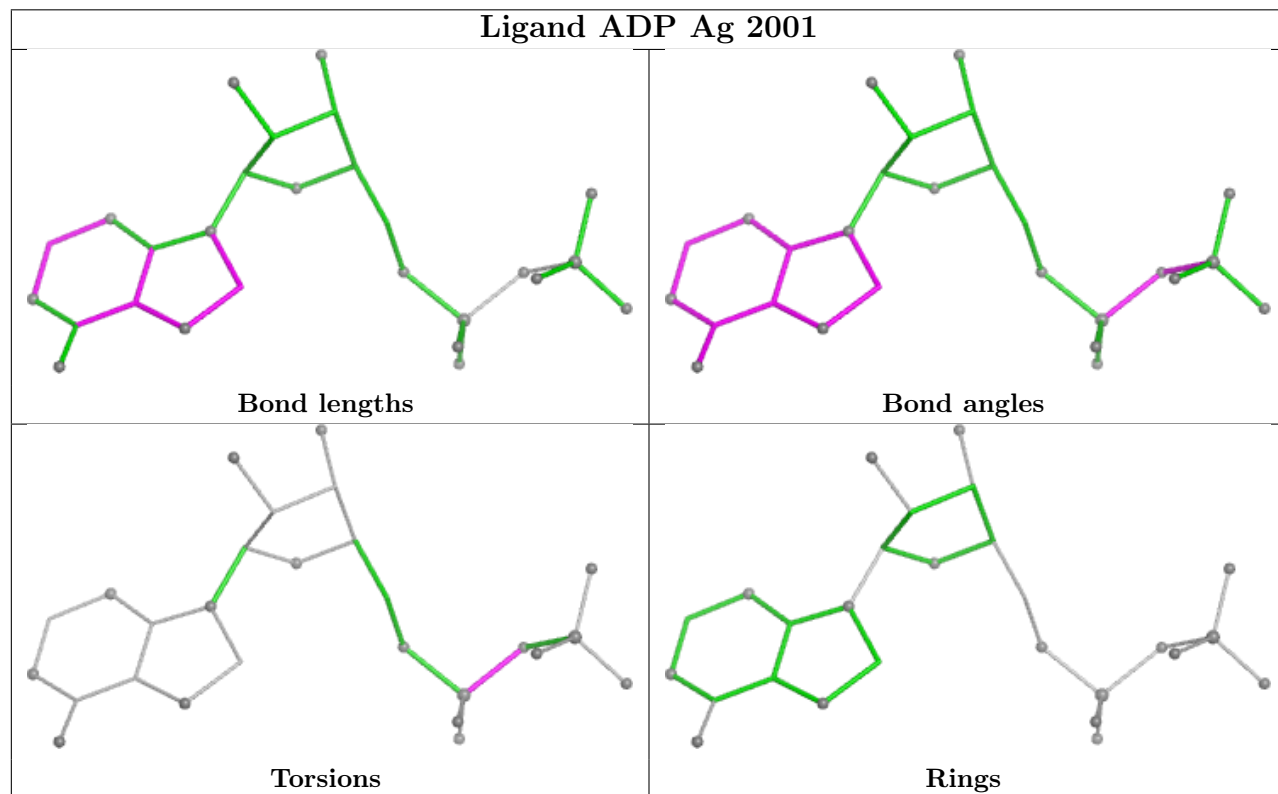
Ligand ADP Bb 4601



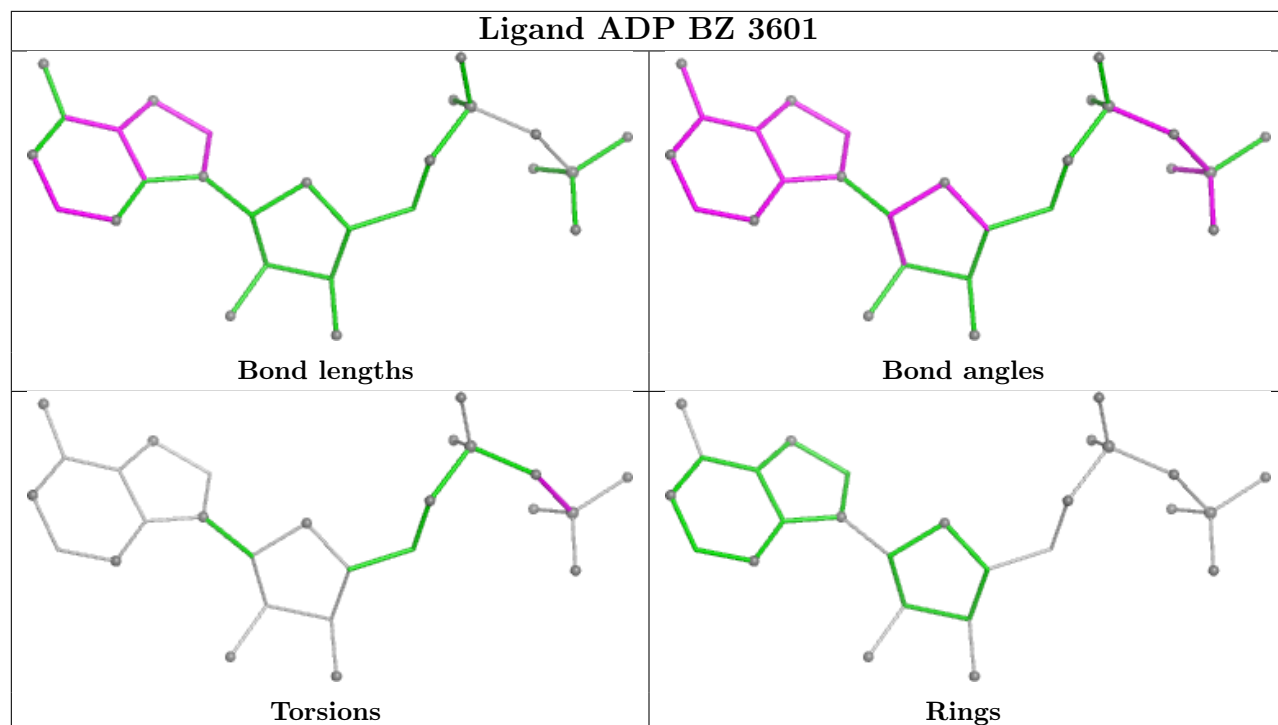
Ligand ADP BA 3601



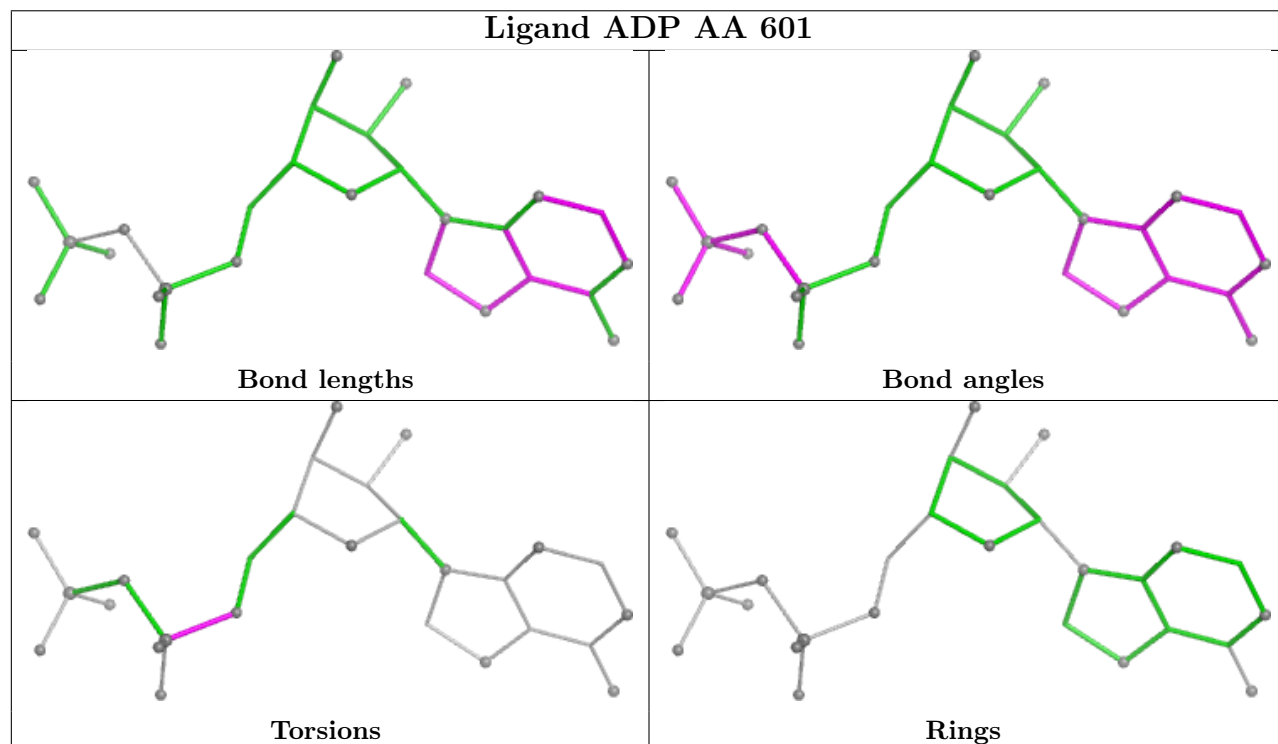
Ligand ADP Ag 2001

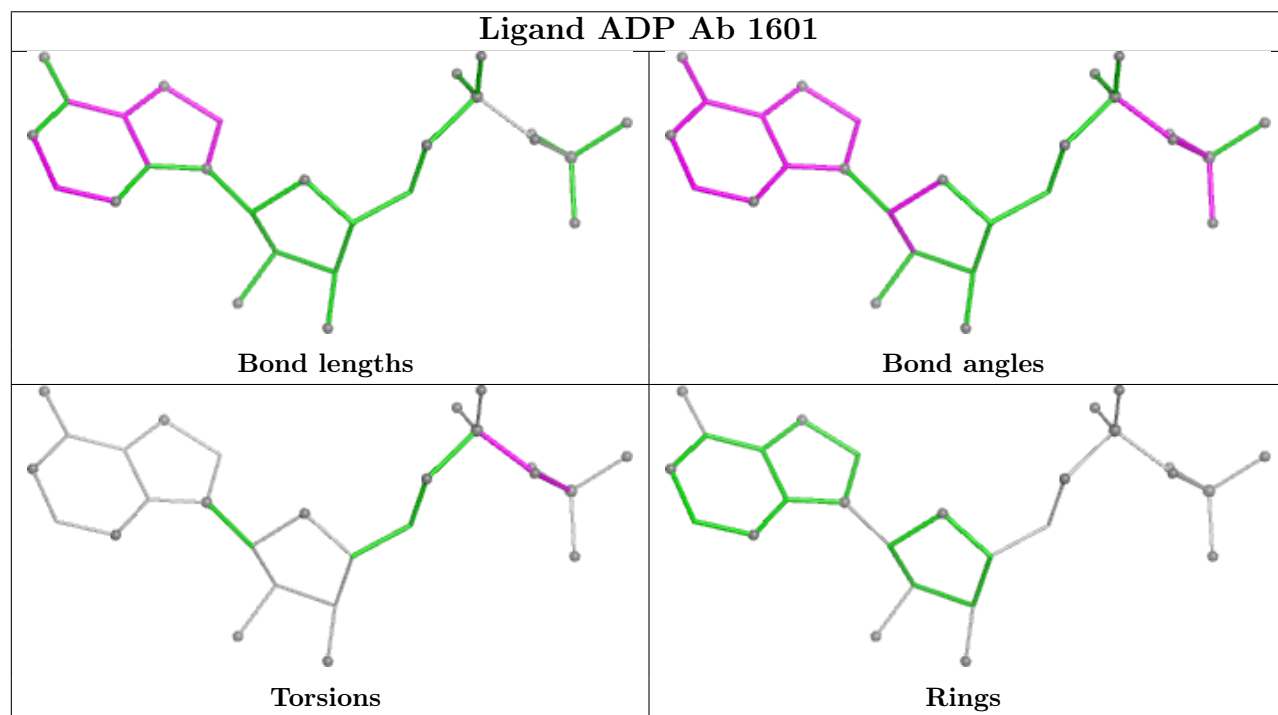
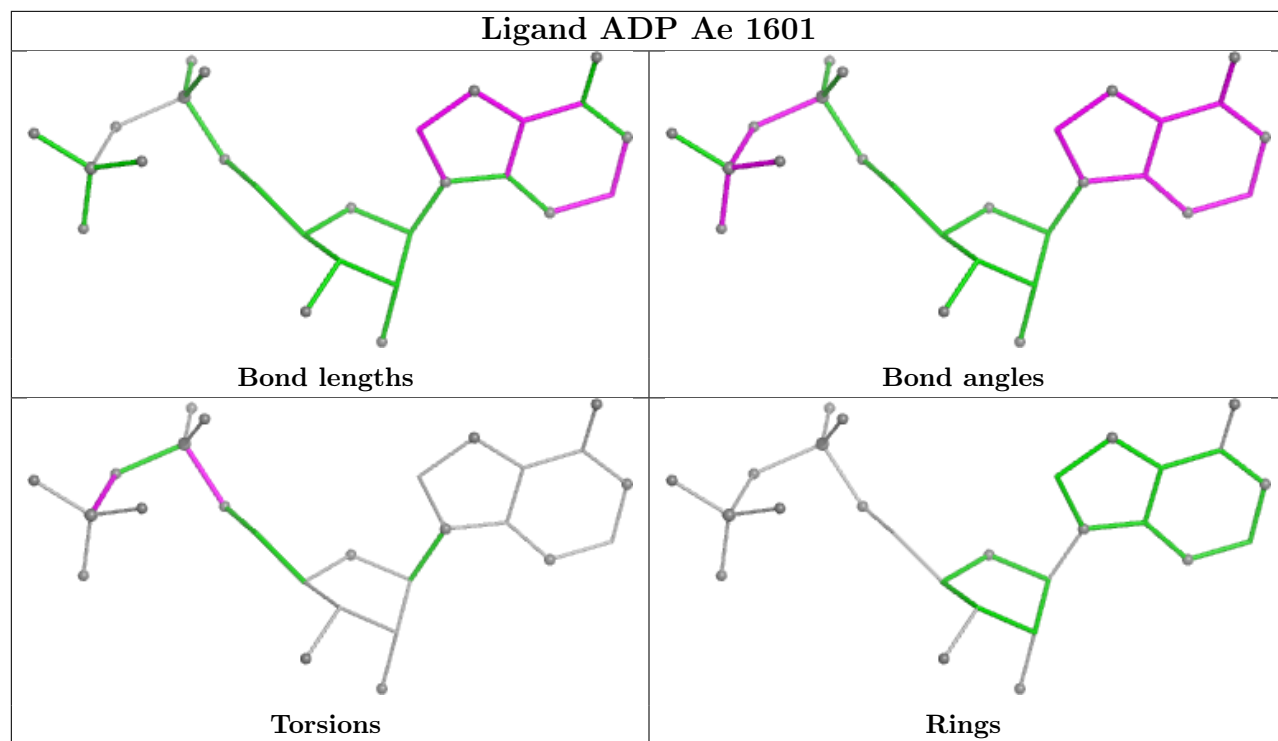


Ligand ADP BZ 3601

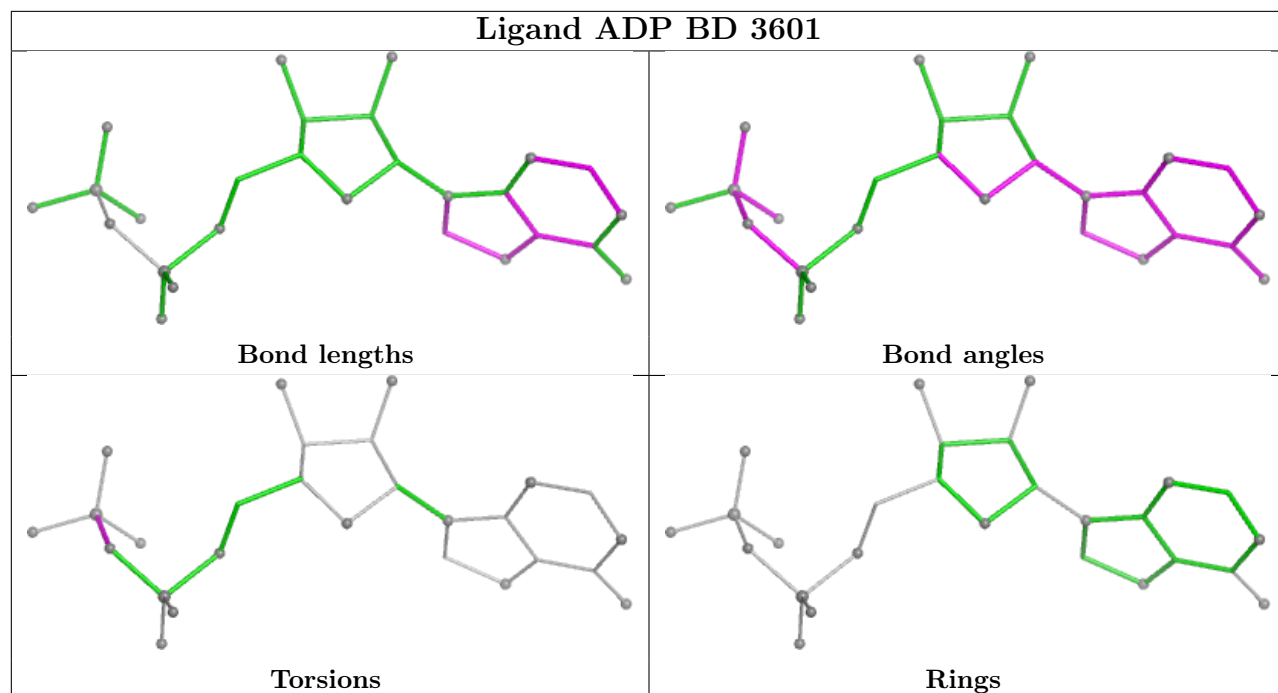


Ligand ADP AA 601

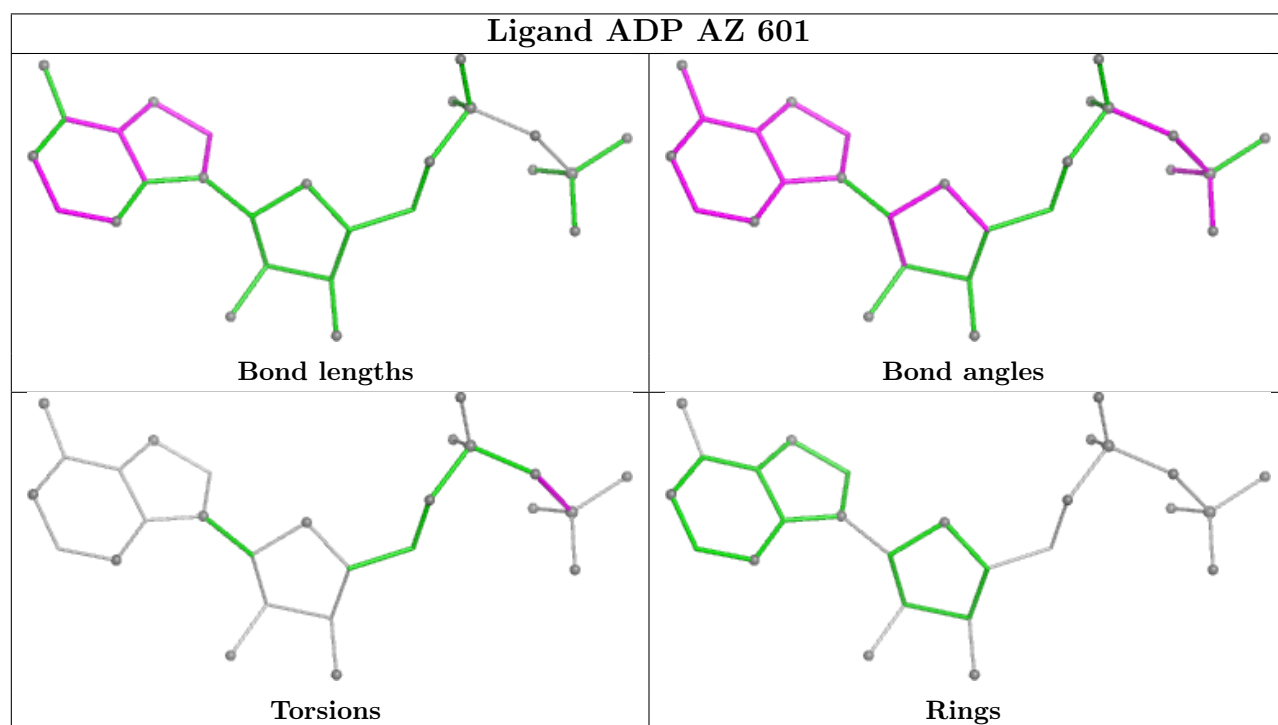




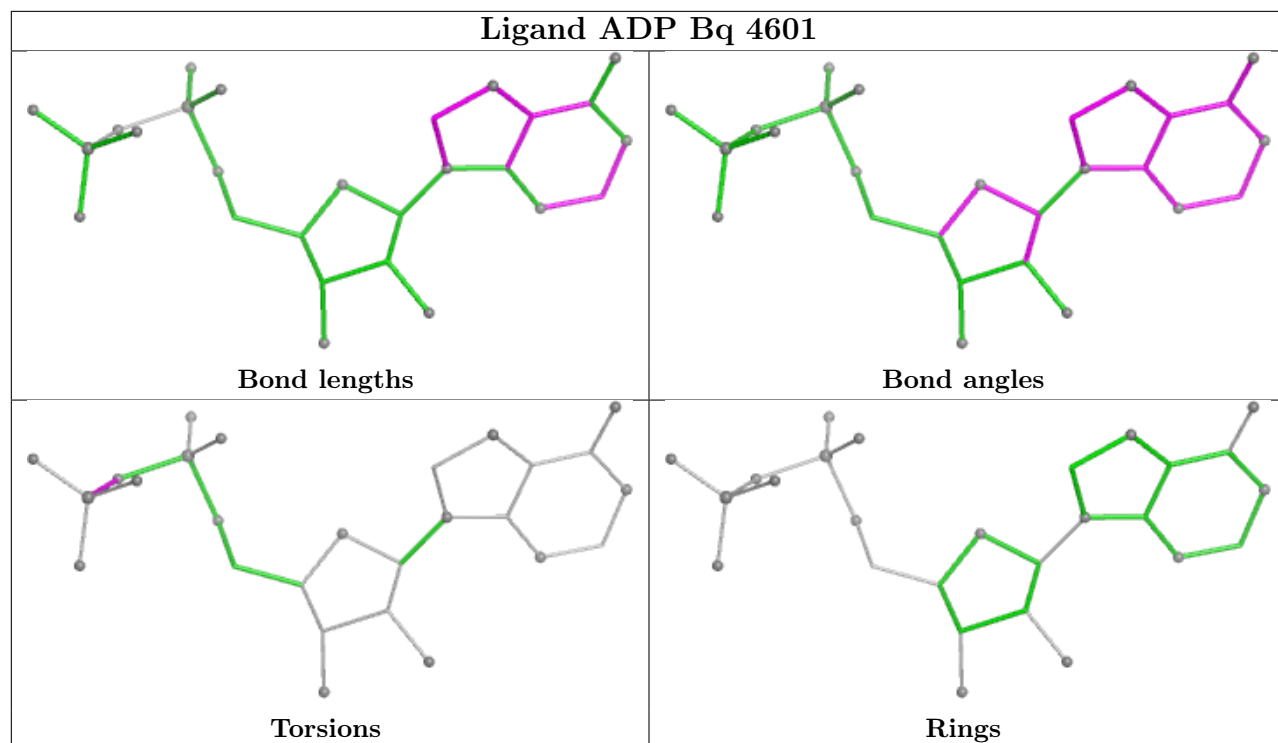
Ligand ADP BD 3601



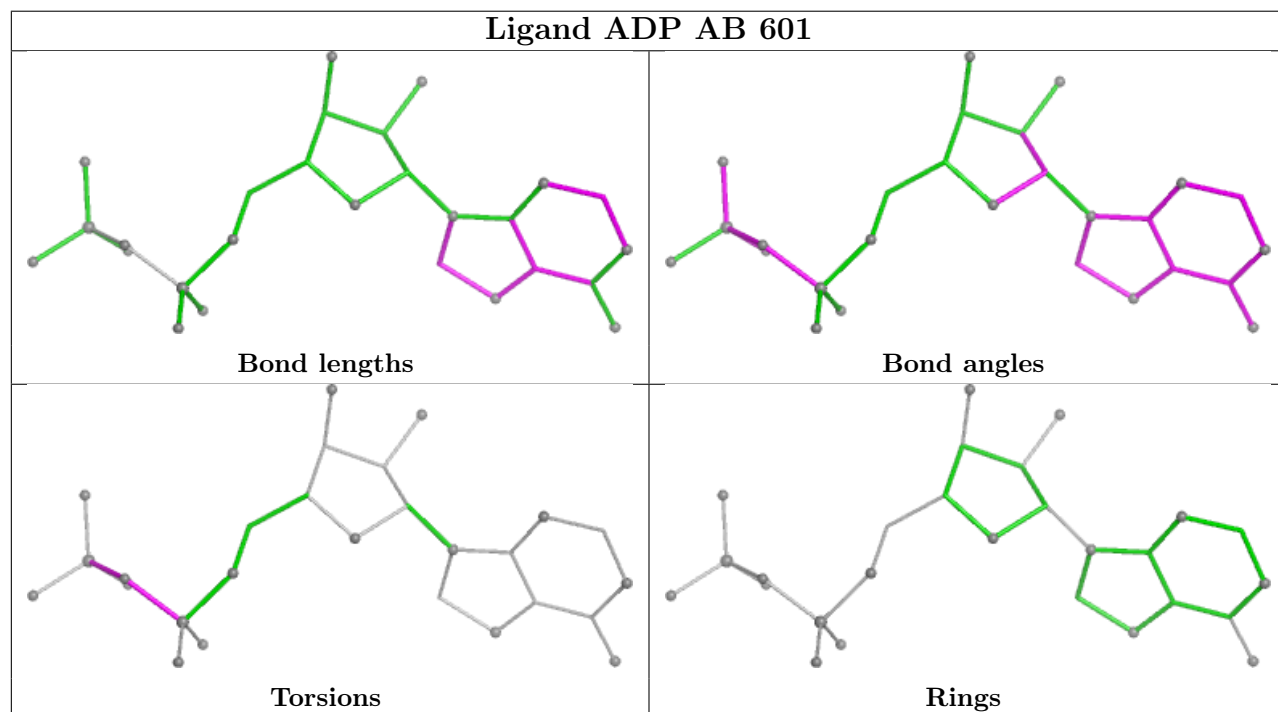
Ligand ADP AZ 601



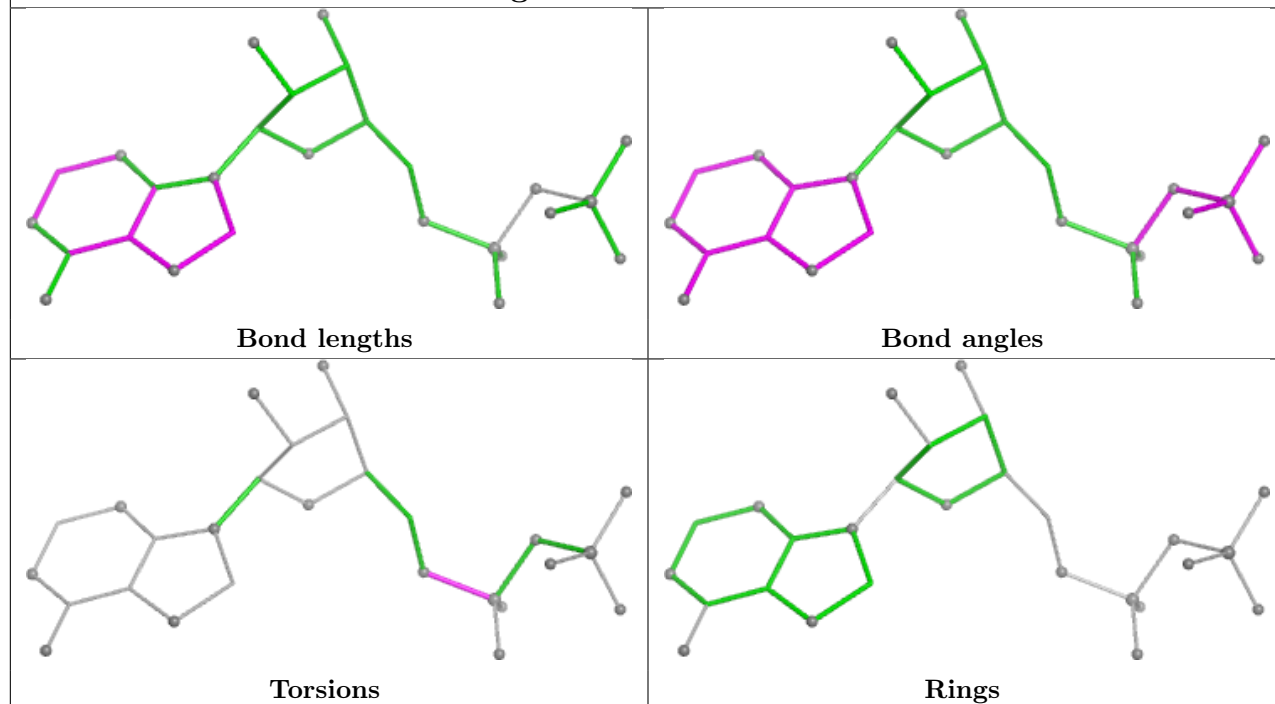
Ligand ADP Bq 4601



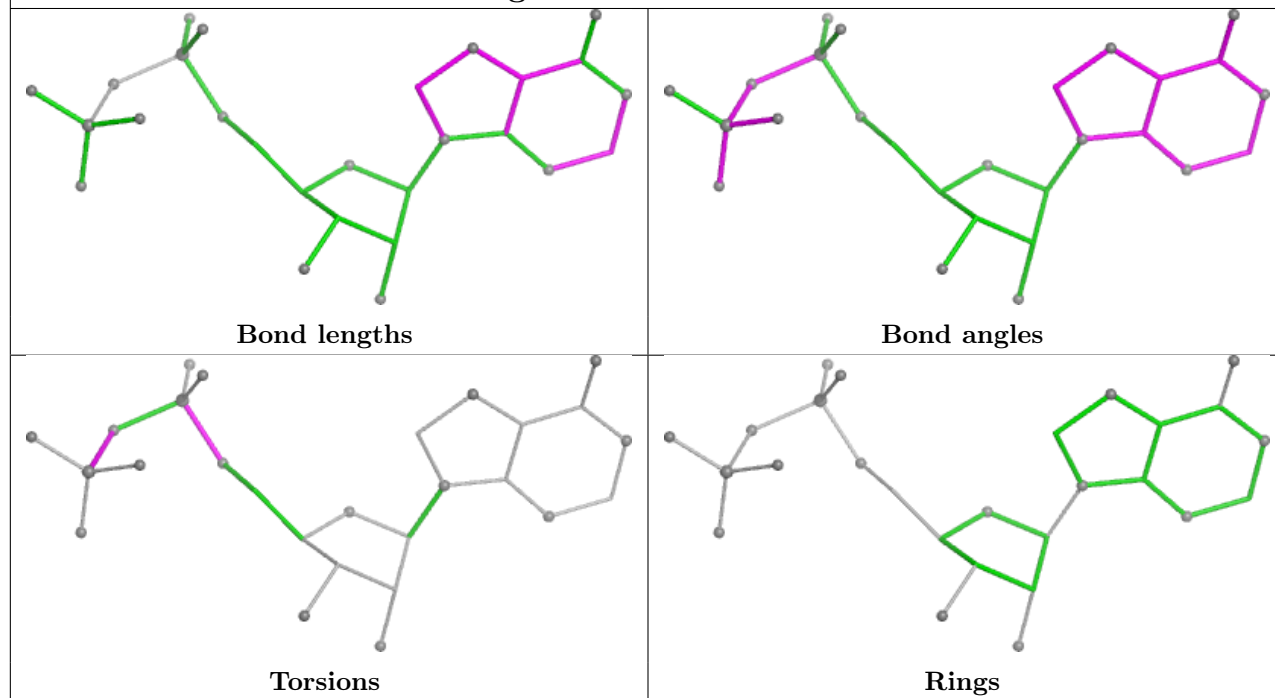
Ligand ADP AB 601



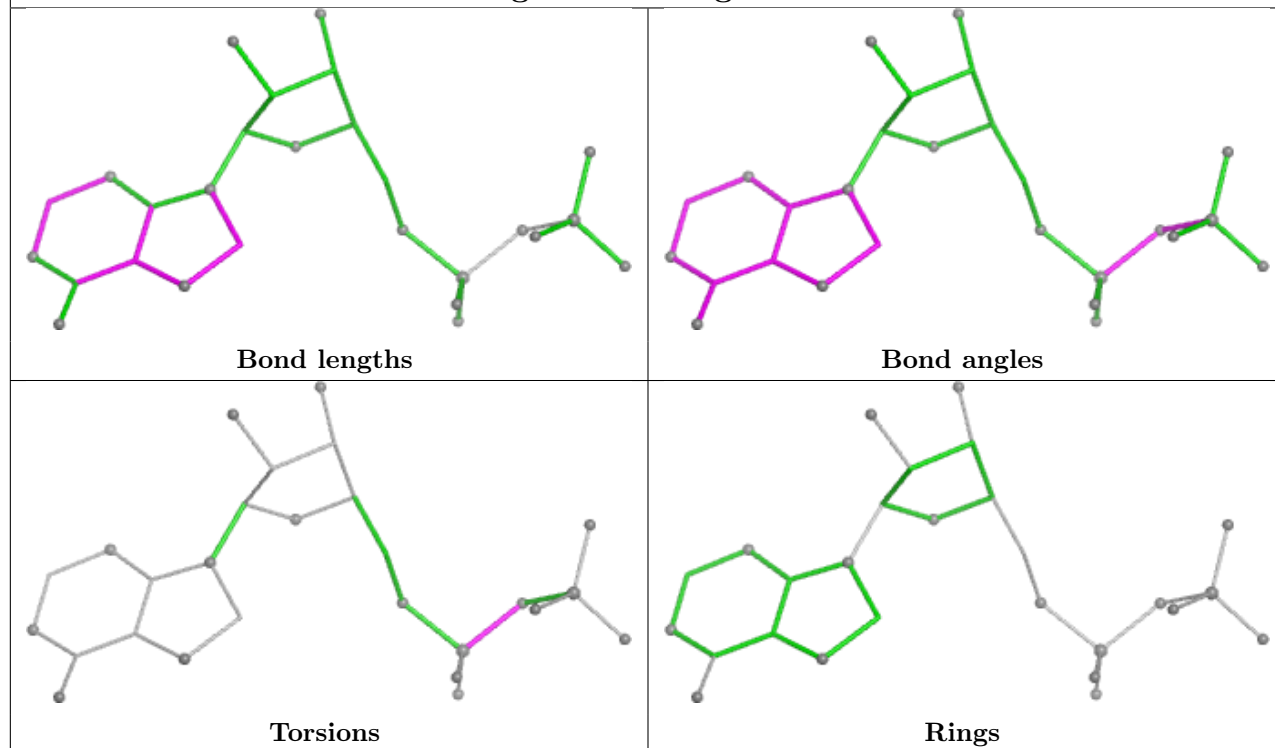
Ligand ADP Aa 1601



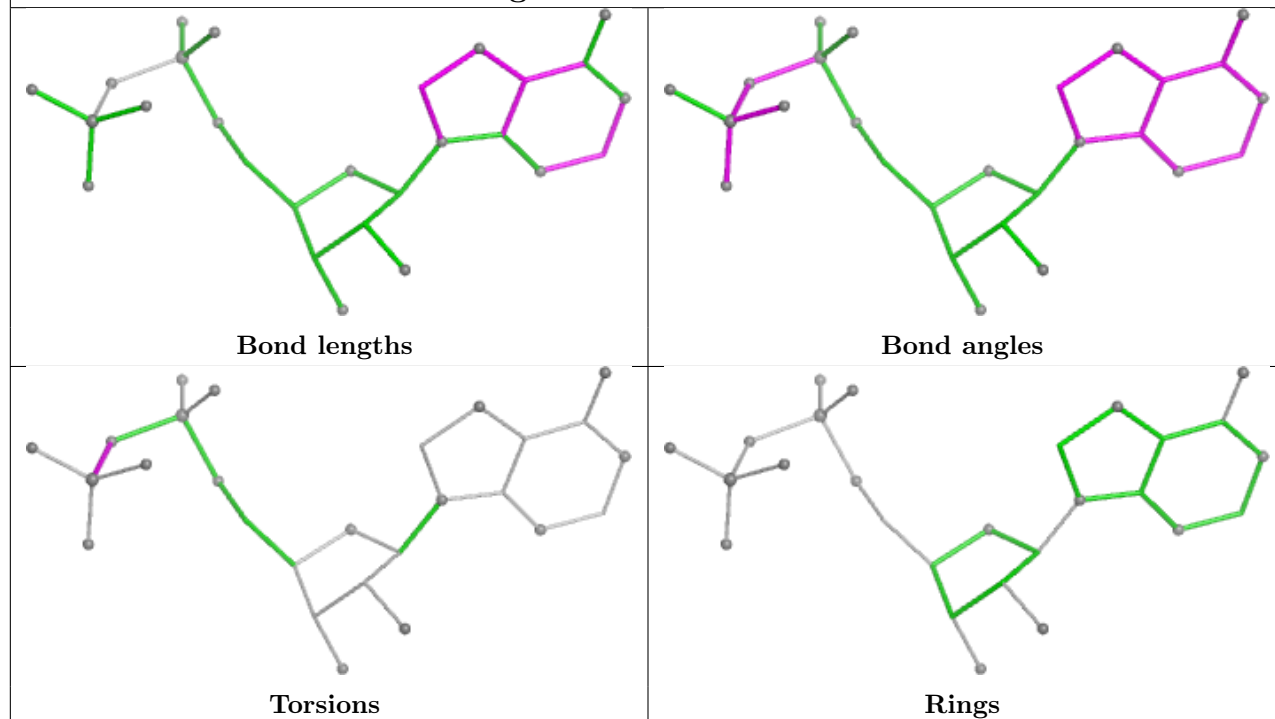
Ligand ADP BE 3601



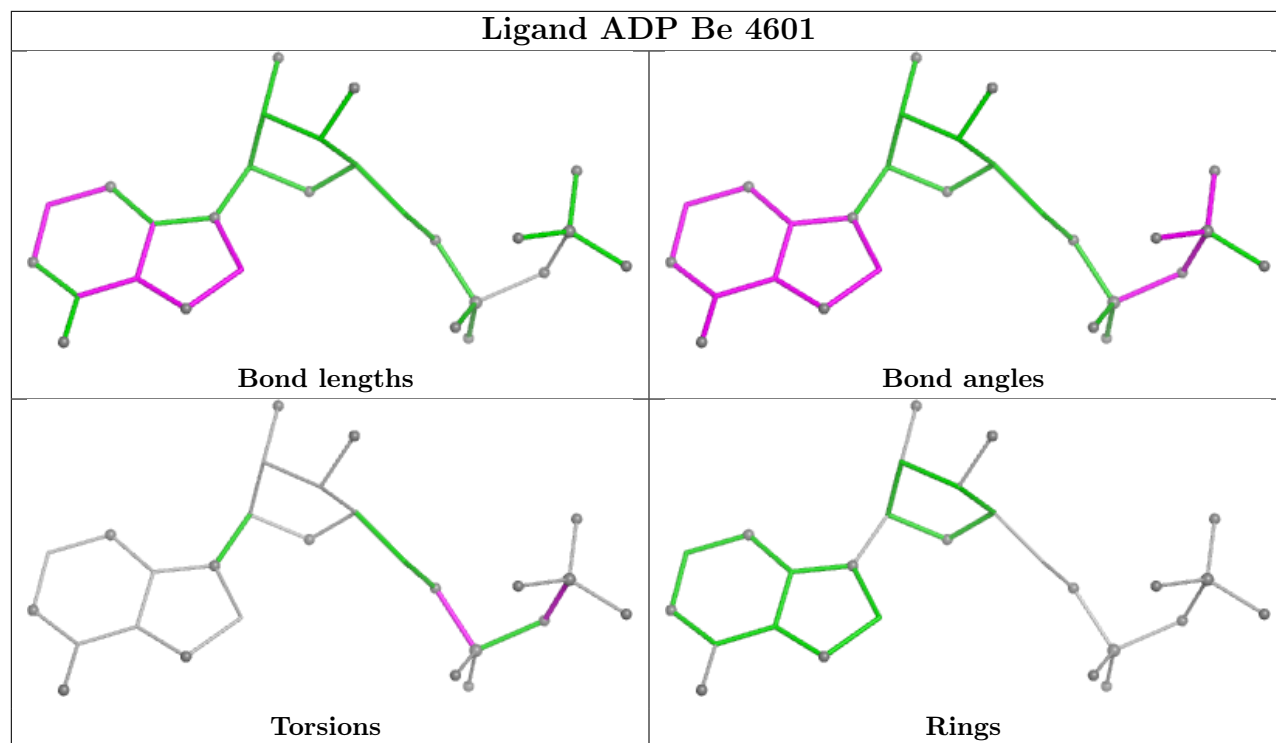
Ligand ADP Bg 5001



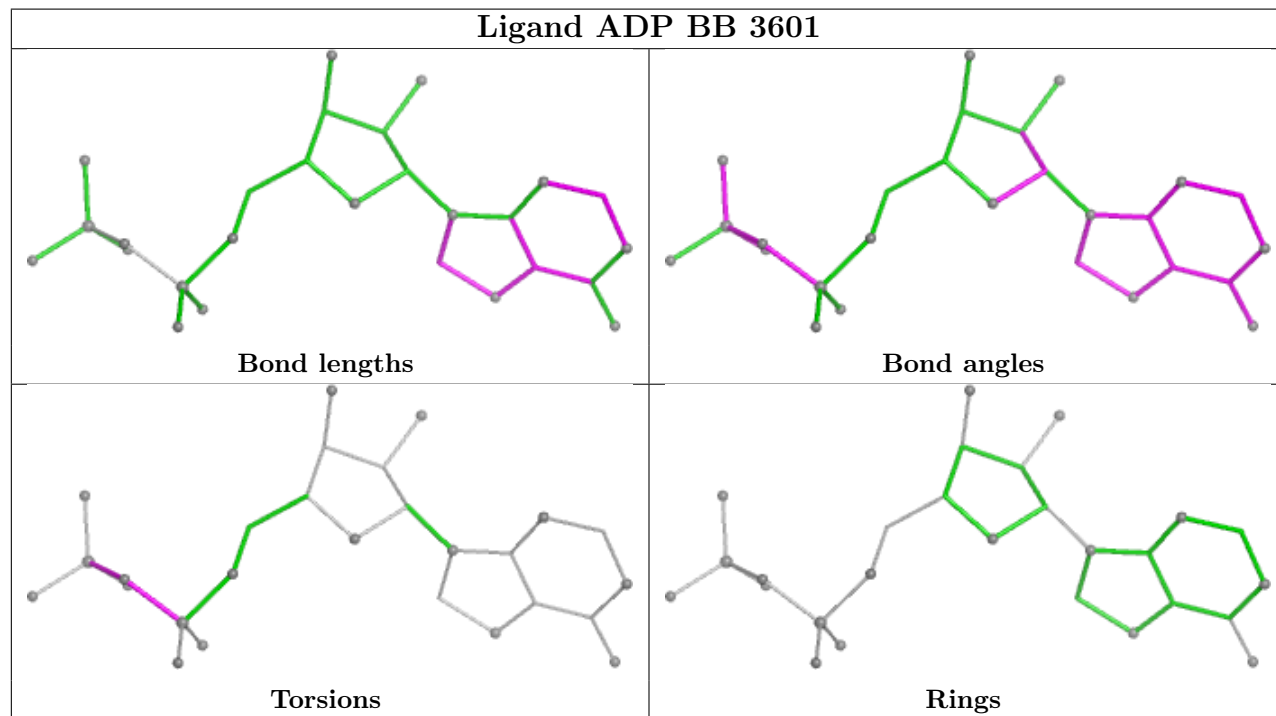
Ligand ADP Ah 1601



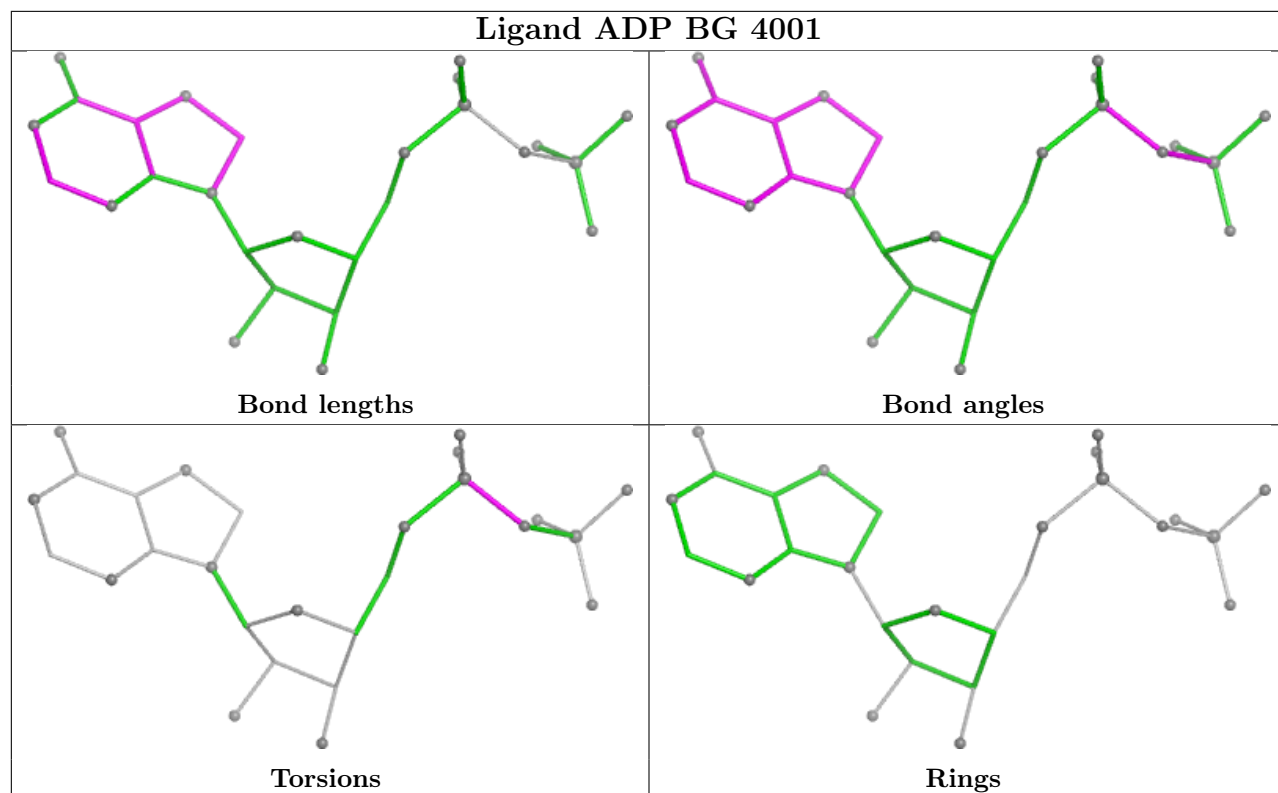
Ligand ADP Be 4601



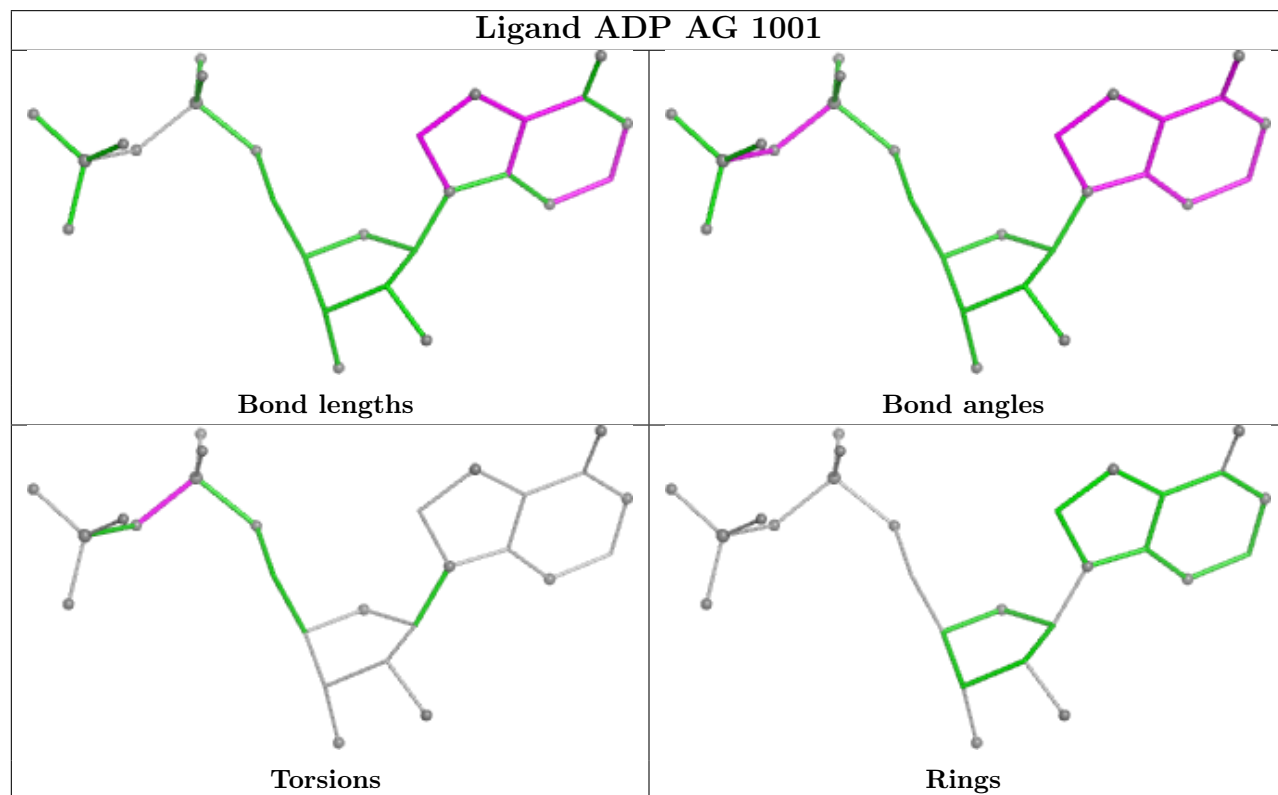
Ligand ADP BB 3601



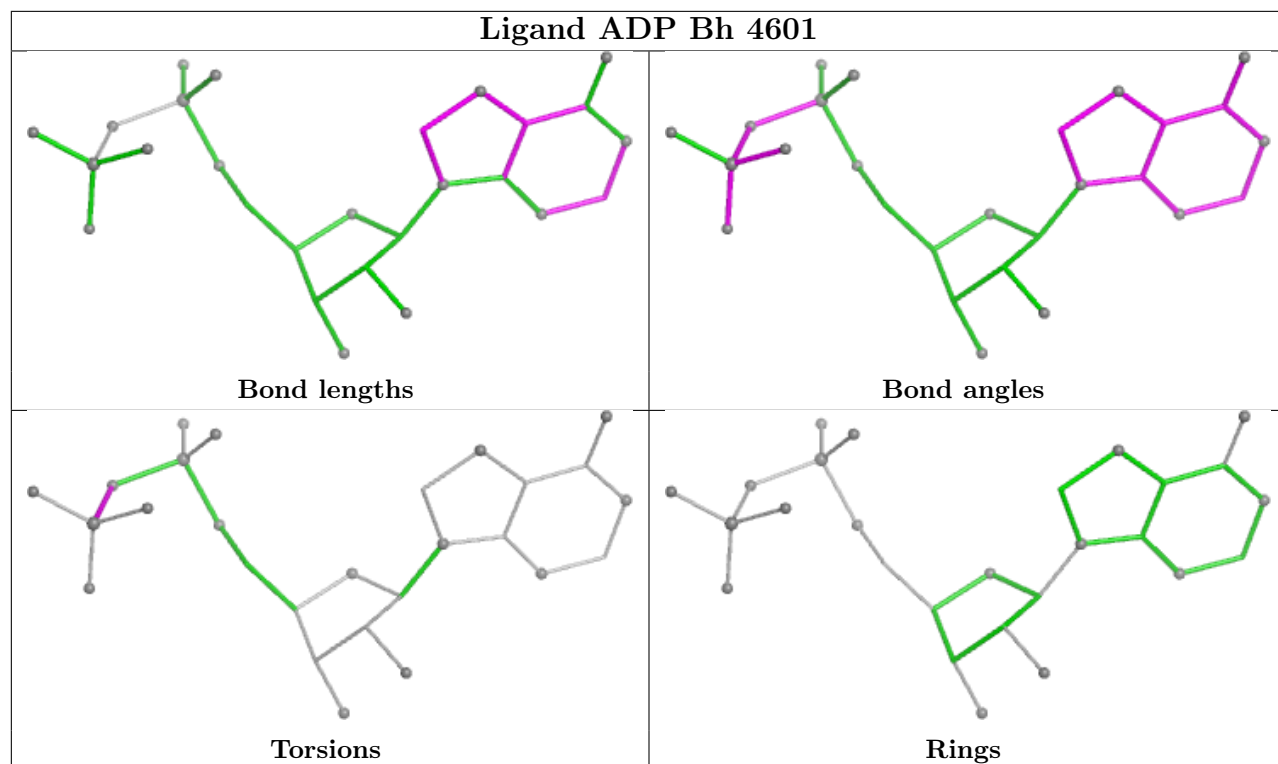
Ligand ADP BG 4001



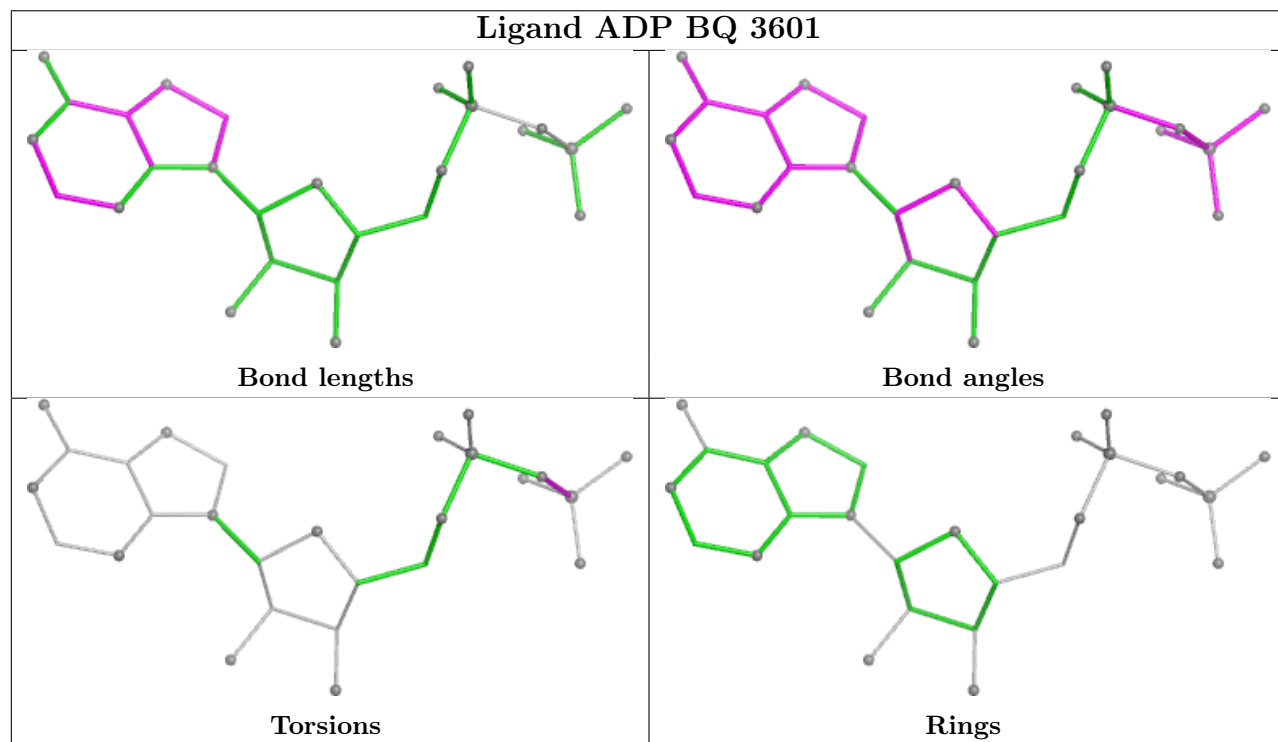
Ligand ADP AG 1001

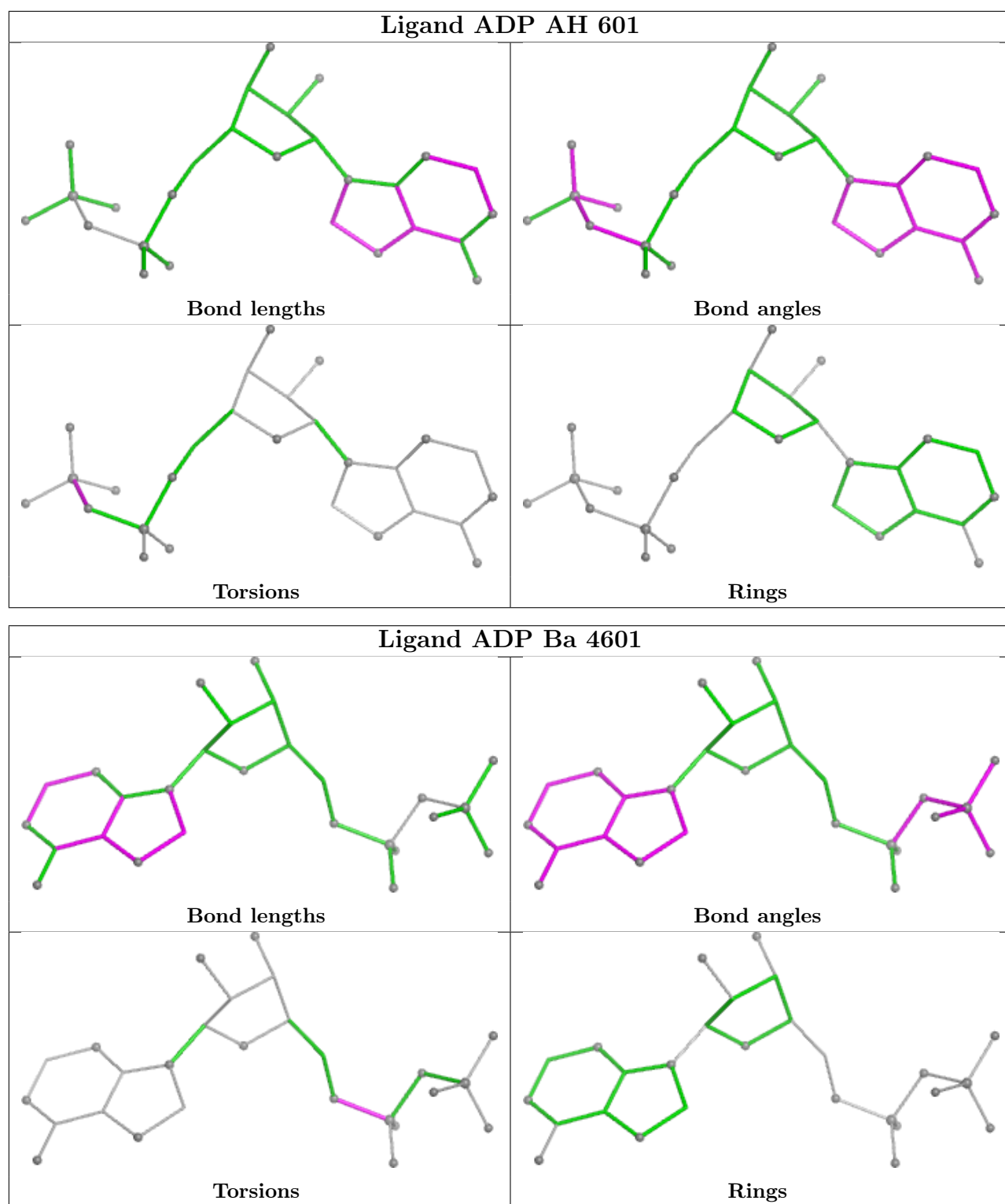


Ligand ADP Bh 4601



Ligand ADP BQ 3601





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	537/559 (96%)	-0.06	1 (0%) 91 81	71, 129, 176, 248	0
1	Aa	537/559 (96%)	0.04	5 (0%) 81 60	71, 129, 176, 248	0
1	BA	537/559 (96%)	-0.08	2 (0%) 88 74	71, 129, 176, 248	0
1	Ba	537/559 (96%)	-0.14	0 100 100	71, 129, 176, 248	0
2	AB	517/527 (98%)	-0.03	1 (0%) 91 81	58, 112, 163, 205	0
2	Ab	517/527 (98%)	-0.06	0 100 100	58, 112, 163, 205	0
2	BB	517/527 (98%)	-0.12	0 100 100	58, 112, 163, 205	0
2	Bb	517/527 (98%)	-0.13	0 100 100	58, 112, 163, 205	0
3	AD	515/528 (97%)	0.03	2 (0%) 88 74	60, 128, 174, 224	0
3	Ad	515/528 (97%)	0.01	5 (0%) 79 58	60, 128, 174, 224	0
3	BD	515/528 (97%)	-0.10	1 (0%) 91 81	60, 128, 174, 224	0
3	Bd	515/528 (97%)	-0.13	1 (0%) 91 81	60, 128, 174, 224	0
4	AE	528/562 (93%)	-0.07	0 100 100	63, 121, 173, 218	0
4	Ae	528/562 (93%)	0.02	1 (0%) 91 81	63, 121, 173, 218	0
4	BE	528/562 (93%)	-0.06	1 (0%) 91 81	63, 121, 173, 218	0
4	Be	528/562 (93%)	-0.10	2 (0%) 88 74	63, 121, 173, 218	0
5	AG	509/590 (86%)	-0.01	2 (0%) 88 74	78, 131, 178, 233	0
5	Ag	509/590 (86%)	0.04	4 (0%) 82 62	78, 131, 178, 233	0
5	BG	509/590 (86%)	-0.06	3 (0%) 85 68	78, 131, 178, 233	0
5	Bg	509/590 (86%)	-0.04	2 (0%) 88 74	78, 131, 178, 233	0
6	AH	519/550 (94%)	-0.03	5 (0%) 79 58	66, 131, 173, 244	0
6	Ah	519/550 (94%)	-0.01	5 (0%) 79 58	66, 131, 173, 244	0
6	BH	519/550 (94%)	-0.11	0 100 100	66, 131, 173, 244	0
6	Bh	519/550 (94%)	-0.09	3 (0%) 85 68	66, 131, 173, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	AQ	523/568 (92%)	0.06	6 (1%) 78 56	71, 138, 182, 249	0
7	Aq	523/568 (92%)	-0.00	3 (0%) 85 68	71, 138, 182, 249	0
7	BQ	523/568 (92%)	-0.07	2 (0%) 88 74	71, 138, 182, 249	0
7	Bq	523/568 (92%)	-0.04	1 (0%) 91 81	71, 138, 182, 249	0
8	AZ	531/546 (97%)	0.10	8 (1%) 72 50	79, 135, 185, 261	0
8	Az	531/546 (97%)	0.03	3 (0%) 85 68	79, 135, 185, 261	0
8	BZ	531/546 (97%)	-0.01	4 (0%) 82 62	79, 135, 185, 261	0
8	Bz	531/546 (97%)	-0.02	6 (1%) 78 56	79, 135, 185, 261	0
All	All	16716/17720 (94%)	-0.04	79 (0%) 87 71	58, 129, 177, 261	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Ag	1384	GLY	6.9
8	AZ	308	VAL	4.8
5	BG	3384	GLY	4.5
8	Bz	4426	LEU	4.1
8	AZ	283	GLU	3.9

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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
10	BEF	Bg	5002	4/4	0.35	0.15	154,176,182,188	0
10	BEF	Ag	2002	4/4	0.48	0.16	154,176,182,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	BEF	AG	1002	4/4	0.49	0.16	154,176,182,188	0
10	BEF	BG	4002	4/4	0.67	0.16	154,176,182,188	0
11	MG	BB	3603	1/1	0.73	0.23	79,79,79,79	0
11	MG	BQ	3603	1/1	0.73	0.19	117,117,117,117	0
11	MG	Bq	4603	1/1	0.76	0.16	117,117,117,117	0
11	MG	Bb	4603	1/1	0.79	0.19	79,79,79,79	0
11	MG	BG	4003	1/1	0.82	0.12	117,117,117,117	0
10	BEF	BQ	3602	4/4	0.82	0.12	154,160,163,170	0
10	BEF	Bz	4602	4/4	0.84	0.09	100,122,147,169	0
10	BEF	Bb	4602	4/4	0.87	0.14	85,91,123,141	0
10	BEF	BZ	3602	4/4	0.87	0.09	100,122,147,169	0
11	MG	AQ	603	1/1	0.88	0.14	117,117,117,117	0
10	BEF	Bq	4602	4/4	0.88	0.12	154,160,163,170	0
10	BEF	AH	602	4/4	0.88	0.09	96,148,149,170	0
10	BEF	Bh	4602	4/4	0.89	0.10	96,148,149,170	0
10	BEF	BB	3602	4/4	0.90	0.09	85,91,123,141	0
11	MG	BH	3603	1/1	0.90	0.08	112,112,112,112	0
10	BEF	BE	3602	4/4	0.90	0.08	109,121,145,150	0
10	BEF	AQ	602	4/4	0.90	0.08	154,160,163,170	0
11	MG	Bh	4603	1/1	0.90	0.10	112,112,112,112	0
10	BEF	Aq	1602	4/4	0.90	0.08	154,160,163,170	0
10	BEF	AE	602	4/4	0.91	0.10	109,121,145,150	0
11	MG	Aq	1603	1/1	0.91	0.11	117,117,117,117	0
10	BEF	Az	1602	4/4	0.91	0.08	100,122,147,169	0
11	MG	Bz	4603	1/1	0.91	0.07	96,96,96,96	0
9	ADP	Ah	1601	27/27	0.92	0.09	29,118,145,160	0
10	BEF	BA	3602	4/4	0.92	0.09	72,141,146,155	0
10	BEF	Ae	1602	4/4	0.92	0.07	109,121,145,150	0
11	MG	Ba	4603	1/1	0.92	0.10	117,117,117,117	0
9	ADP	Bg	5001	27/27	0.93	0.10	66,124,161,173	0
11	MG	AG	1003	1/1	0.93	0.14	117,117,117,117	0
9	ADP	AQ	601	27/27	0.93	0.10	55,126,167,172	0
9	ADP	AG	1001	27/27	0.93	0.11	66,124,161,173	0
9	ADP	Aq	1601	27/27	0.93	0.08	55,126,167,172	0
9	ADP	Az	1601	27/27	0.93	0.08	91,121,146,151	0
10	BEF	AZ	602	4/4	0.93	0.10	100,122,147,169	0
10	BEF	Ab	1602	4/4	0.93	0.09	85,91,123,141	0
10	BEF	Ad	1602	4/4	0.93	0.09	103,113,151,153	0
10	BEF	Bd	4602	4/4	0.93	0.08	103,113,151,153	0
9	ADP	BG	4001	27/27	0.93	0.11	66,124,161,173	0
9	ADP	BH	3601	27/27	0.93	0.09	29,118,145,160	0
9	ADP	BQ	3601	27/27	0.93	0.10	55,126,167,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ADP	BZ	3601	27/27	0.94	0.07	91,121,146,151	0
9	ADP	AA	601	27/27	0.94	0.09	32,114,157,179	0
9	ADP	Bh	4601	27/27	0.94	0.09	29,118,145,160	0
9	ADP	Bq	4601	27/27	0.94	0.08	55,126,167,172	0
9	ADP	Ad	1601	27/27	0.94	0.07	78,119,143,177	0
11	MG	Ad	1603	1/1	0.94	0.07	78,78,78,78	0
11	MG	Ae	1603	1/1	0.94	0.05	88,88,88,88	0
9	ADP	Ag	2001	27/27	0.94	0.12	66,124,161,173	0
11	MG	BA	3603	1/1	0.94	0.06	117,117,117,117	0
10	BEF	AB	602	4/4	0.95	0.09	85,91,123,141	0
10	BEF	AD	602	4/4	0.95	0.08	103,113,151,153	0
9	ADP	Ae	1601	27/27	0.95	0.11	30,104,142,184	0
9	ADP	AB	601	27/27	0.95	0.10	55,93,132,149	0
9	ADP	AZ	601	27/27	0.95	0.09	91,121,146,151	0
11	MG	Az	1603	1/1	0.95	0.06	96,96,96,96	0
9	ADP	Ab	1601	27/27	0.95	0.09	55,93,132,149	0
9	ADP	Bd	4601	27/27	0.95	0.06	78,119,143,177	0
10	BEF	Aa	1602	4/4	0.95	0.09	72,141,146,155	0
9	ADP	AH	601	27/27	0.95	0.10	29,118,145,160	0
10	BEF	Be	4602	4/4	0.95	0.08	109,121,145,150	0
9	ADP	BA	3601	27/27	0.95	0.08	32,114,157,179	0
9	ADP	BB	3601	27/27	0.95	0.09	55,93,132,149	0
9	ADP	Bz	4601	27/27	0.95	0.07	91,121,146,151	0
10	BEF	AA	602	4/4	0.95	0.07	72,141,146,155	0
11	MG	AB	603	1/1	0.95	0.10	79,79,79,79	0
10	BEF	BH	3602	4/4	0.96	0.05	96,148,149,170	0
9	ADP	Be	4601	27/27	0.96	0.07	30,104,142,184	0
9	ADP	AD	601	27/27	0.96	0.08	78,119,143,177	0
11	MG	BD	3603	1/1	0.96	0.10	78,78,78,78	0
11	MG	AD	603	1/1	0.96	0.07	78,78,78,78	0
9	ADP	BD	3601	27/27	0.96	0.07	78,119,143,177	0
9	ADP	BE	3601	27/27	0.96	0.08	30,104,142,184	0
11	MG	BZ	3603	1/1	0.96	0.05	96,96,96,96	0
11	MG	Aa	1603	1/1	0.96	0.06	117,117,117,117	0
10	BEF	BD	3602	4/4	0.96	0.06	103,113,151,153	0
11	MG	Be	4603	1/1	0.96	0.06	88,88,88,88	0
9	ADP	Bb	4601	27/27	0.96	0.09	55,93,132,149	0
11	MG	Ah	1603	1/1	0.96	0.08	112,112,112,112	0
9	ADP	Aa	1601	27/27	0.96	0.08	32,114,157,179	0
11	MG	AE	603	1/1	0.97	0.09	88,88,88,88	0
11	MG	Ag	2003	1/1	0.97	0.04	117,117,117,117	0
10	BEF	Ah	1602	4/4	0.97	0.06	96,148,149,170	0

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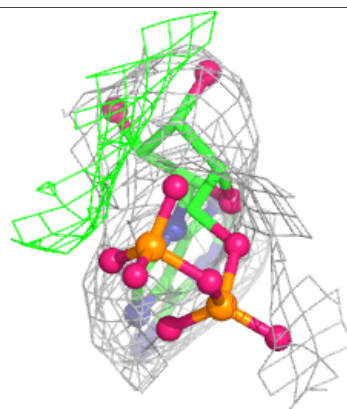
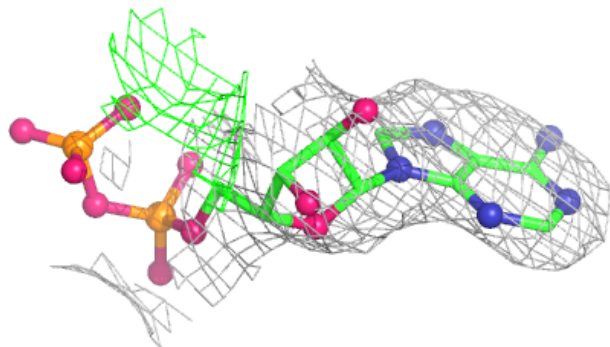
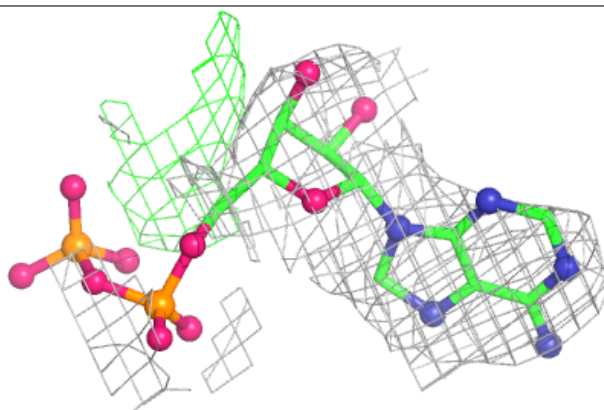
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MG	AH	603	1/1	0.97	0.11	112,112,112,112	0
9	ADP	AE	601	27/27	0.97	0.07	30,104,142,184	0
11	MG	Bd	4603	1/1	0.97	0.05	78,78,78,78	0
11	MG	AZ	603	1/1	0.97	0.06	96,96,96,96	0
11	MG	Bg	5003	1/1	0.97	0.05	117,117,117,117	0
10	BEF	Ba	4602	4/4	0.97	0.07	72,141,146,155	0
11	MG	Ab	1603	1/1	0.97	0.07	79,79,79,79	0
9	ADP	Ba	4601	27/27	0.97	0.08	32,114,157,179	0
11	MG	AA	603	1/1	0.98	0.10	117,117,117,117	0
11	MG	BE	3603	1/1	0.99	0.06	88,88,88,88	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.

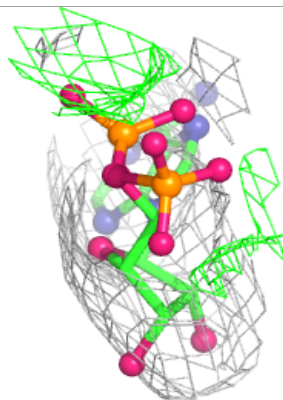
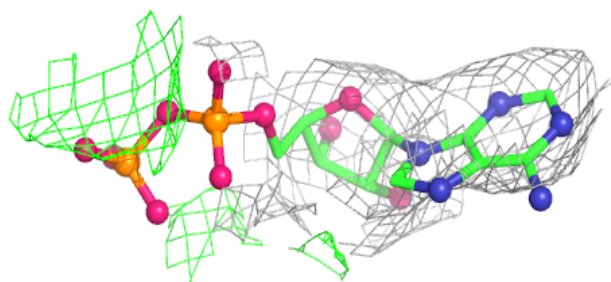
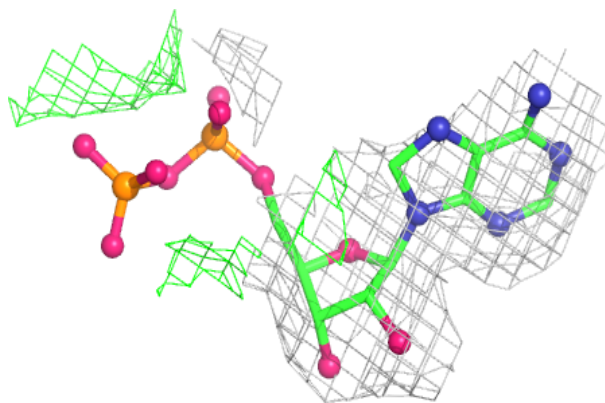
Electron density around ADP Ah 1601:

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

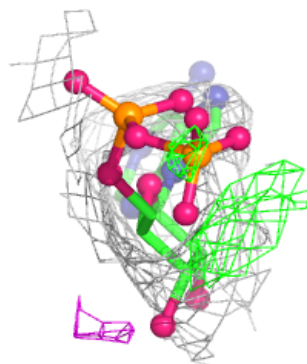
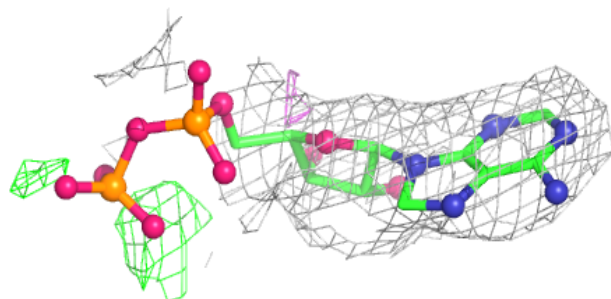
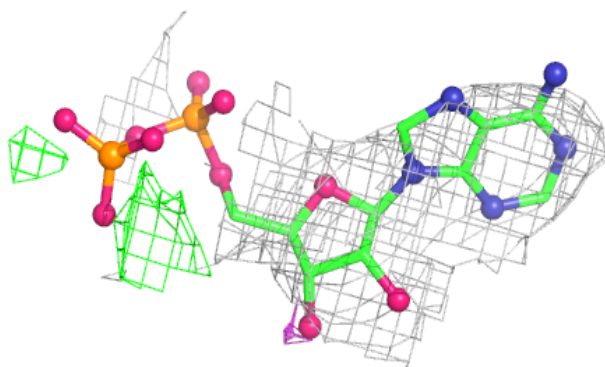


Electron density around ADP Bg 5001:

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

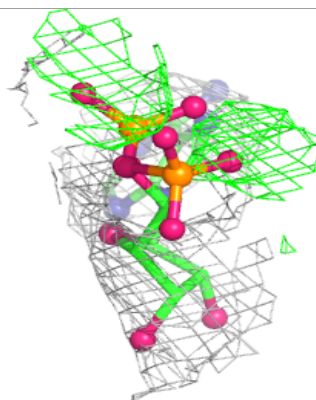
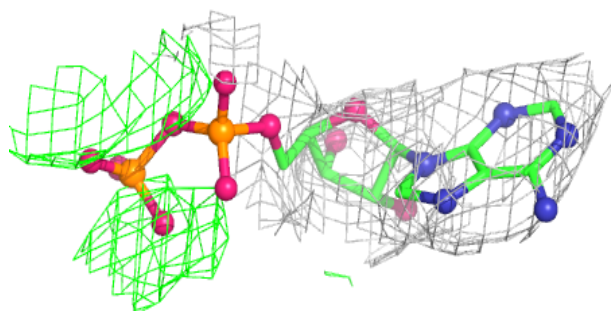
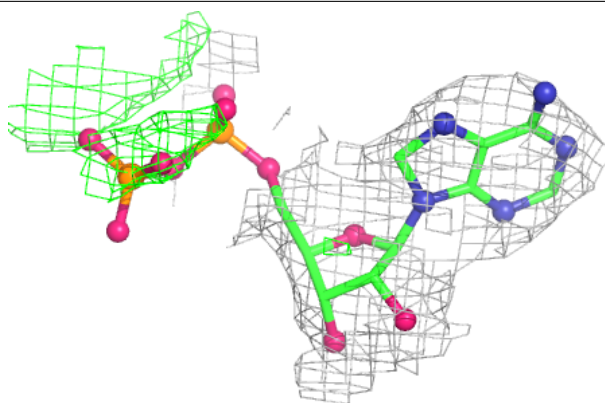
**Electron density around ADP AQ 601:**

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

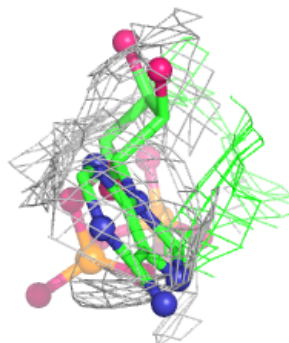
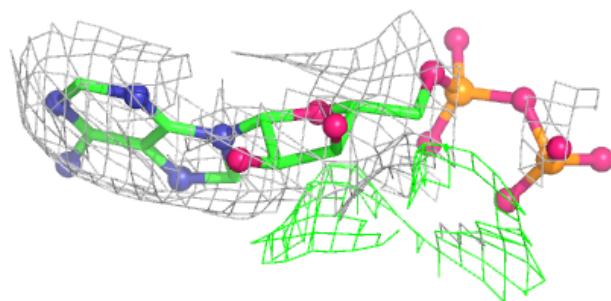
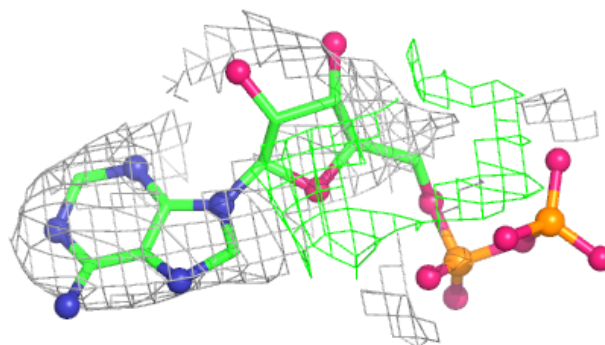


Electron density around ADP AG 1001:

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

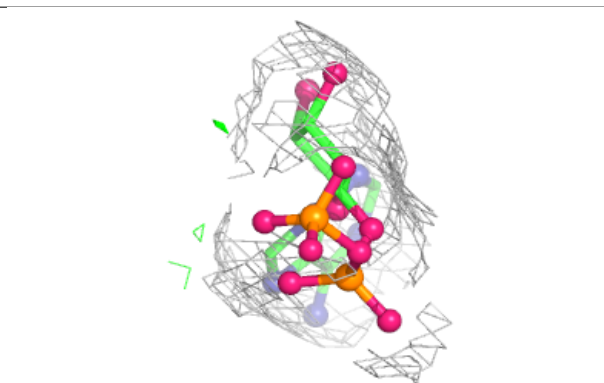
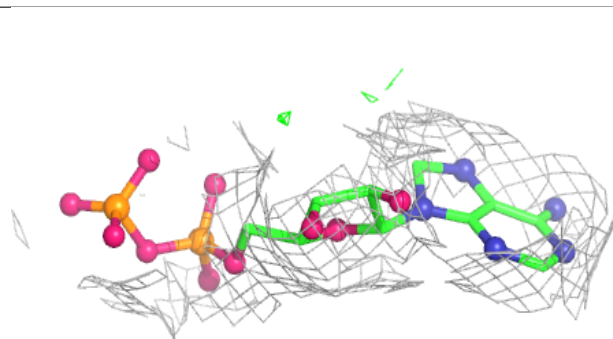
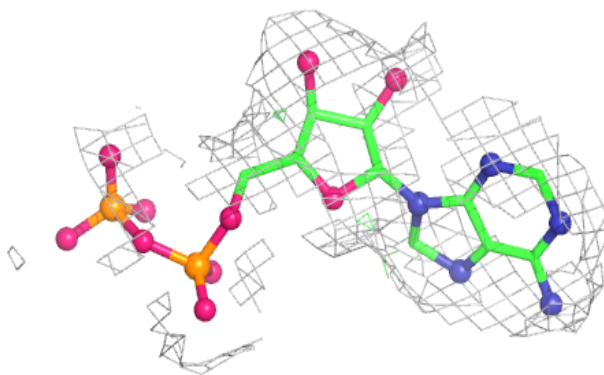
**Electron density around ADP Aq 1601:**

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

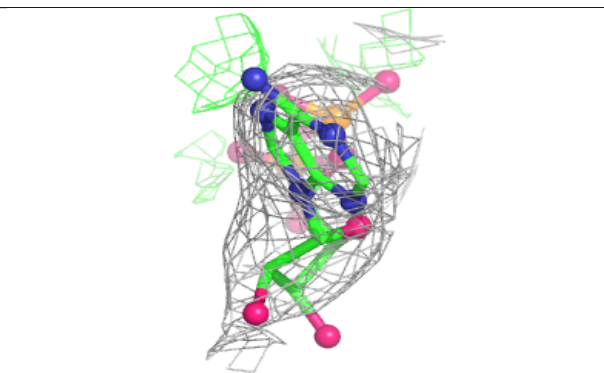
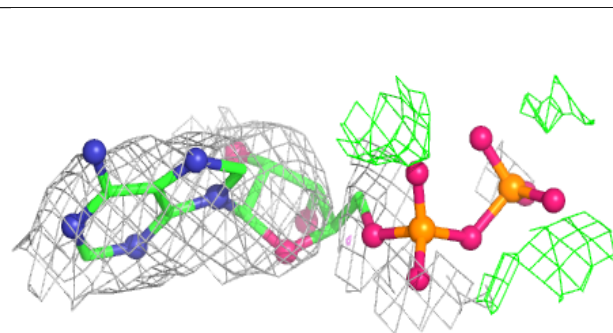
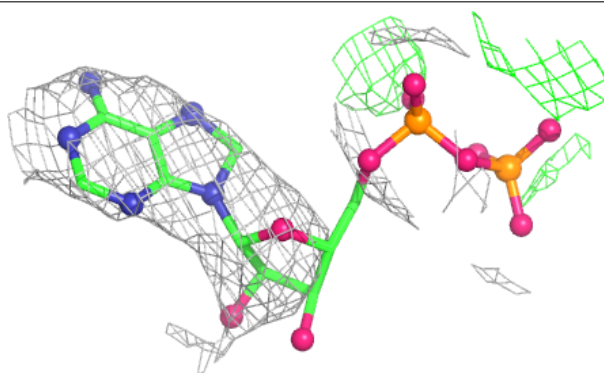


Electron density around ADP Az 1601:

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

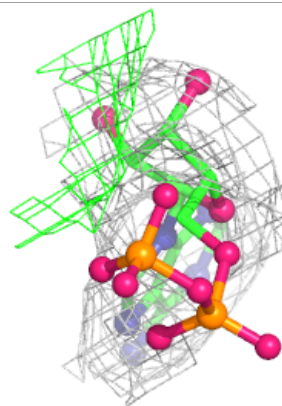
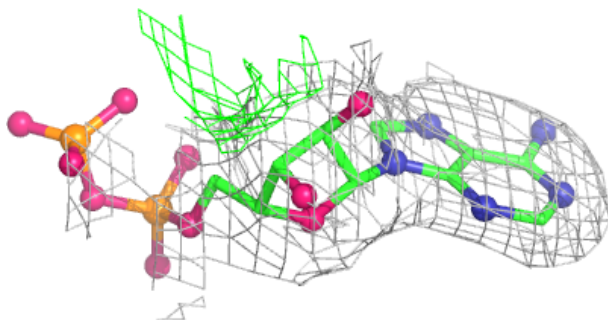
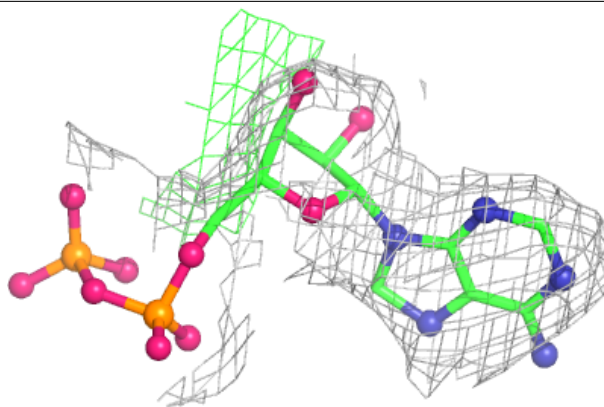
**Electron density around ADP BG 4001:**

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

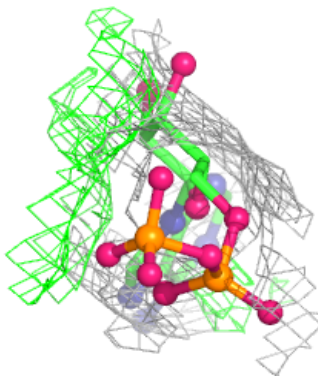
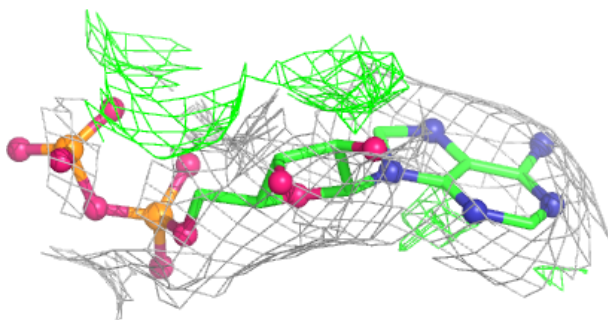
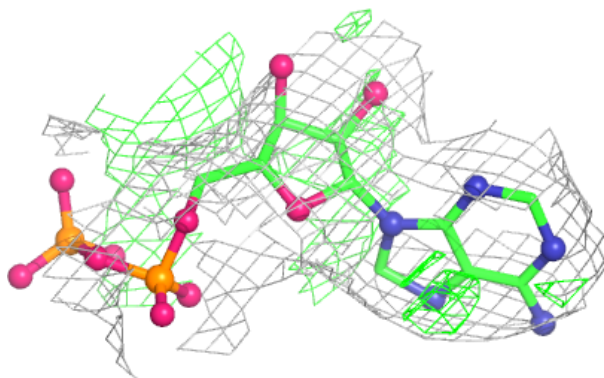


Electron density around ADP BH 3601:

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

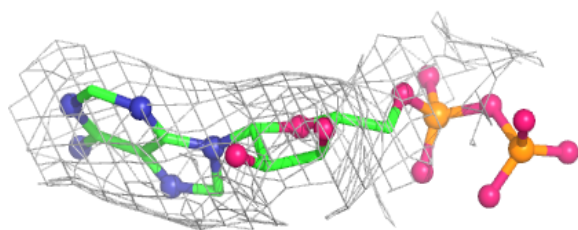
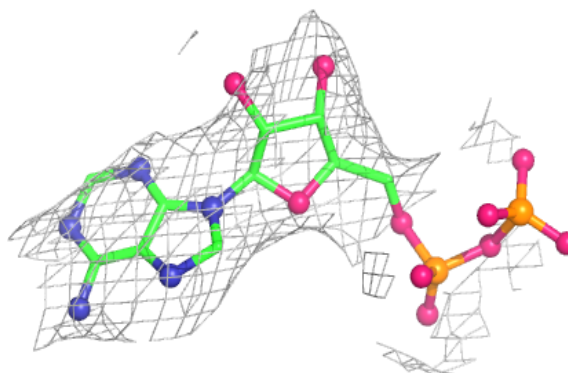
**Electron density around ADP BQ 3601:**

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

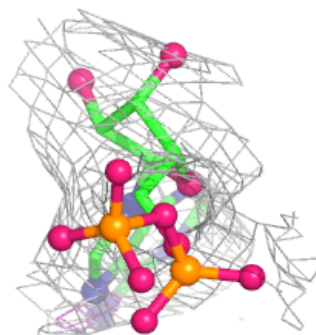
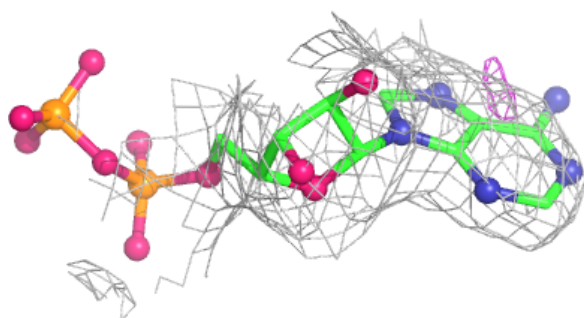
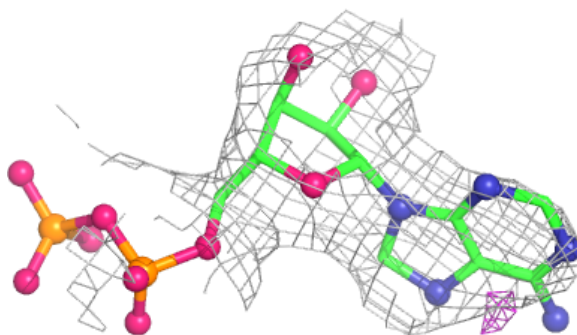


Electron density around ADP BZ 3601:

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

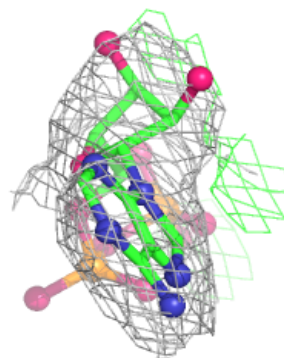
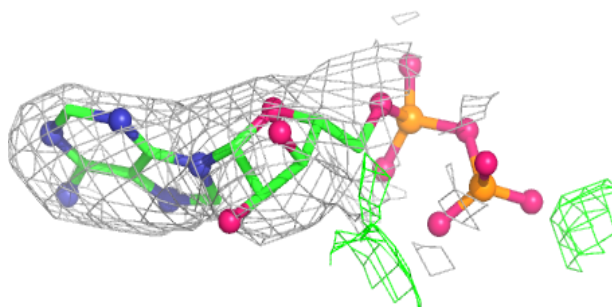
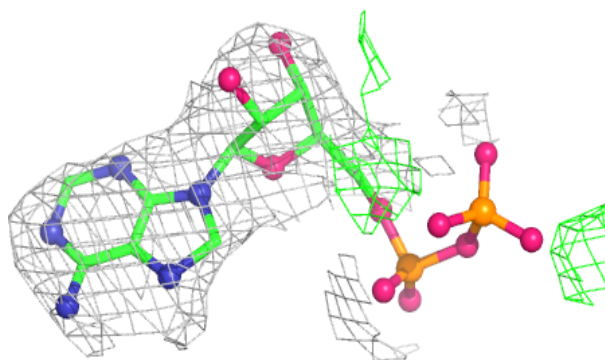
**Electron density around ADP AA 601:**

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

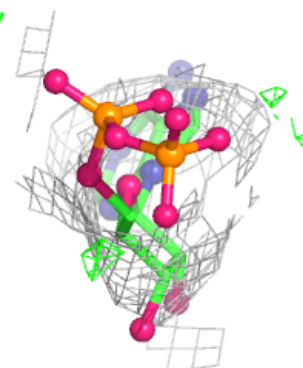
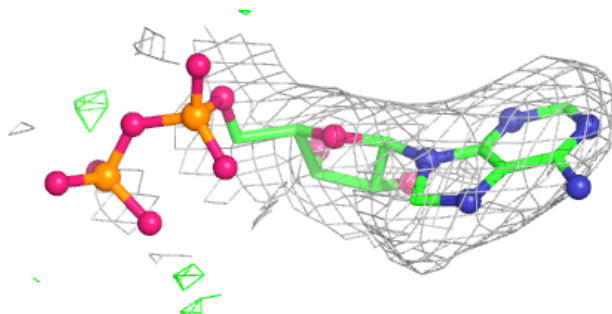
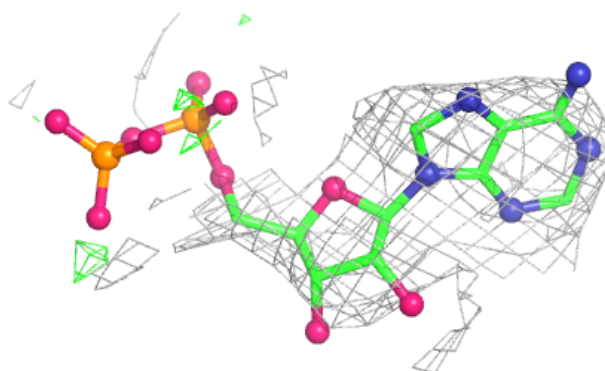


Electron density around ADP Bh 4601:

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

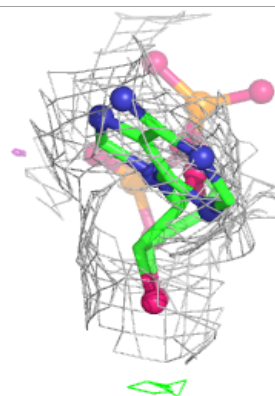
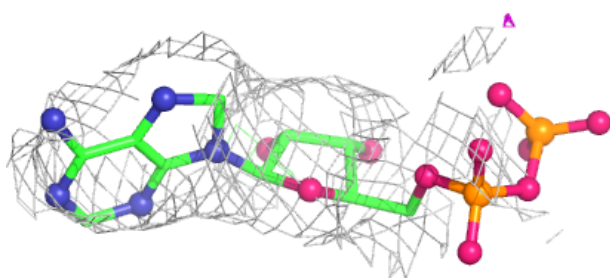
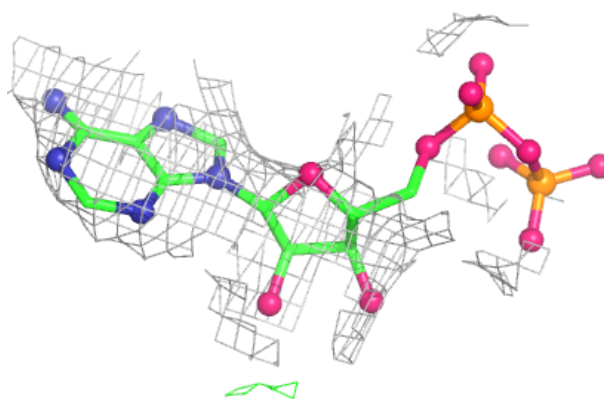
**Electron density around ADP Bq 4601:**

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

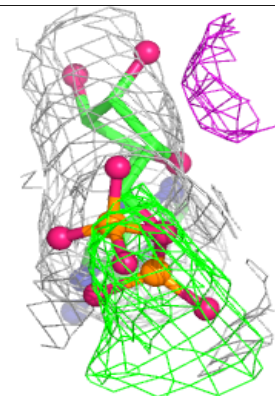
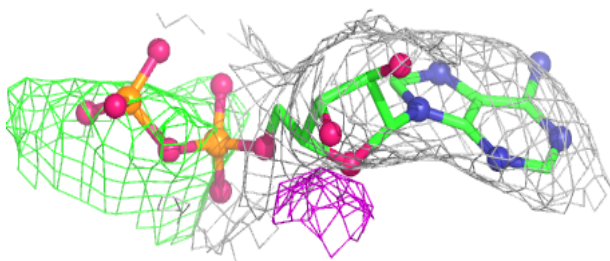
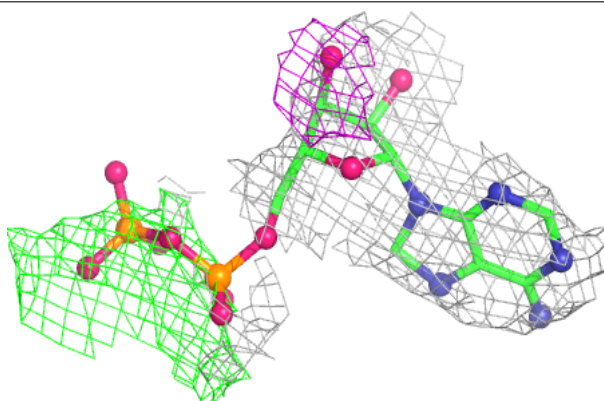


Electron density around ADP Ad 1601:

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

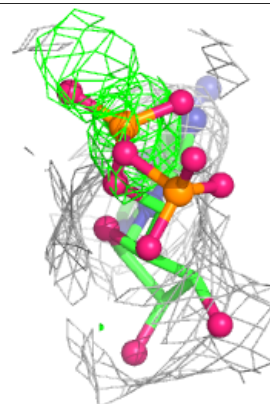
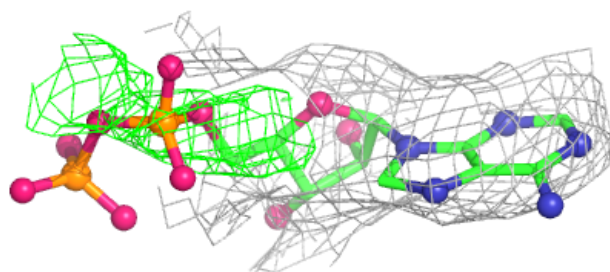
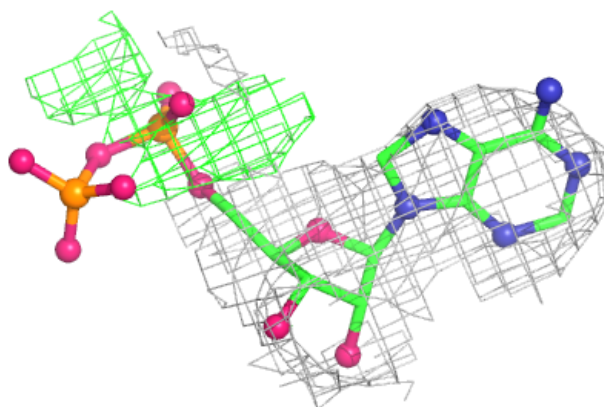
**Electron density around ADP Ag 2001:**

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

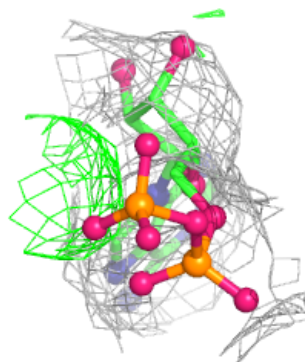
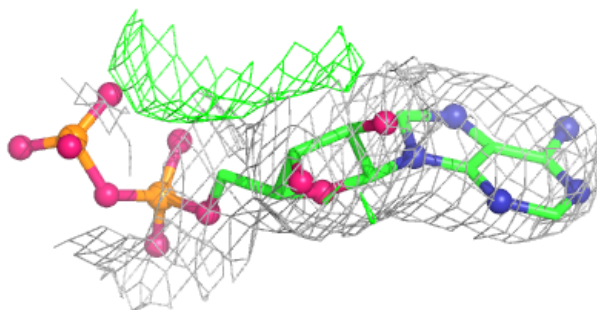
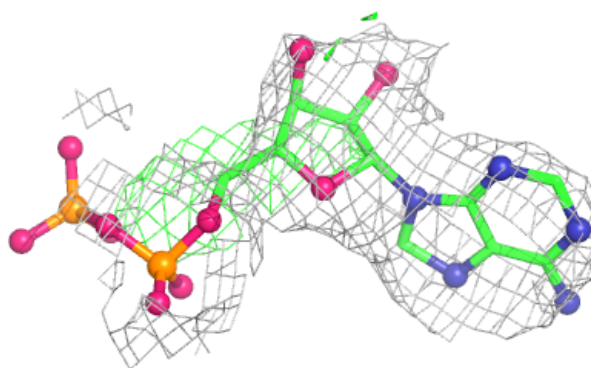


Electron density around ADP Ae 1601:

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

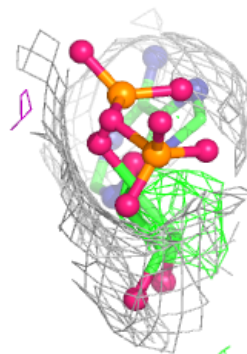
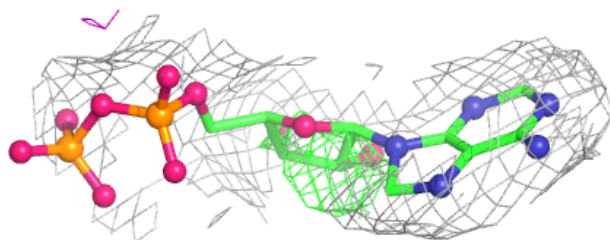
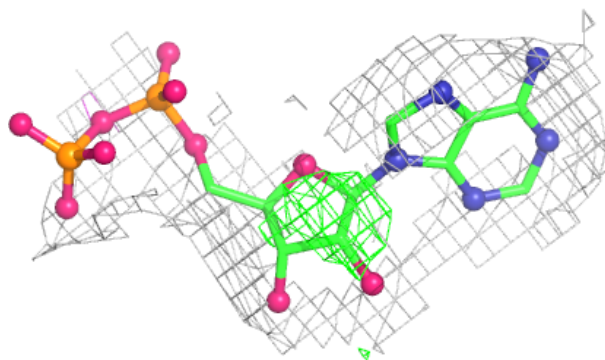
**Electron density around ADP AB 601:**

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

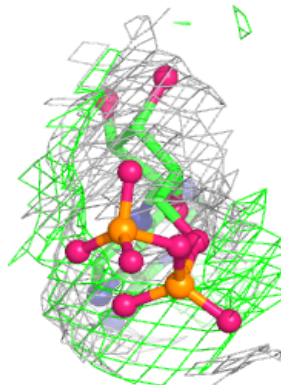
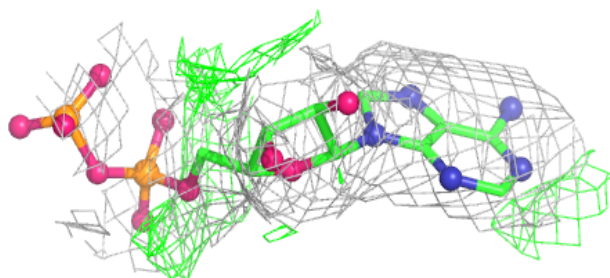


Electron density around ADP AZ 601:

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

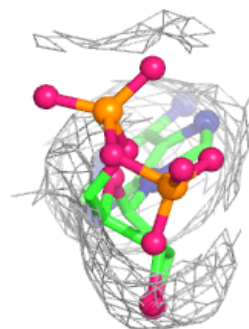
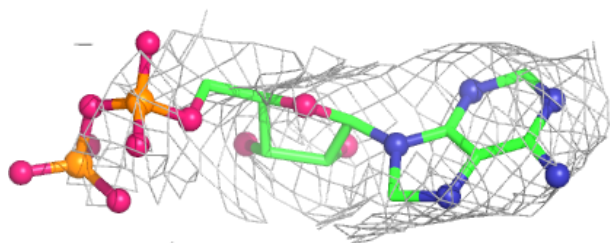
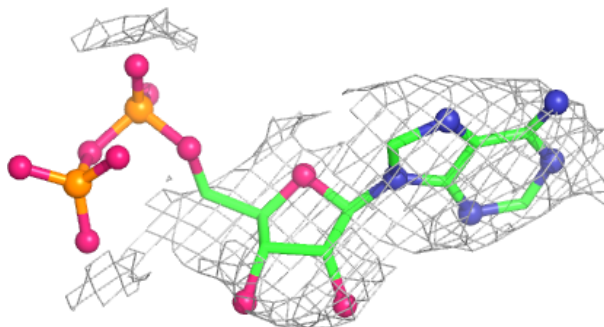
**Electron density around ADP Ab 1601:**

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

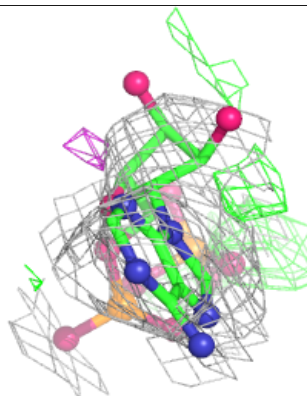
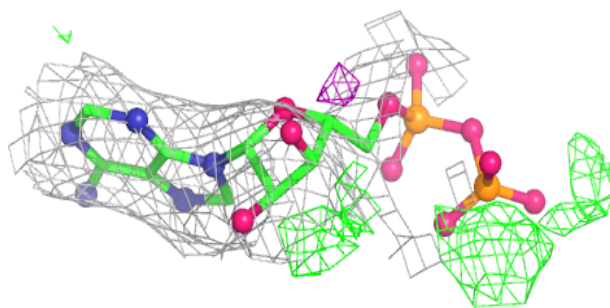
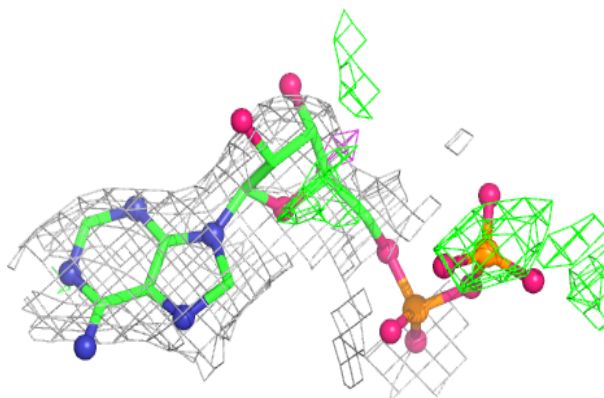


Electron density around ADP Bd 4601:

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

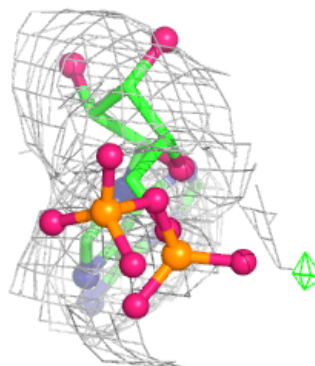
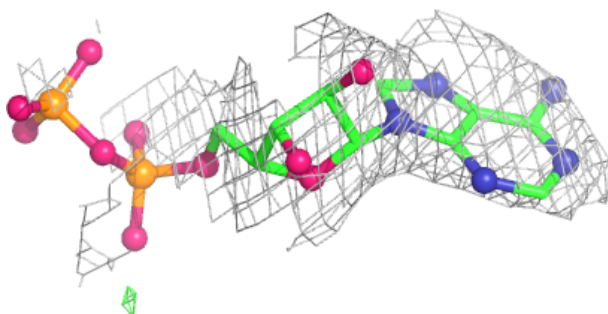
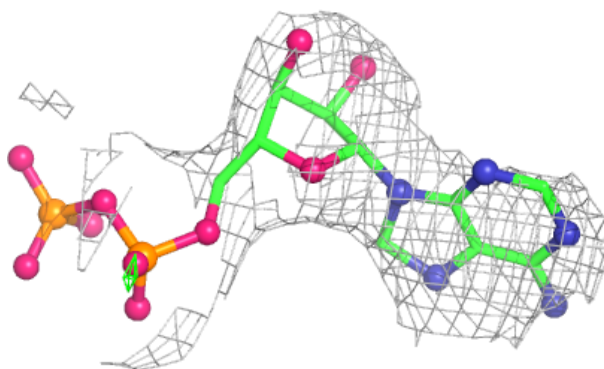
**Electron density around ADP AH 601:**

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

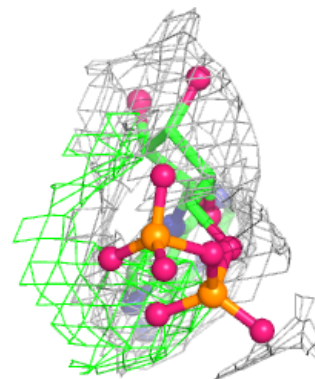
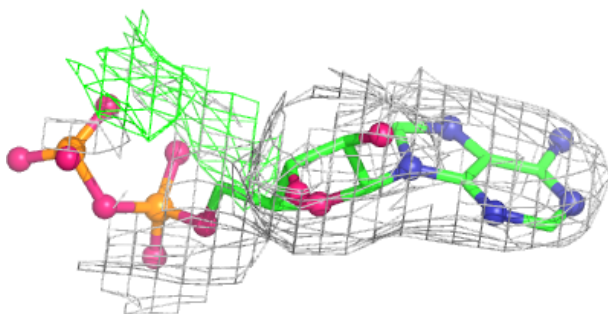
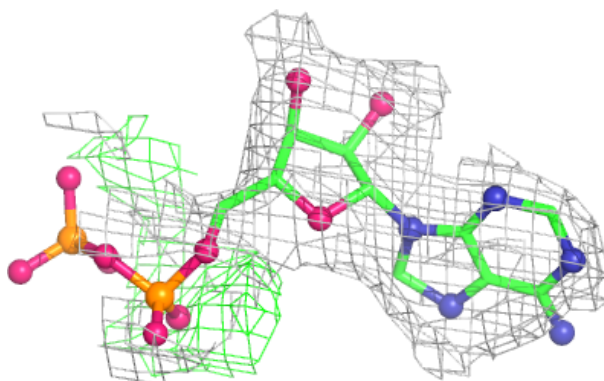


Electron density around ADP BA 3601:

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

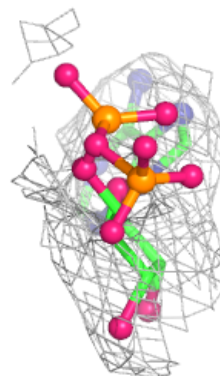
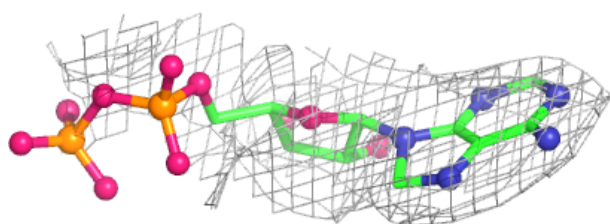
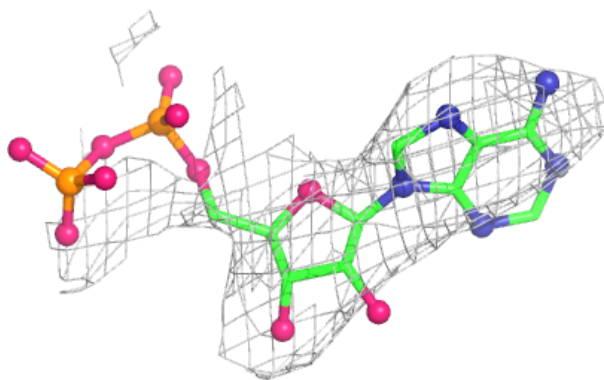
**Electron density around ADP BB 3601:**

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

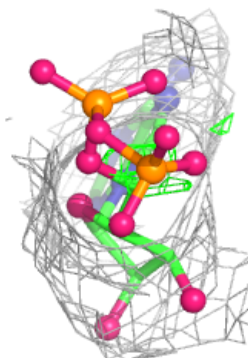
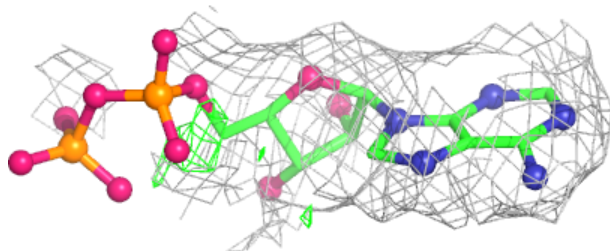
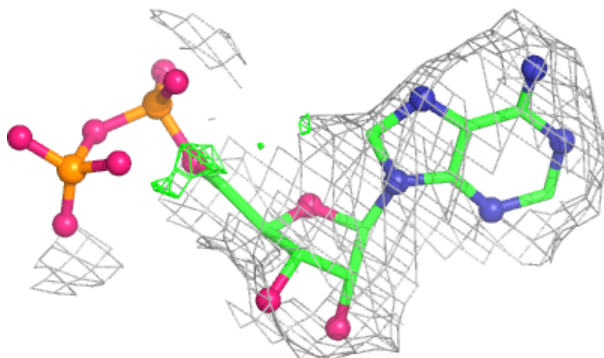


Electron density around ADP Bz 4601:

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

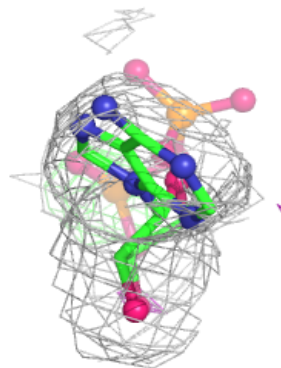
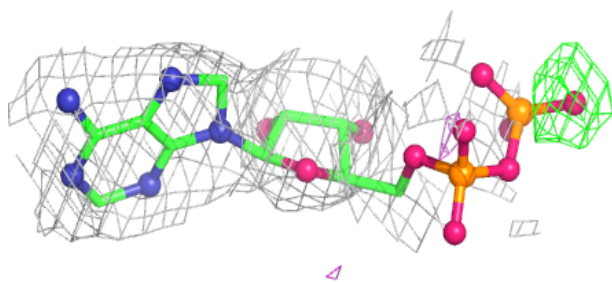
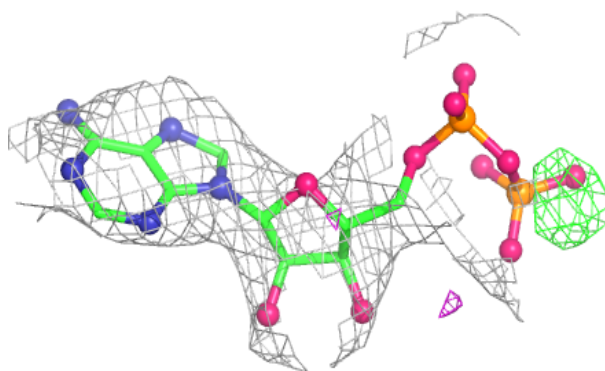
**Electron density around ADP Be 4601:**

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

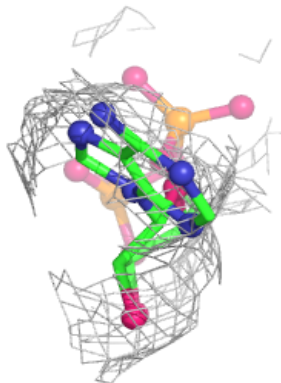
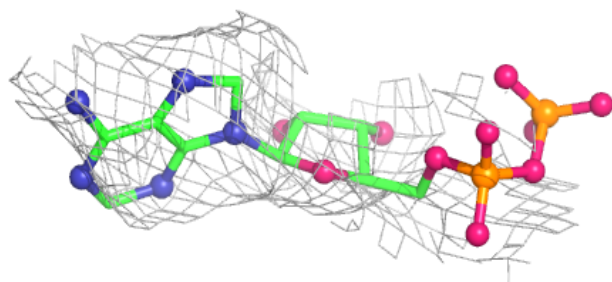
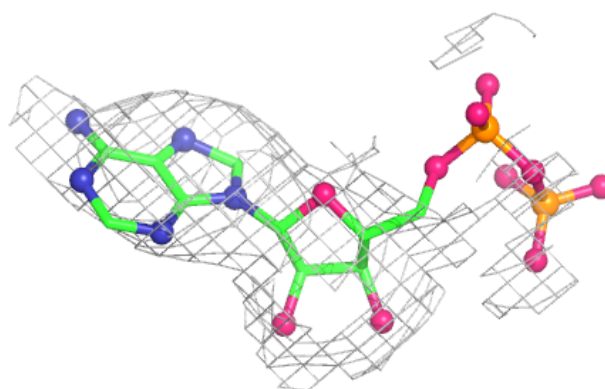


Electron density around ADP AD 601:

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

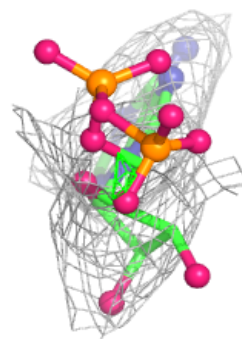
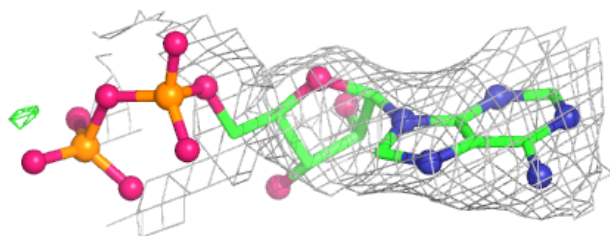
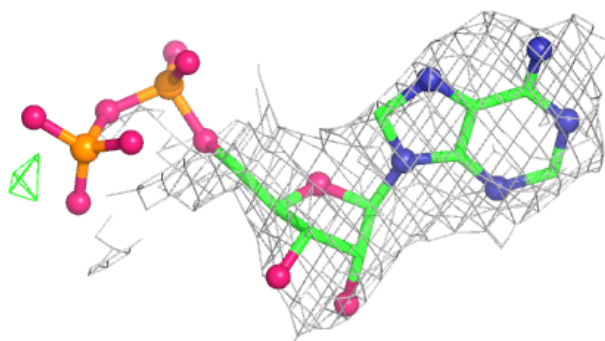
**Electron density around ADP BD 3601:**

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

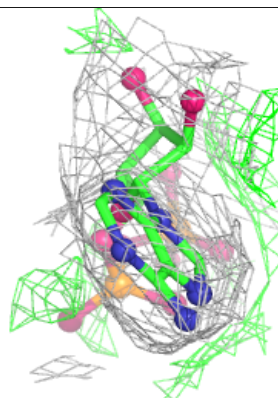
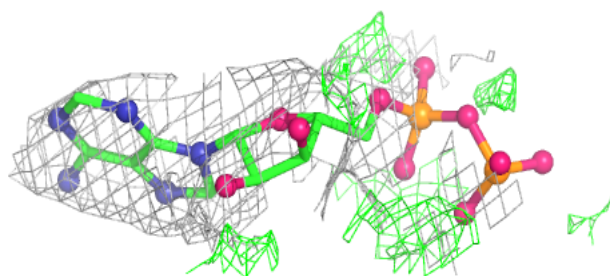
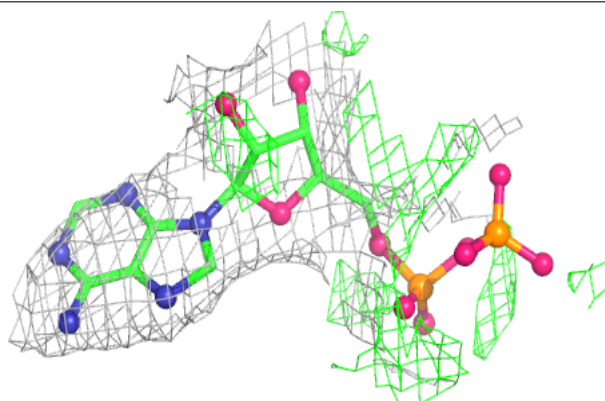


Electron density around ADP BE 3601:

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

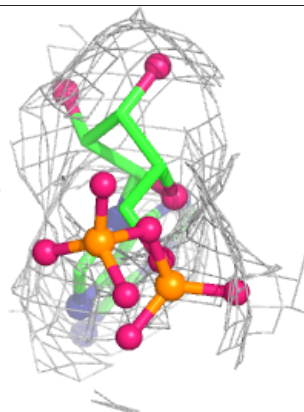
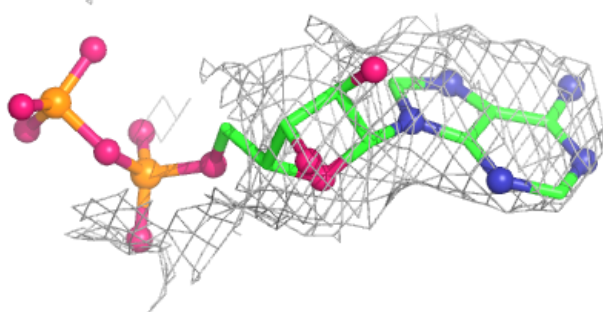
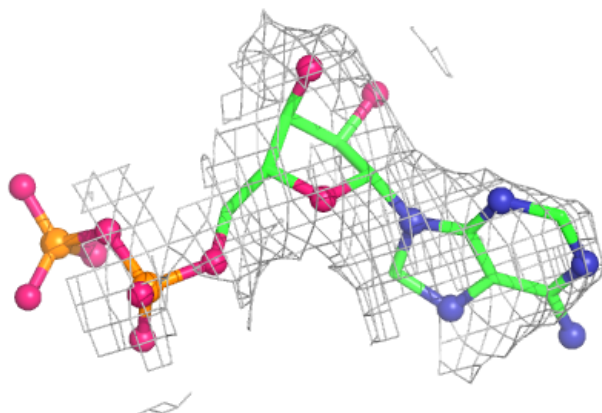
**Electron density around ADP Bb 4601:**

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

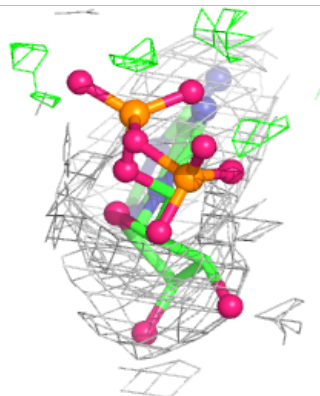
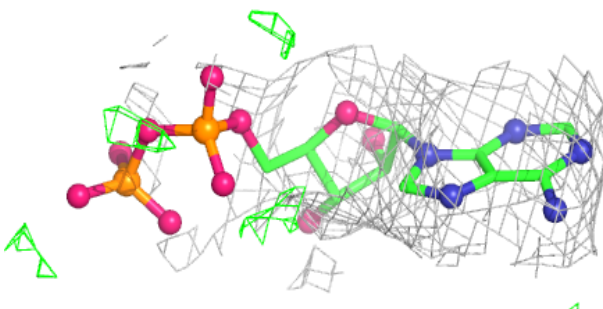
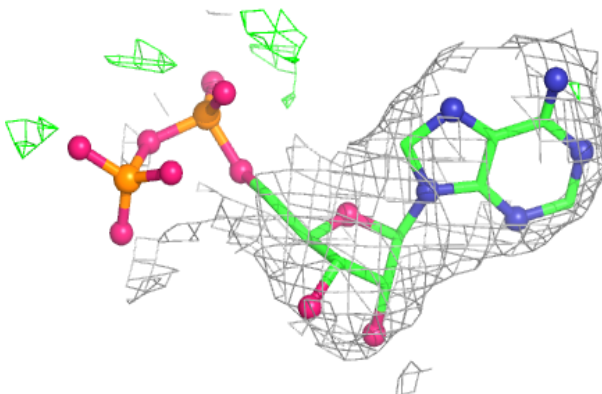


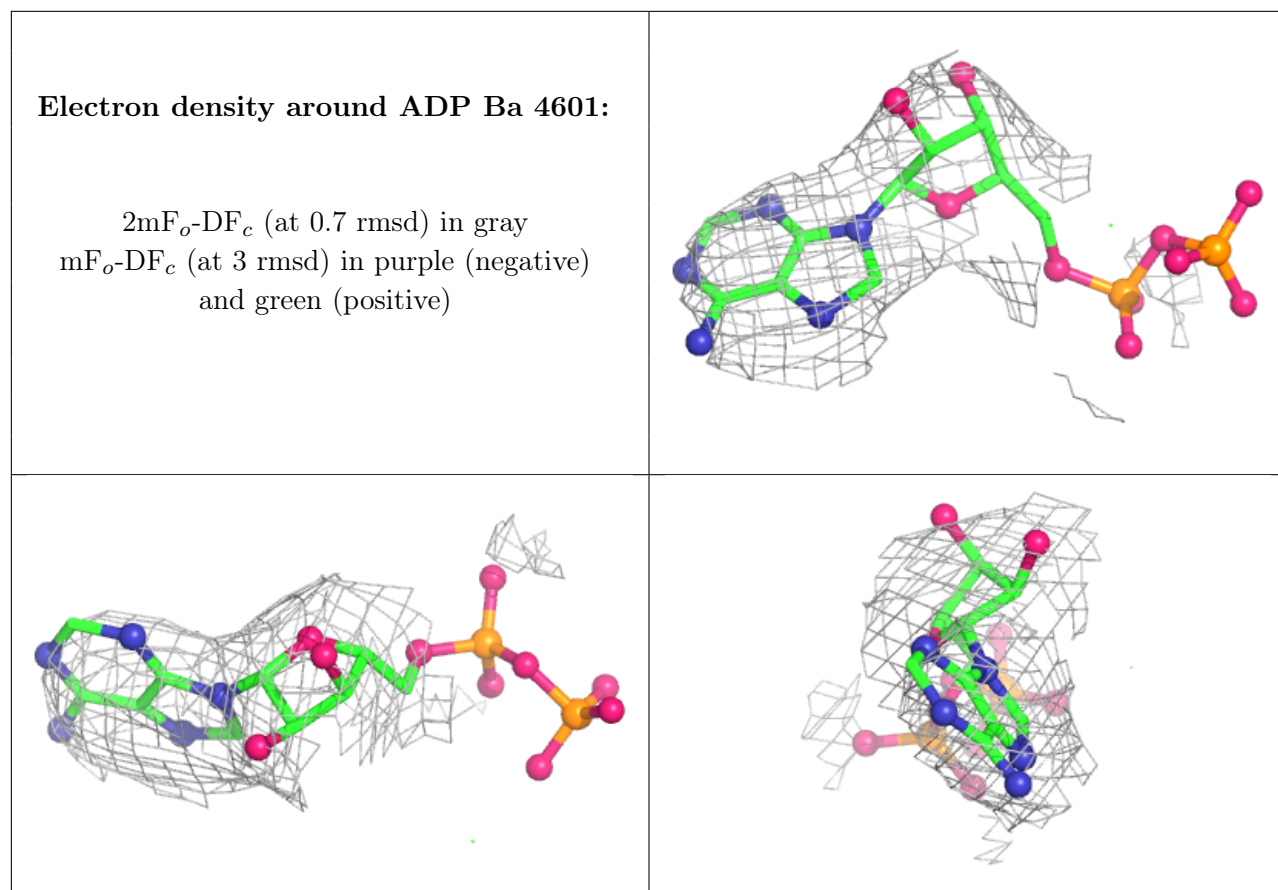
Electron density around ADP Aa 1601:

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

**Electron density around ADP AE 601:**

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





5.5 Other polymers [i](#)

There are no such residues in this entry.