



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:22 am BST

PDB ID : 5HKK  
Title : Caldalaklibacillus thermarum F1-ATPase (wild type)  
Authors : Ferguson, S.A.; Cook, G.M.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2016-01-14  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

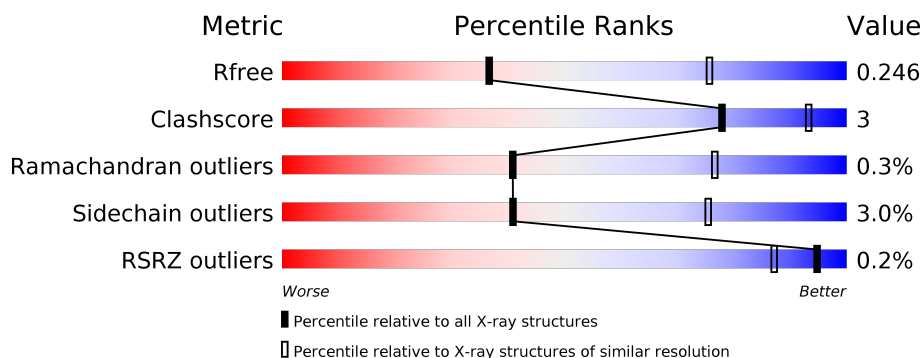
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>82%</span> <span>12%</span> <span>• 5%</span> </div> </div>
1	B	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 86%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>86%</span> <span>8%</span> <span>• 5%</span> </div> </div>
1	C	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 8%, green 85%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span></span> <span>85%</span> <span>8%</span> <span>• 5%</span> </div> </div>
1	I	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 10%, green 84%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span></span> <span>84%</span> <span>10%</span> <span>• 6%</span> </div> </div>
1	J	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 8%, green 86%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span></span> <span>86%</span> <span>8%</span> <span>• 5%</span> </div> </div>
1	K	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 10%, green 84%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span></span> <span>84%</span> <span>10%</span> <span>• 5%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	462	<div><div></div><div>92%</div><div>8%</div></div>
2	E	462	<div><div></div><div>87%</div><div>11%</div><div></div></div>
2	F	462	<div><div></div><div>95%</div><div>5%</div></div>
2	L	462	<div><div></div><div>92%</div><div>7%</div><div></div></div>
2	M	462	<div><div></div><div>88%</div><div>11%</div><div></div></div>
2	N	462	<div><div></div><div>94%</div><div>6%</div></div>
3	G	286	<div><div></div><div>91%</div><div>8%</div><div></div></div>
3	O	286	<div><div>%</div><div></div><div>90%</div><div>9%</div><div></div></div>
4	H	135	<div><div></div><div>91%</div><div>7%</div><div></div></div>
4	P	135	<div><div>%</div><div></div><div>89%</div><div>9%</div><div></div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 50225 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3647	2300	629	704	14			
1	B	475	Total	C	N	O	S	0	0	0
			3646	2298	629	705	14			
1	C	476	Total	C	N	O	S	0	0	0
			3651	2301	630	706	14			
1	I	474	Total	C	N	O	S	0	0	0
			3640	2295	628	703	14			
1	J	475	Total	C	N	O	S	0	0	0
			3646	2298	629	705	14			
1	K	478	Total	C	N	O	S	0	0	0
			3665	2311	632	708	14			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	E	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	F	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	L	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	M	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	N	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			

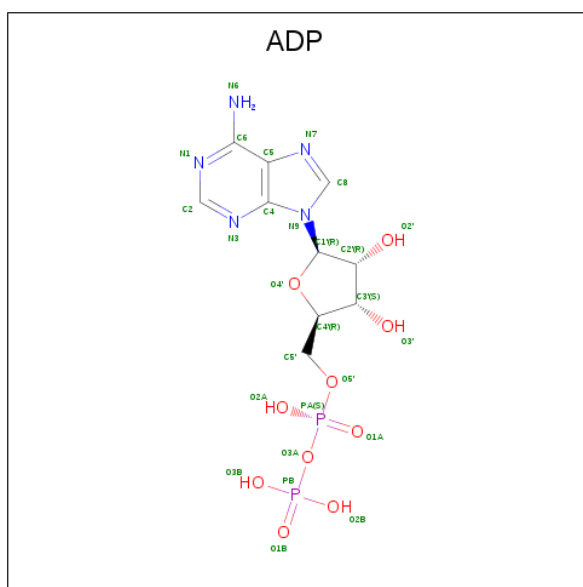
- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	284	Total	C	N	O	S	0	0	0
			2221	1398	386	428	9			
3	O	284	Total	C	N	O	S	0	0	0
			2221	1398	386	428	9			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	132	Total	C	N	O	S	0	0	0
			1031	647	190	193	1			
4	P	132	Total	C	N	O	S	0	0	0
			1031	647	190	193	1			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	N	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

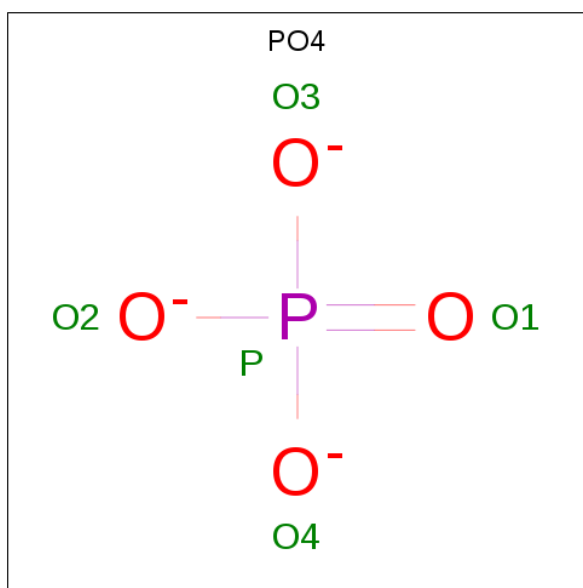
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Mg 1	0	0
6	J	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0
6	K	1	Total 1	Mg 1	0	0
6	B	1	Total 1	Mg 1	0	0
6	I	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0
6	A	1	Total 1	Mg 1	0	0
6	N	1	Total 1	Mg 1	0	0
6	O	1	Total 1	Mg 1	0	0
6	L	1	Total 1	Mg 1	0	0
6	F	1	Total 1	Mg 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



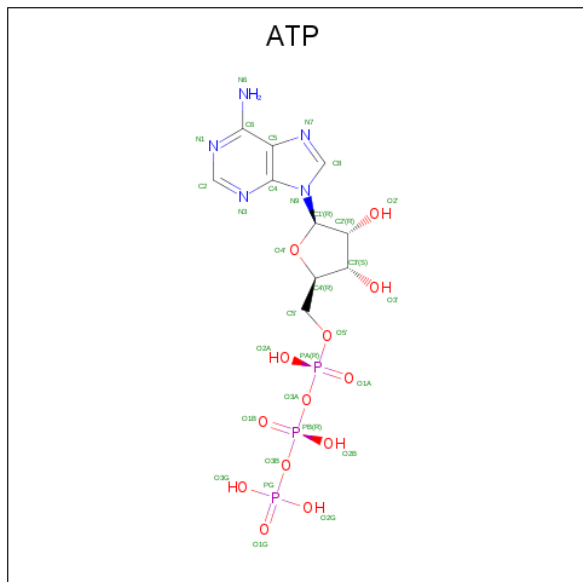
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	20	Total	O	0	0
			20	20		
10	B	21	Total	O	0	0
			21	21		
10	C	23	Total	O	0	0
			23	23		
10	D	30	Total	O	0	0
			30	30		
10	E	24	Total	O	0	0
			24	24		
10	F	26	Total	O	0	0
			26	26		
10	G	6	Total	O	0	0
			6	6		
10	H	6	Total	O	0	0
			6	6		

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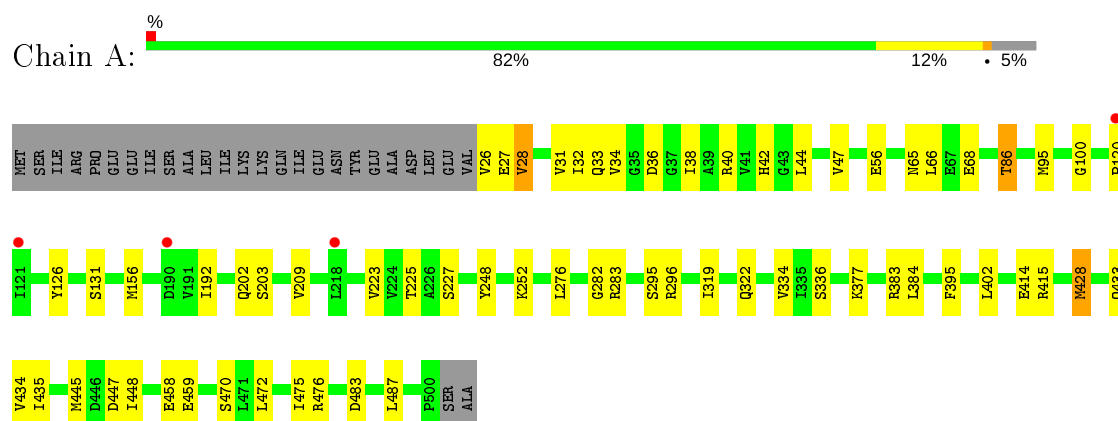
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	13	Total 13	O 13	0	0
10	J	13	Total 13	O 13	0	0
10	K	24	Total 24	O 24	0	0
10	L	30	Total 30	O 30	0	0
10	M	10	Total 10	O 10	0	0
10	N	31	Total 31	O 31	0	0
10	O	4	Total 4	O 4	0	0
10	P	5	Total 5	O 5	0	0

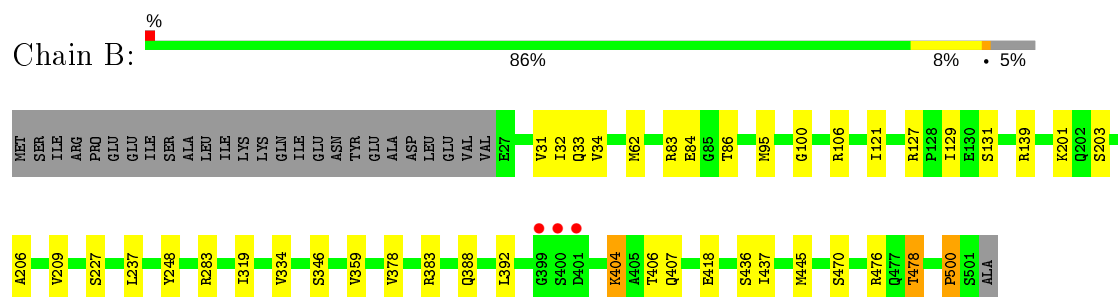
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

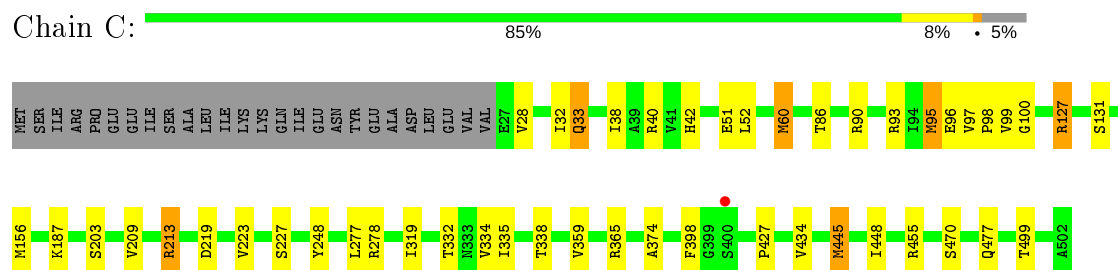
- Molecule 1: ATP synthase subunit alpha



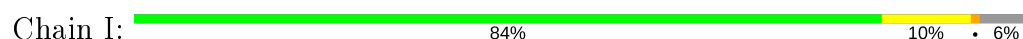
- Molecule 1: ATP synthase subunit alpha

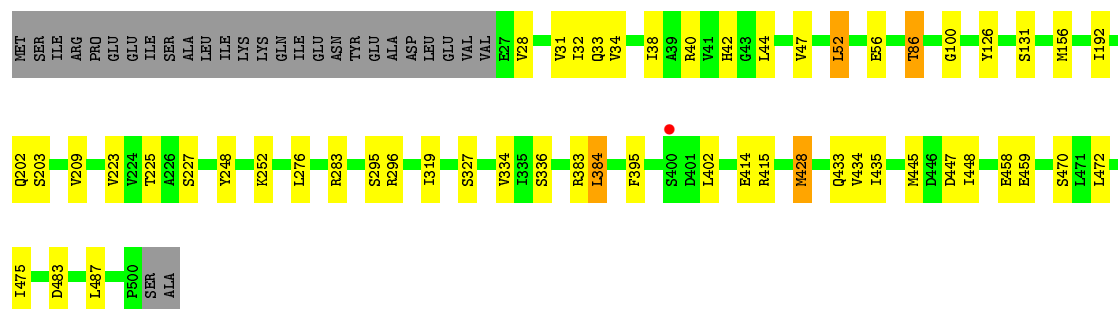


- Molecule 1: ATP synthase subunit alpha



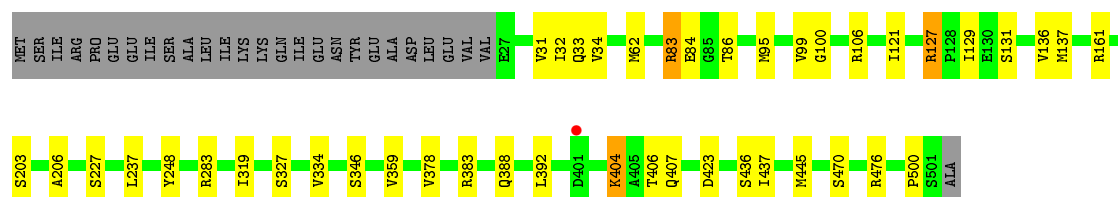
- Molecule 1: ATP synthase subunit alpha





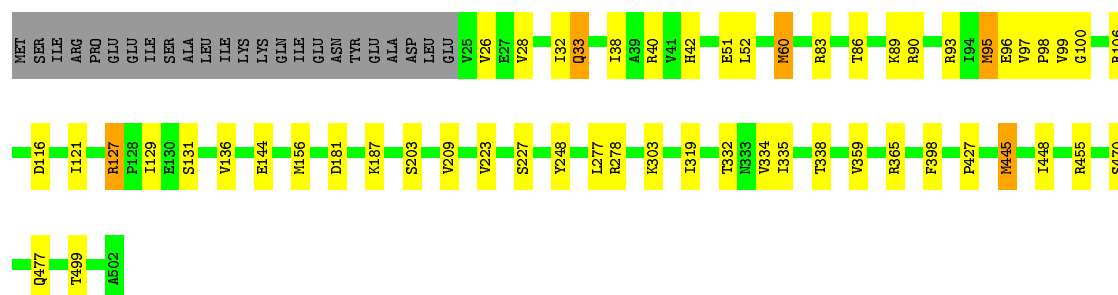
- Molecule 1: ATP synthase subunit alpha

Chain J: 86% 8% 5%



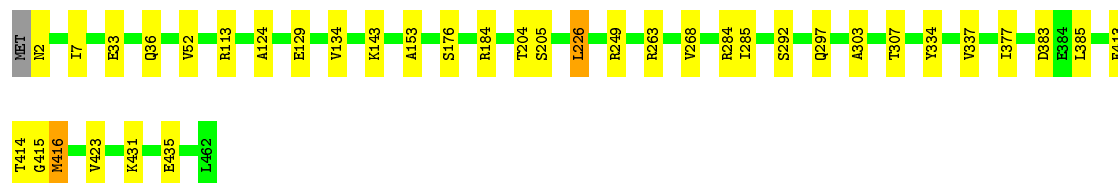
- Molecule 1: ATP synthase subunit alpha

Chain K: 84% 10% 5%



- Molecule 2: ATP synthase subunit beta

Chain D: 92% 8%



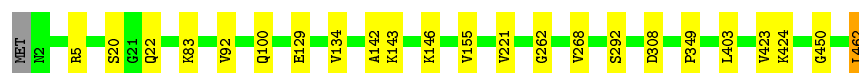
- Molecule 2: ATP synthase subunit beta

Chain E: 87% 11%





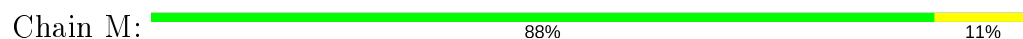
- Molecule 2: ATP synthase subunit beta



- Molecule 2: ATP synthase subunit beta



- Molecule 2: ATP synthase subunit beta



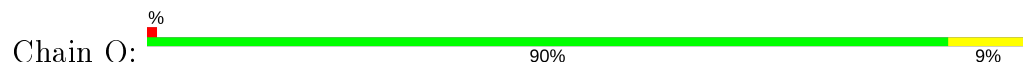
- Molecule 2: ATP synthase subunit beta

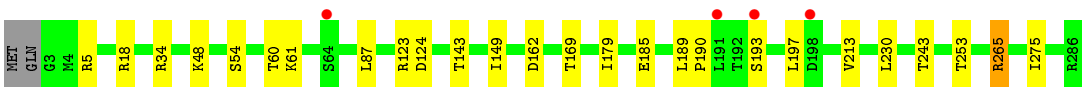


- Molecule 3: ATP synthase gamma chain

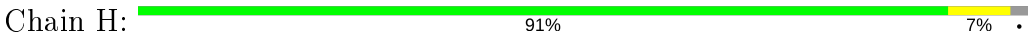


- Molecule 3: ATP synthase gamma chain

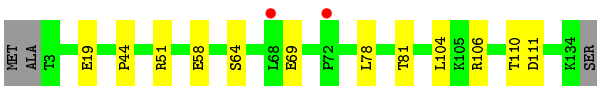
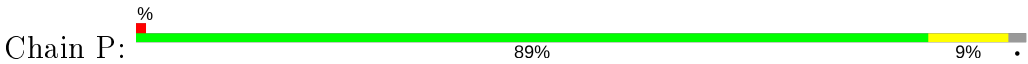




● Molecule 4: ATP synthase epsilon chain



● Molecule 4: ATP synthase epsilon chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.82Å 130.79Å 210.39Å 90.00° 107.97° 90.00°	Depositor
Resolution (Å)	62.16 – 3.00 64.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (62.16-3.00) 95.0 (64.30-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0144	Depositor
R, $R_{free}$	0.203 , 0.246 0.205 , 0.246	Depositor DCC
$R_{free}$ test set	7274 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	50225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GOL, MG, PO4, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	0/3706	0.83	8/5016 (0.2%)
1	B	0.55	0/3705	0.80	2/5014 (0.0%)
1	C	0.58	0/3710	0.79	4/5021 (0.1%)
1	I	0.57	0/3699	0.83	9/5006 (0.2%)
1	J	0.55	0/3705	0.80	2/5014 (0.0%)
1	K	0.59	0/3724	0.78	2/5041 (0.0%)
2	D	0.57	0/3581	0.76	0/4852
2	E	0.65	0/3581	0.85	7/4852 (0.1%)
2	F	0.55	0/3581	0.78	3/4852 (0.1%)
2	L	0.57	0/3581	0.78	3/4852 (0.1%)
2	M	0.66	0/3581	0.84	6/4852 (0.1%)
2	N	0.56	0/3581	0.79	2/4852 (0.0%)
3	G	0.50	0/2254	0.70	0/3042
3	O	0.50	0/2254	0.69	1/3042 (0.0%)
4	H	0.50	0/1042	0.79	0/1404
4	P	0.48	0/1042	0.78	0/1404
All	All	0.57	0/50327	0.79	49/68116 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	I	296	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	478	THR	CA-CB-CG2	7.87	123.42	112.40
2	E	383	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	I	126	TYR	CB-CG-CD1	7.18	125.31	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	144	GLY	Peptide
2	M	144	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3647	0	3683	35	0
1	B	3646	0	3679	18	0
1	C	3651	0	3684	23	0
1	I	3640	0	3674	30	0
1	J	3646	0	3679	21	0
1	K	3665	0	3702	29	0
2	D	3521	0	3529	23	0
2	E	3521	0	3530	33	0
2	F	3521	0	3529	10	0
2	L	3521	0	3529	21	0
2	M	3521	0	3530	30	0
2	N	3521	0	3529	17	0
3	G	2221	0	2261	12	0
3	O	2221	0	2261	16	0
4	H	1031	0	1089	2	0
4	P	1031	0	1089	6	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	4	0
5	E	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	27	0	12	0	0
5	I	27	0	12	0	0
5	J	27	0	12	0	0
5	K	27	0	12	0	0
5	L	27	0	12	3	0
5	M	27	0	12	0	0
5	N	27	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	A	6	0	8	2	0
8	E	5	0	0	0	0
8	M	5	0	0	0	0
9	H	31	0	12	0	0
9	P	31	0	12	0	0
10	A	20	0	0	1	0
10	B	21	0	0	1	0
10	C	23	0	0	1	0
10	D	30	0	0	4	0
10	E	24	0	0	1	0
10	F	26	0	0	2	0
10	G	6	0	0	0	0
10	H	6	0	0	0	0
10	I	13	0	0	0	0
10	J	13	0	0	1	0
10	K	24	0	0	5	0
10	L	30	0	0	2	0
10	M	10	0	0	0	0
10	N	31	0	0	4	0
10	O	4	0	0	0	0
10	P	5	0	0	0	0
All	All	50225	0	50153	285	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 285 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:J:84:GLU:HB3	2:M:23:LEU:HD13	1.60	0.84
2:L:176:SER:HB2	2:L:204:THR:HG22	1.61	0.82
2:D:176:SER:HB2	2:D:204:THR:HG22	1.62	0.82
2:M:285:ILE:HG21	2:M:295:SER:HB2	1.70	0.72
1:B:84:GLU:HB3	2:E:23:LEU:HD13	1.69	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	473/502 (94%)	465 (98%)	6 (1%)	2 (0%)	34	72
1	B	473/502 (94%)	463 (98%)	9 (2%)	1 (0%)	47	82
1	C	474/502 (94%)	465 (98%)	9 (2%)	0	100	100
1	I	472/502 (94%)	465 (98%)	6 (1%)	1 (0%)	47	82
1	J	473/502 (94%)	463 (98%)	9 (2%)	1 (0%)	47	82
1	K	476/502 (95%)	465 (98%)	11 (2%)	0	100	100
2	D	459/462 (99%)	443 (96%)	15 (3%)	1 (0%)	47	82
2	E	459/462 (99%)	441 (96%)	16 (4%)	2 (0%)	34	72
2	F	459/462 (99%)	441 (96%)	16 (4%)	2 (0%)	34	72
2	L	459/462 (99%)	443 (96%)	15 (3%)	1 (0%)	47	82
2	M	459/462 (99%)	443 (96%)	14 (3%)	2 (0%)	34	72
2	N	459/462 (99%)	442 (96%)	15 (3%)	2 (0%)	34	72
3	G	282/286 (99%)	268 (95%)	12 (4%)	2 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	282/286 (99%)	268 (95%)	12 (4%)	2 (1%)	22	60
4	H	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
4	P	130/135 (96%)	127 (98%)	3 (2%)	0	100	100
All	All	6419/6626 (97%)	6227 (97%)	173 (3%)	19 (0%)	41	76

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	28	VAL
1	I	28	VAL
3	O	61	LYS
2	E	20	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/413 (94%)	373 (96%)	16 (4%)	30	67
1	B	389/413 (94%)	374 (96%)	15 (4%)	32	69
1	C	389/413 (94%)	375 (96%)	14 (4%)	35	70
1	I	388/413 (94%)	375 (97%)	13 (3%)	37	72
1	J	389/413 (94%)	376 (97%)	13 (3%)	38	73
1	K	391/413 (95%)	377 (96%)	14 (4%)	35	70
2	D	375/376 (100%)	366 (98%)	9 (2%)	49	79
2	E	375/376 (100%)	364 (97%)	11 (3%)	42	76
2	F	375/376 (100%)	367 (98%)	8 (2%)	53	82
2	L	375/376 (100%)	366 (98%)	9 (2%)	49	79
2	M	375/376 (100%)	364 (97%)	11 (3%)	42	76
2	N	375/376 (100%)	367 (98%)	8 (2%)	53	82
3	G	237/239 (99%)	234 (99%)	3 (1%)	69	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	237/239 (99%)	234 (99%)	3 (1%)	69	89
4	H	111/113 (98%)	105 (95%)	6 (5%)	22	57
4	P	111/113 (98%)	104 (94%)	7 (6%)	18	51
All	All	5281/5438 (97%)	5121 (97%)	160 (3%)	41	75

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	462	LEU
1	I	428	MET
2	N	349	PRO
3	G	110	LYS
4	H	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	172	HIS
3	G	187	GLN
3	O	65	HIS
2	E	8	GLN
3	G	65	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	ADP	A	601	6	24,29,29	1.17	2 (8%)	29,45,45	1.34	4 (13%)
5	ADP	N	600	6	24,29,29	1.09	1 (4%)	29,45,45	1.36	3 (10%)
5	ADP	C	600	6	24,29,29	1.04	2 (8%)	29,45,45	1.39	4 (13%)
5	ADP	L	600	6	24,29,29	1.15	1 (4%)	29,45,45	1.50	5 (17%)
5	ADP	M	501	-	24,29,29	1.19	3 (12%)	29,45,45	1.53	4 (13%)
9	ATP	H	201	6	26,33,33	1.05	3 (11%)	31,52,52	1.53	6 (19%)
5	ADP	K	600	6	24,29,29	0.98	1 (4%)	29,45,45	1.26	3 (10%)
5	ADP	E	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.53	4 (13%)
8	PO4	E	502	-	4,4,4	0.88	0	6,6,6	0.91	0
9	ATP	P	201	6	26,33,33	0.89	1 (3%)	31,52,52	1.51	7 (22%)
5	ADP	B	600	6	24,29,29	1.02	2 (8%)	29,45,45	1.50	5 (17%)
8	PO4	M	502	-	4,4,4	1.07	0	6,6,6	0.47	0
5	ADP	F	600	6	24,29,29	1.13	2 (8%)	29,45,45	1.48	5 (17%)
7	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.90	0
5	ADP	D	600	6	24,29,29	1.15	2 (8%)	29,45,45	1.49	5 (17%)
5	ADP	I	600	6	24,29,29	1.07	2 (8%)	29,45,45	1.72	7 (24%)
5	ADP	J	600	6	24,29,29	1.02	2 (8%)	29,45,45	1.57	2 (6%)

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
5	ADP	A	601	6	-	3/12/32/32	0/3/3/3
5	ADP	N	600	6	-	6/12/32/32	0/3/3/3
5	ADP	C	600	6	-	0/12/32/32	0/3/3/3
5	ADP	L	600	6	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	M	501	-	-	0/12/32/32	0/3/3/3
9	ATP	H	201	6	-	5/18/38/38	0/3/3/3
5	ADP	K	600	6	-	1/12/32/32	0/3/3/3
5	ADP	E	501	-	-	3/12/32/32	0/3/3/3
9	ATP	P	201	6	-	5/18/38/38	0/3/3/3
5	ADP	B	600	6	-	0/12/32/32	0/3/3/3
5	ADP	F	600	6	-	5/12/32/32	0/3/3/3
7	GOL	A	603	-	-	0/4/4/4	-
5	ADP	D	600	6	-	3/12/32/32	0/3/3/3
5	ADP	I	600	6	-	1/12/32/32	0/3/3/3
5	ADP	J	600	6	-	1/12/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	600	ADP	C5-C4	3.24	1.49	1.40
5	M	501	ADP	C5-C4	3.20	1.49	1.40
5	D	600	ADP	C5-C4	2.85	1.48	1.40
5	L	600	ADP	C5-C4	2.78	1.48	1.40
9	H	201	ATP	C5-C4	2.78	1.48	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	ADP	N3-C2-N1	-4.38	121.83	128.68
5	F	600	ADP	PA-O3A-PB	-4.04	118.95	132.83
5	C	600	ADP	N3-C2-N1	-3.93	122.54	128.68
9	H	201	ATP	C4-C5-N7	-3.92	105.31	109.40
9	P	201	ATP	N3-C2-N1	-3.87	122.63	128.68

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

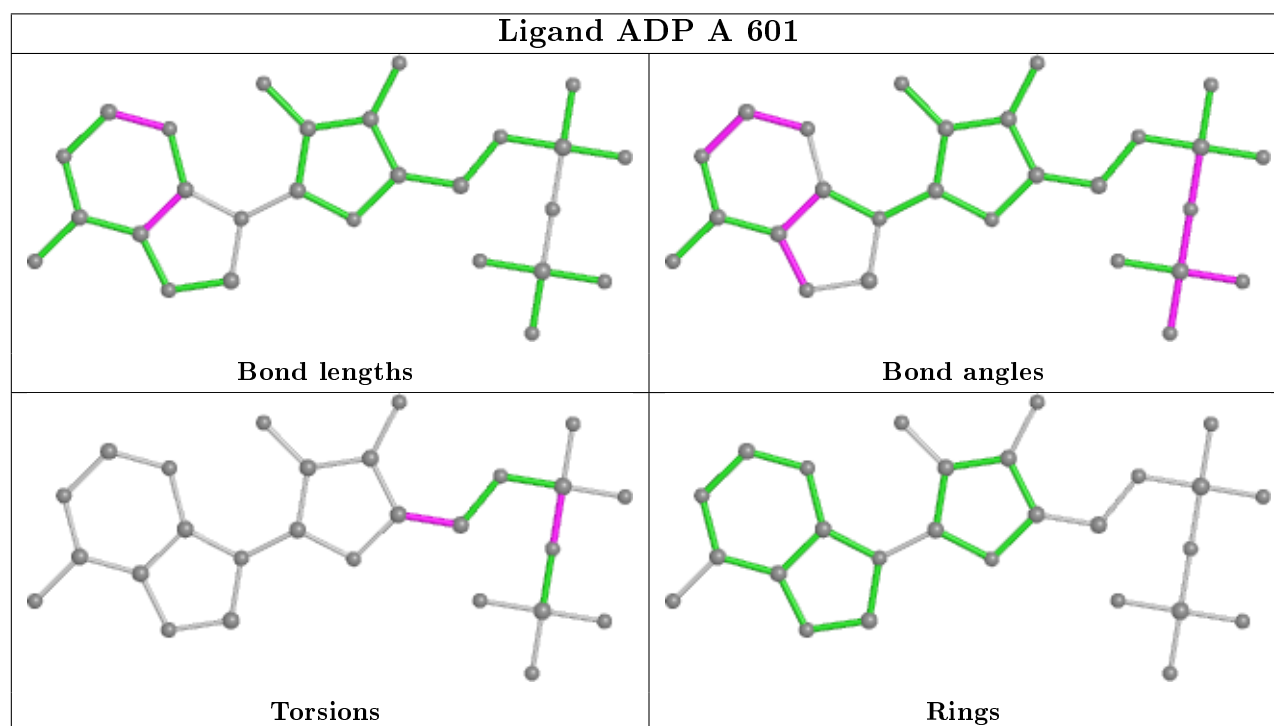
Mol	Chain	Res	Type	Atoms
9	H	201	ATP	PB-O3B-PG-O3G
5	E	501	ADP	C5'-O5'-PA-O2A
5	F	600	ADP	C5'-O5'-PA-O1A
5	F	600	ADP	C5'-O5'-PA-O2A
5	F	600	ADP	C5'-O5'-PA-O3A

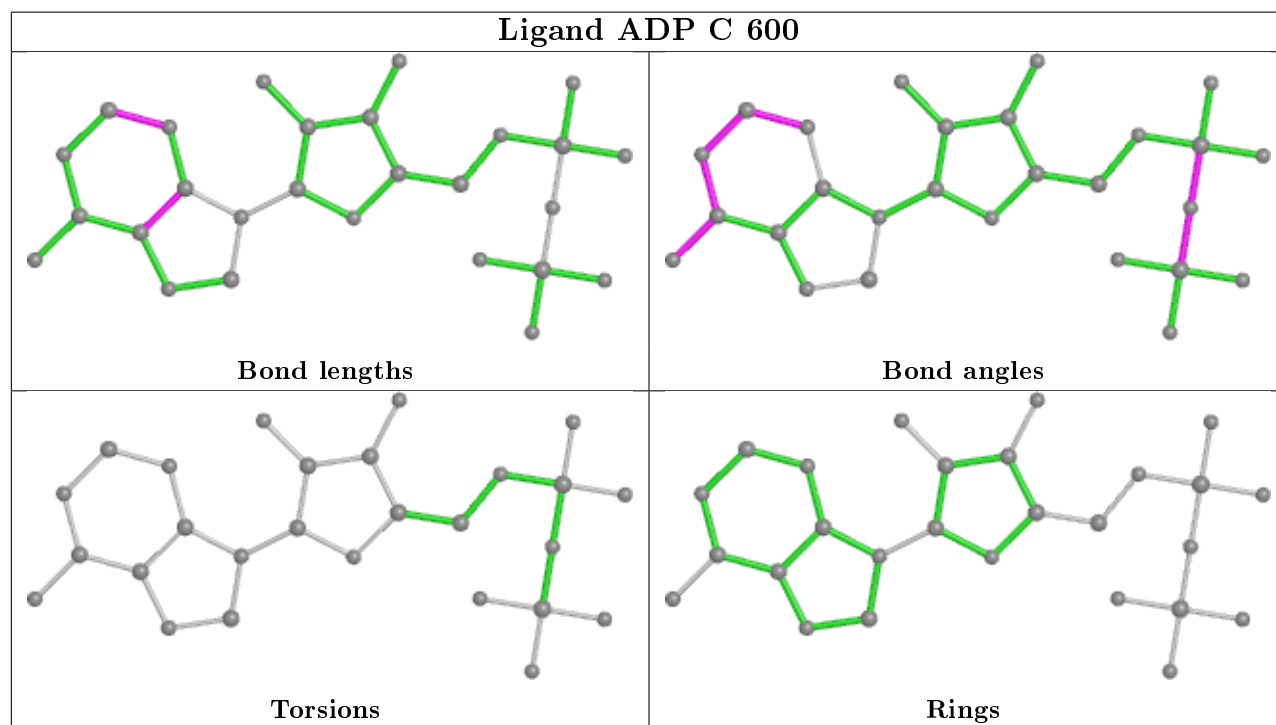
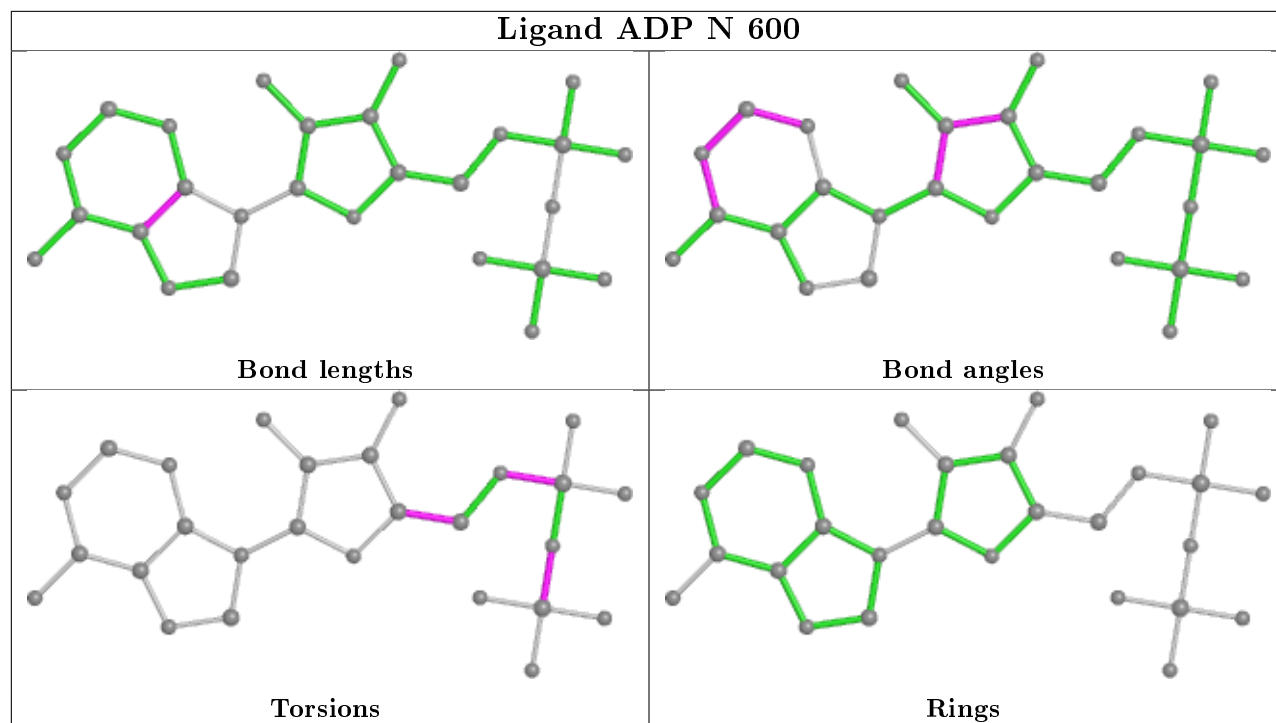
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	600	ADP	3	0
7	A	603	GOL	2	0
5	D	600	ADP	4	0

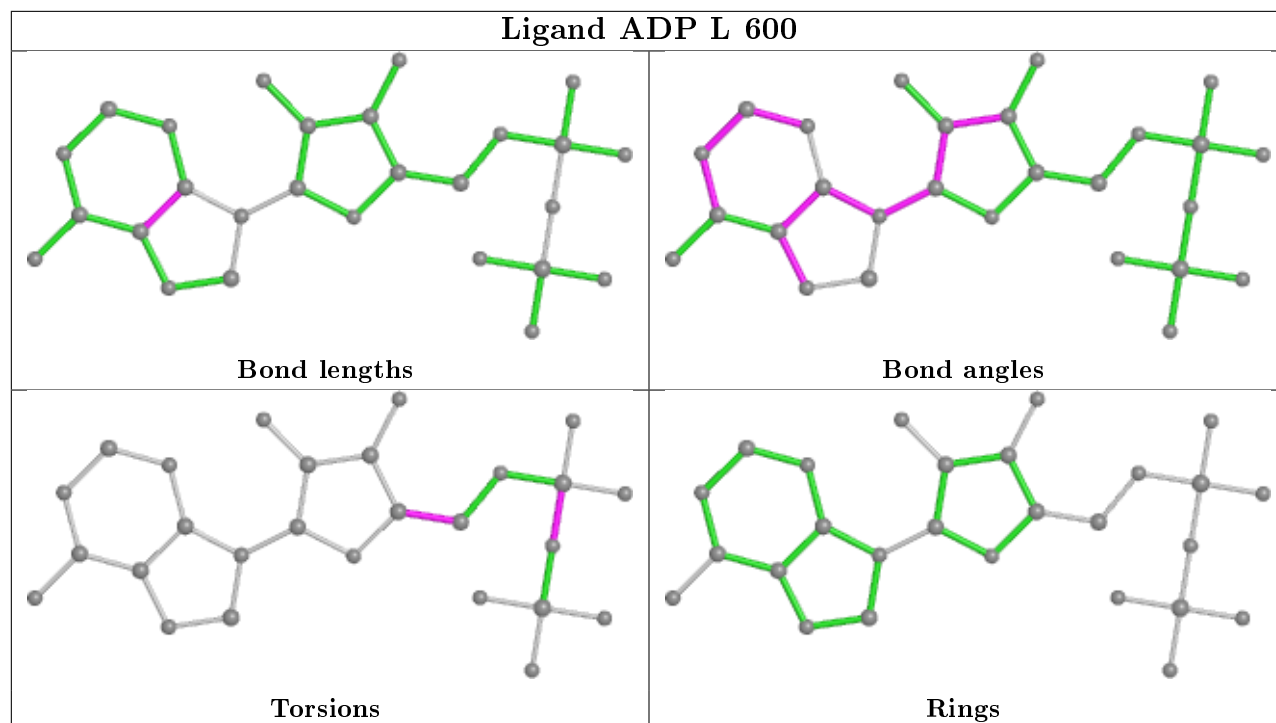
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



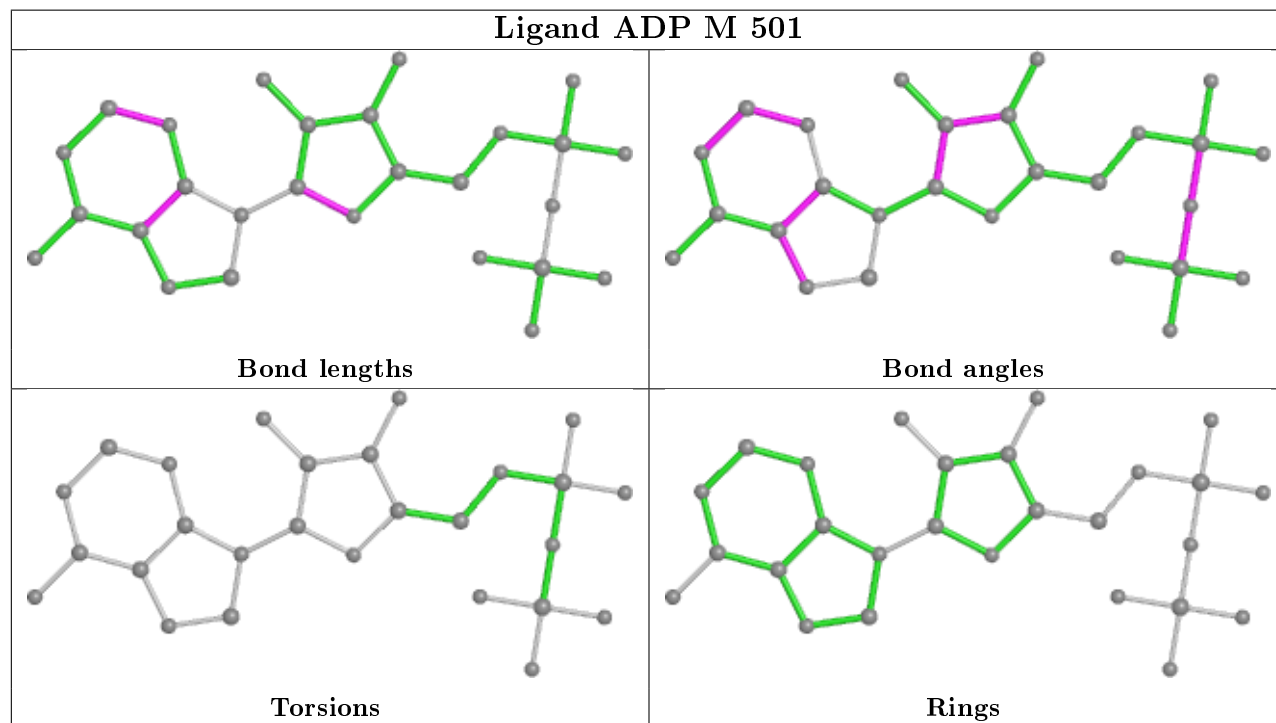


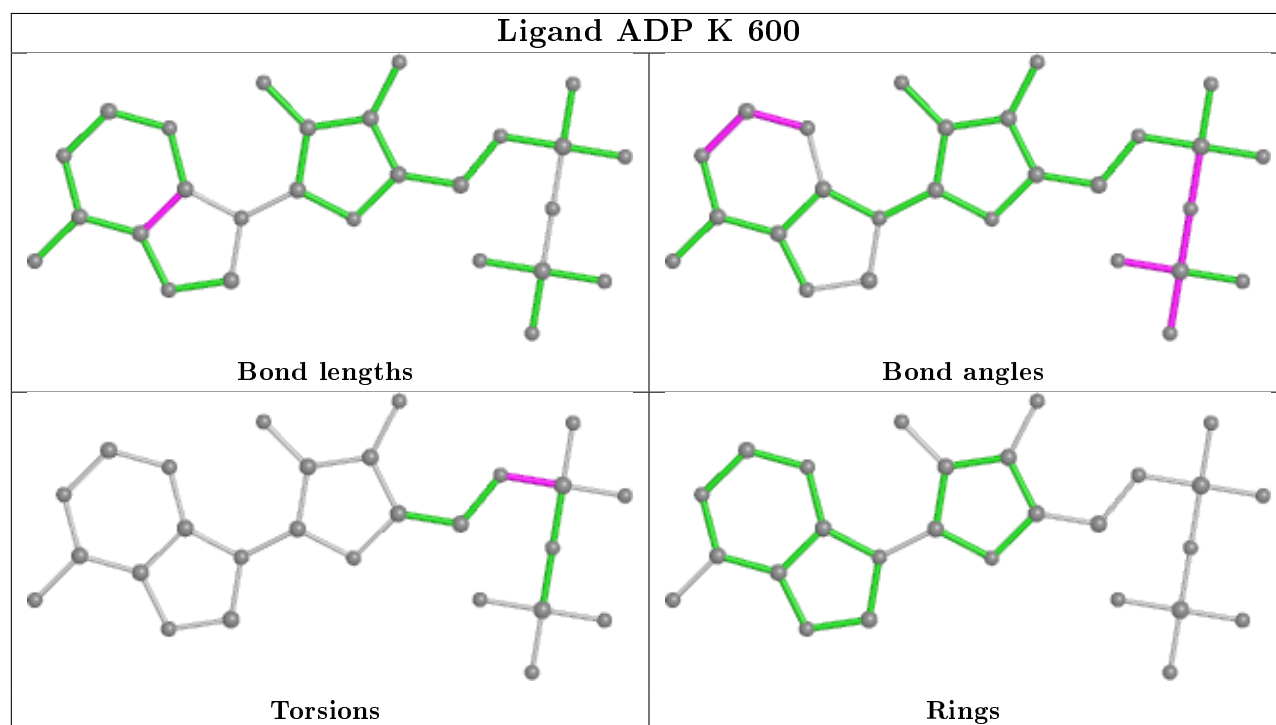
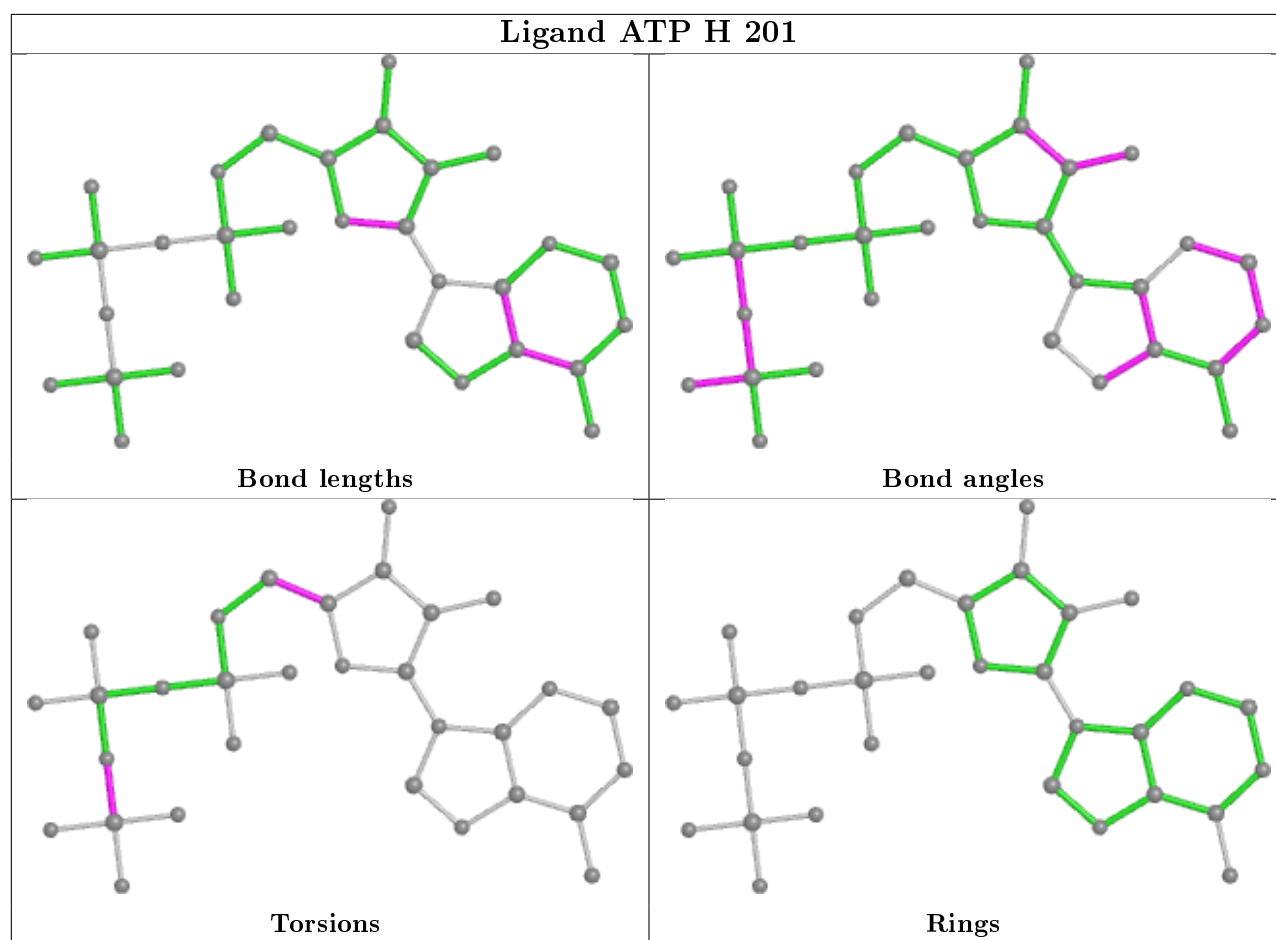


## Ligand ADP L 600

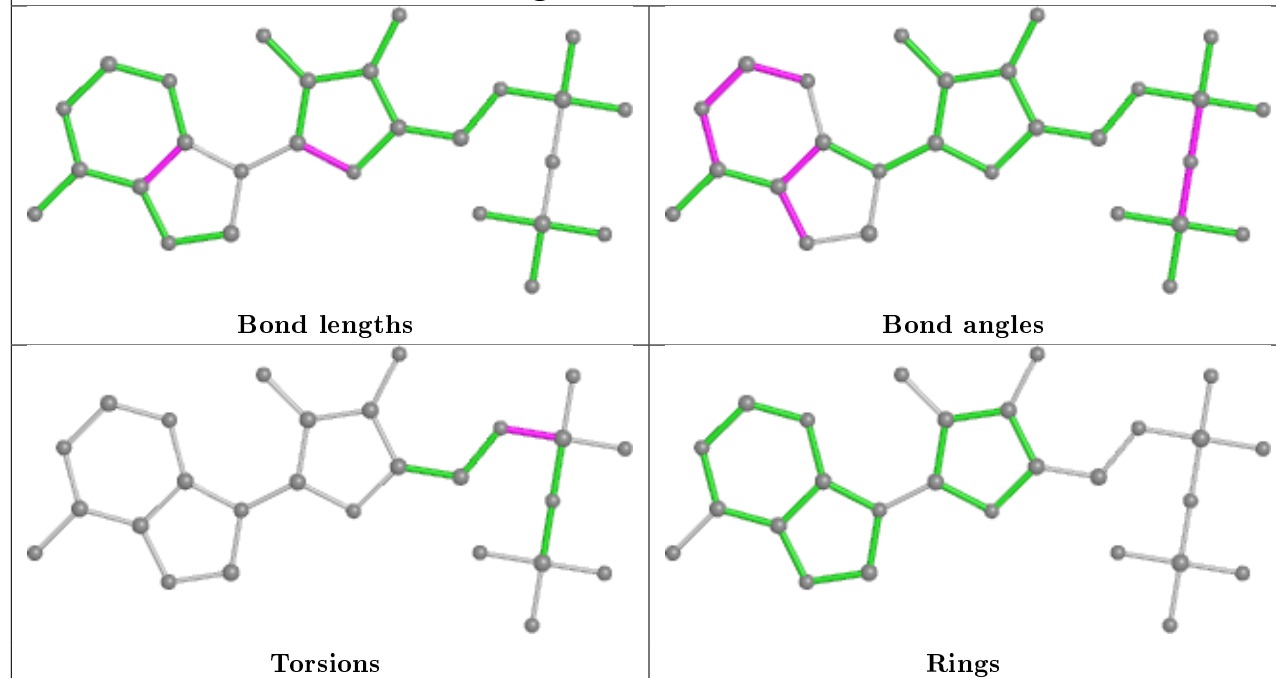


## Ligand ADP M 501

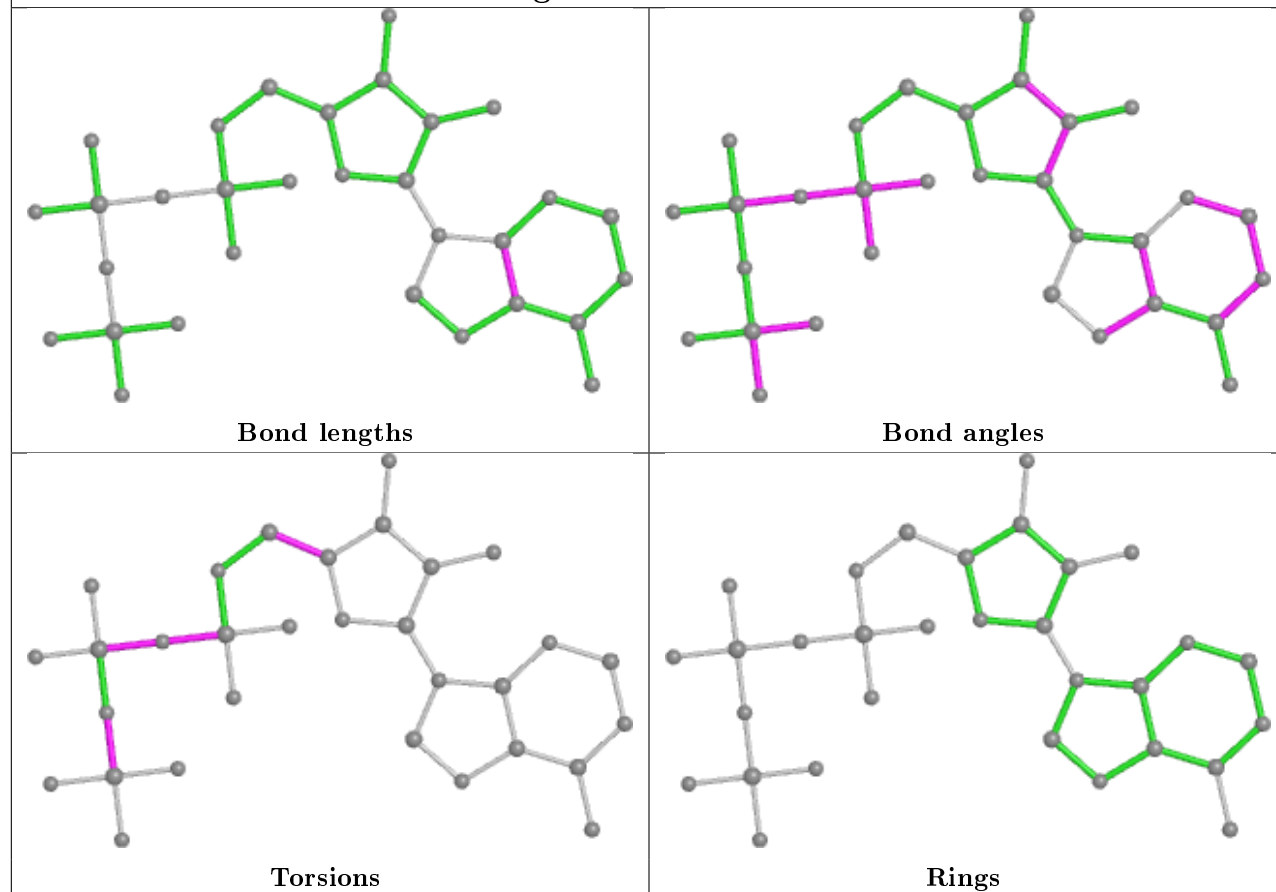


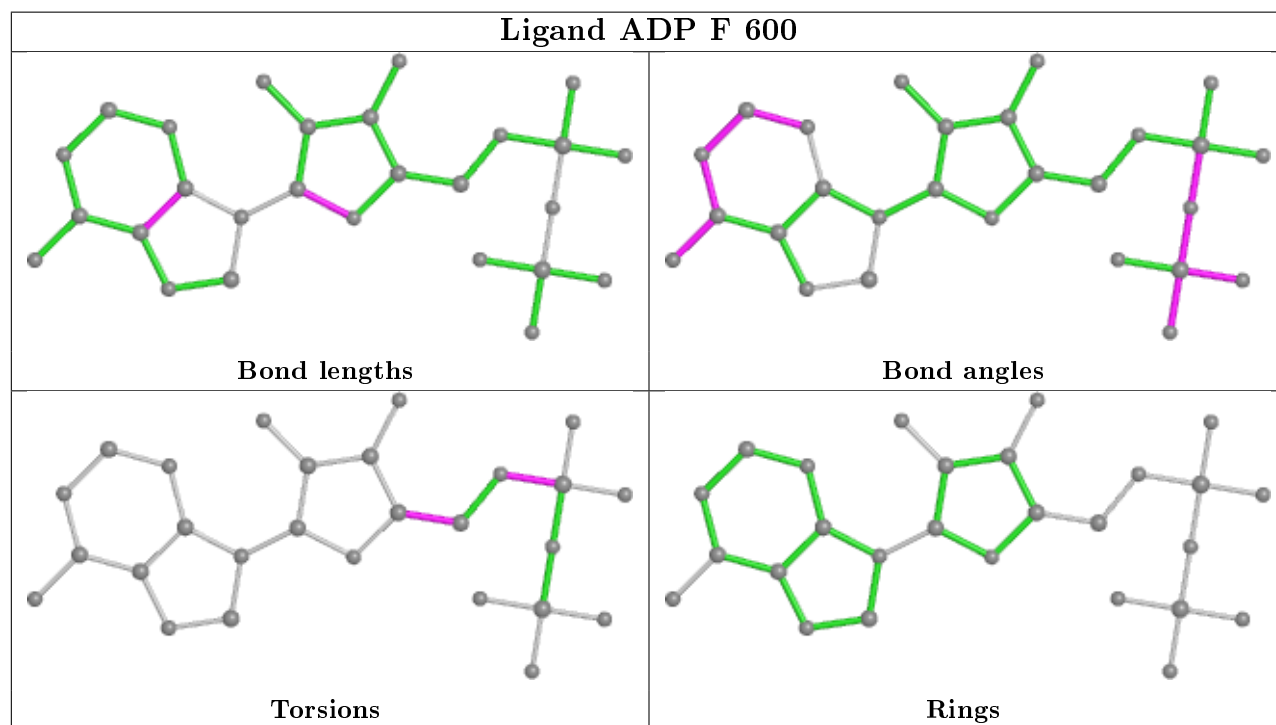
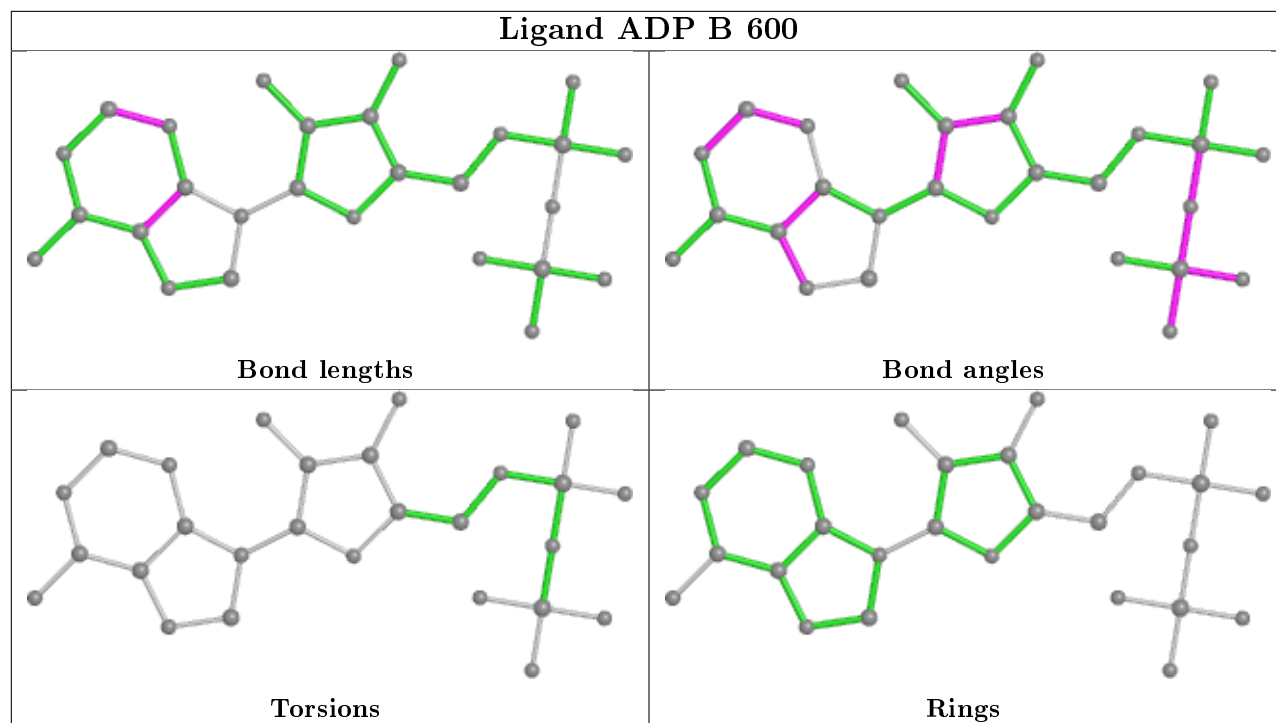


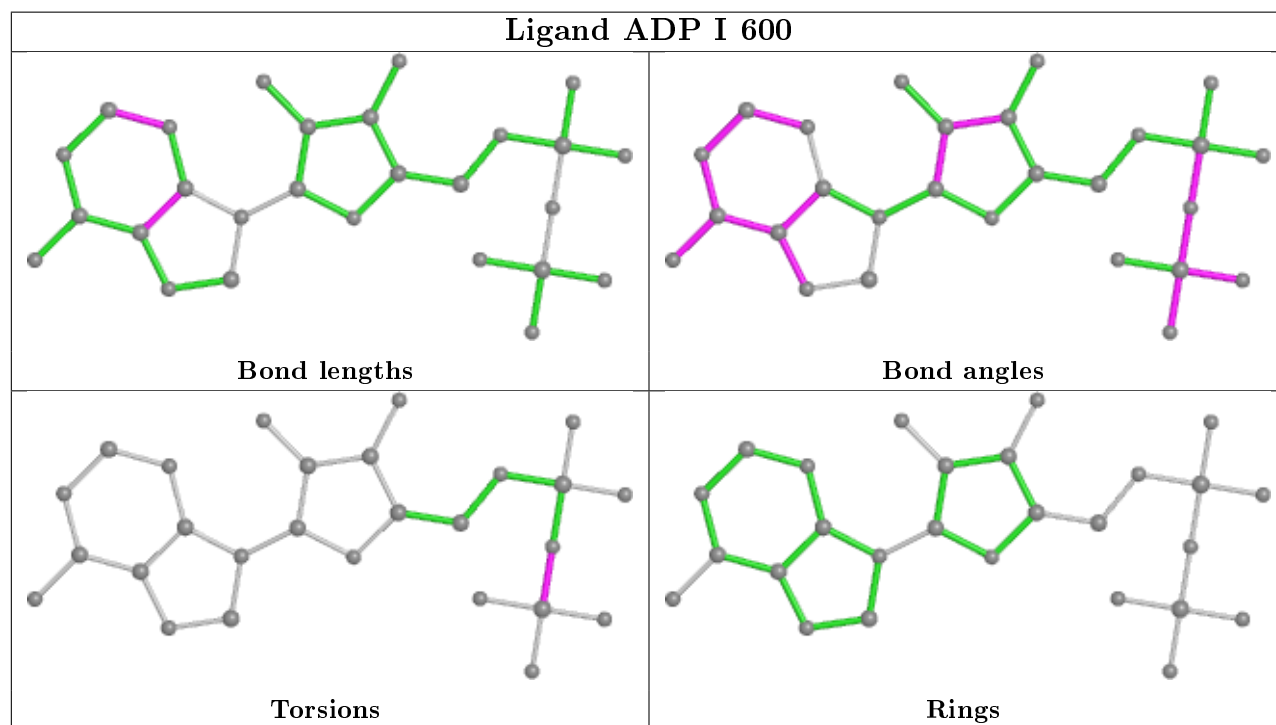
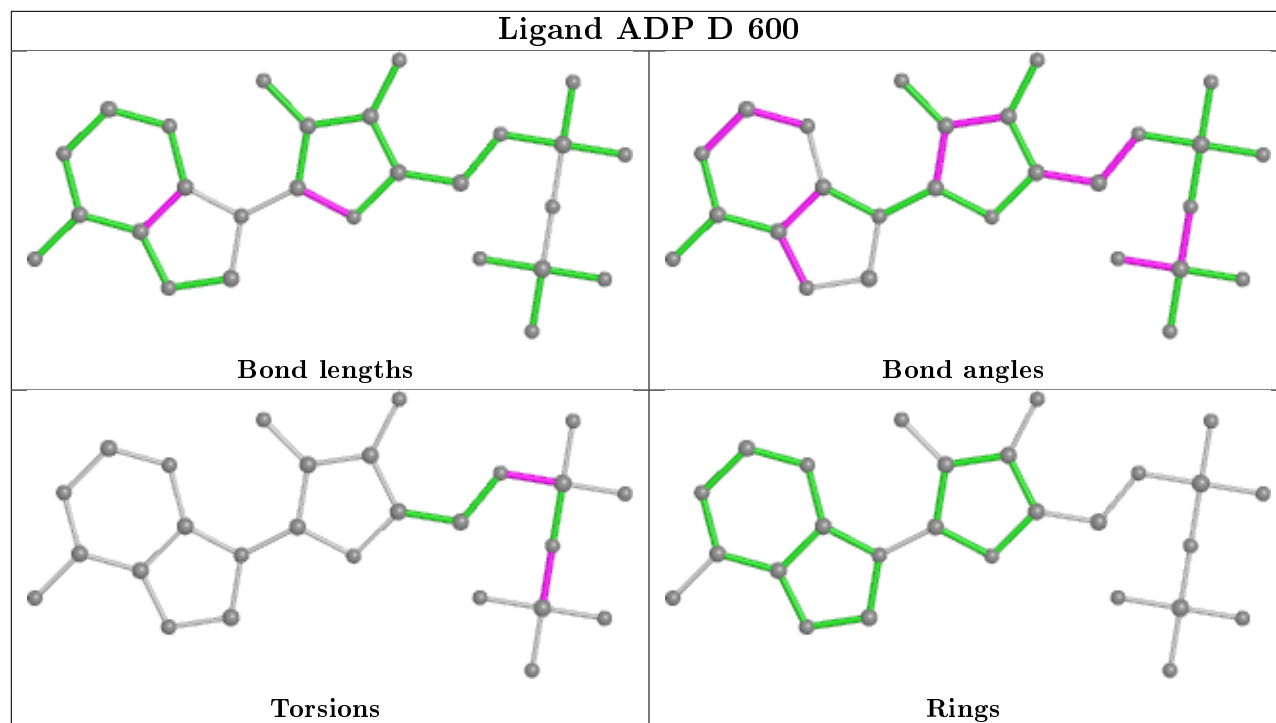
## Ligand ADP E 501

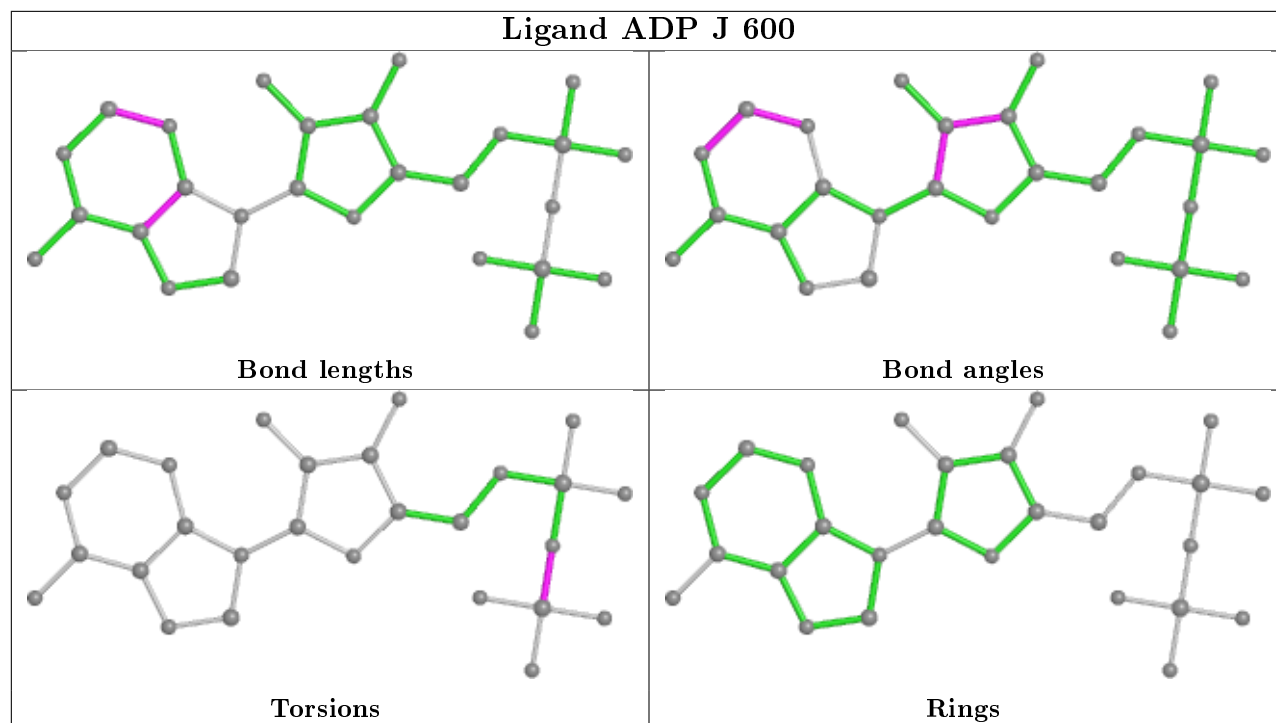


## Ligand ATP P 201









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	475/502 (94%)	-0.16	4 (0%) 86 65	34, 59, 91, 111	0
1	B	475/502 (94%)	-0.27	3 (0%) 89 72	28, 49, 84, 117	0
1	C	476/502 (94%)	-0.50	1 (0%) 95 87	29, 47, 70, 103	0
1	I	474/502 (94%)	-0.46	1 (0%) 95 87	27, 46, 76, 110	0
1	J	475/502 (94%)	-0.33	1 (0%) 95 87	26, 47, 84, 120	0
1	K	478/502 (95%)	-0.55	0 100 100	24, 39, 59, 114	0
2	D	461/462 (99%)	-0.41	0 100 100	31, 52, 77, 94	0
2	E	461/462 (99%)	-0.45	0 100 100	30, 47, 75, 113	0
2	F	461/462 (99%)	-0.46	0 100 100	28, 48, 81, 96	0
2	L	461/462 (99%)	-0.43	0 100 100	22, 44, 72, 85	0
2	M	461/462 (99%)	-0.49	0 100 100	26, 43, 74, 118	0
2	N	461/462 (99%)	-0.55	0 100 100	26, 40, 70, 103	0
3	G	284/286 (99%)	-0.16	0 100 100	28, 48, 76, 106	0
3	O	284/286 (99%)	-0.13	4 (1%) 75 49	24, 55, 98, 115	0
4	H	132/135 (97%)	-0.37	0 100 100	34, 49, 72, 96	0
4	P	132/135 (97%)	0.23	2 (1%) 73 46	52, 73, 102, 117	0
All	All	6451/6626 (97%)	-0.38	16 (0%) 95 87	22, 47, 82, 120	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	401	ASP	3.4
1	B	399	GLY	2.7
1	C	400	SER	2.6
4	P	72	PRO	2.5
1	B	401	ASP	2.5

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	D	601	1/1	0.87	0.14	67,67,67,67	0
5	ADP	M	501	27/27	0.87	0.24	52,54,59,60	27
6	MG	O	601	1/1	0.90	0.19	30,30,30,30	0
6	MG	B	601	1/1	0.90	0.08	26,26,26,26	0
7	GOL	A	603	6/6	0.91	0.31	50,52,52,54	0
5	ADP	E	501	27/27	0.92	0.20	35,37,49,50	27
6	MG	K	601	1/1	0.92	0.12	24,24,24,24	0
6	MG	I	601	1/1	0.92	0.08	30,30,30,30	0
6	MG	G	601	1/1	0.94	0.13	30,30,30,30	0
5	ADP	L	600	27/27	0.94	0.23	44,74,81,84	0
6	MG	A	602	1/1	0.94	0.14	35,35,35,35	0
9	ATP	P	201	31/31	0.95	0.17	48,67,72,72	0
5	ADP	D	600	27/27	0.96	0.19	42,72,80,83	0
5	ADP	A	601	27/27	0.96	0.17	40,46,50,52	0
6	MG	L	601	1/1	0.96	0.11	52,52,52,52	0
8	PO4	E	502	5/5	0.96	0.14	50,50,52,54	0
5	ADP	B	600	27/27	0.96	0.13	31,39,44,45	0
5	ADP	K	600	27/27	0.97	0.14	23,27,31,31	0
5	ADP	I	600	27/27	0.97	0.13	31,34,35,41	0
5	ADP	F	600	27/27	0.97	0.14	30,38,41,42	0
5	ADP	J	600	27/27	0.97	0.14	29,35,37,39	0
6	MG	N	601	1/1	0.97	0.05	34,34,34,34	0
6	MG	F	601	1/1	0.98	0.07	32,32,32,32	0
9	ATP	H	201	31/31	0.98	0.13	31,35,44,45	0
5	ADP	N	600	27/27	0.98	0.11	29,36,39,40	0
6	MG	J	601	1/1	0.98	0.09	25,25,25,25	0
5	ADP	C	600	27/27	0.98	0.13	27,30,33,36	0

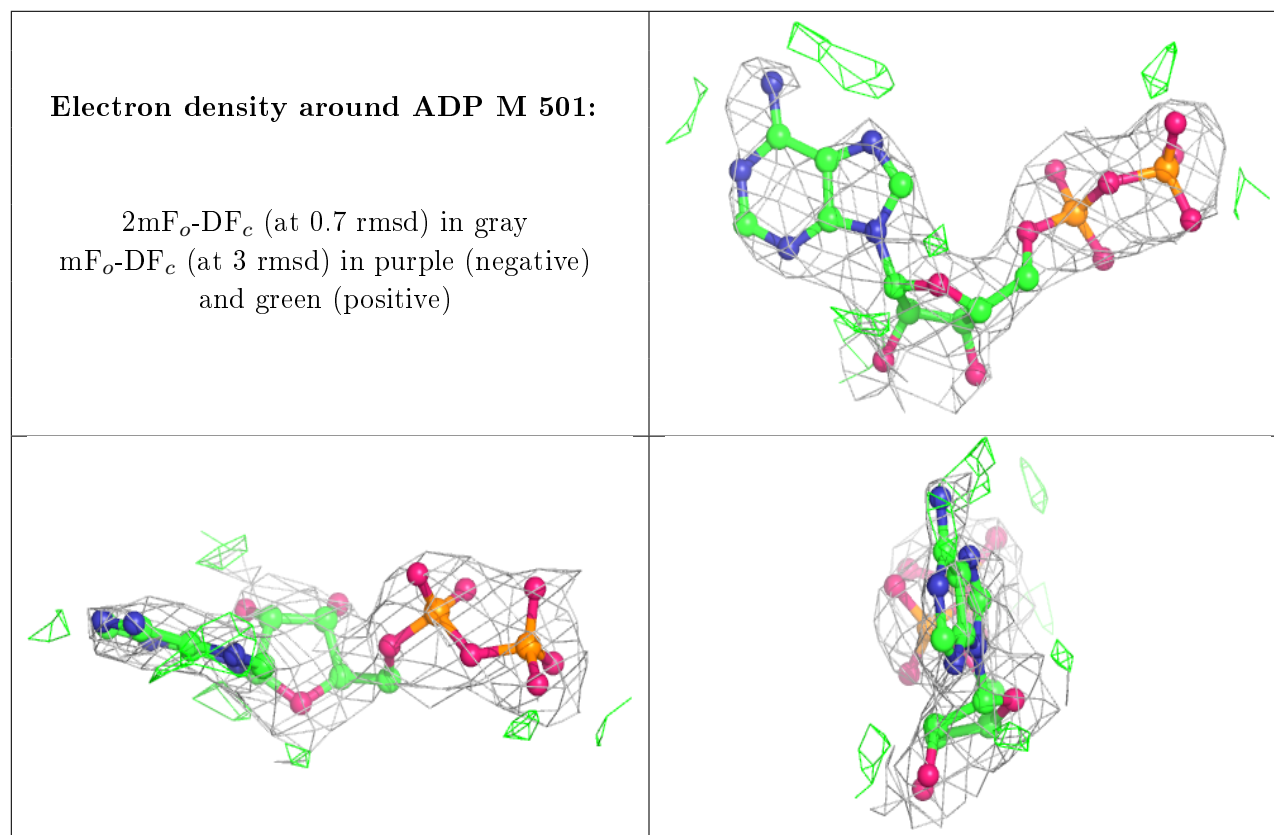
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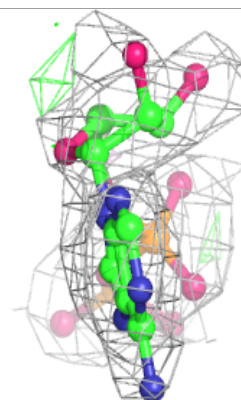
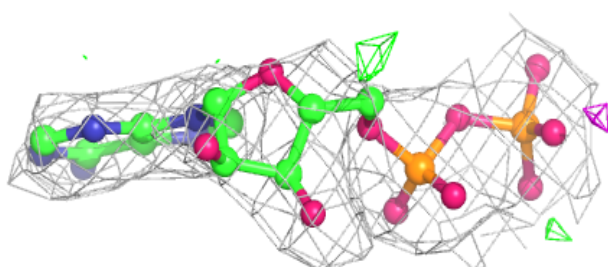
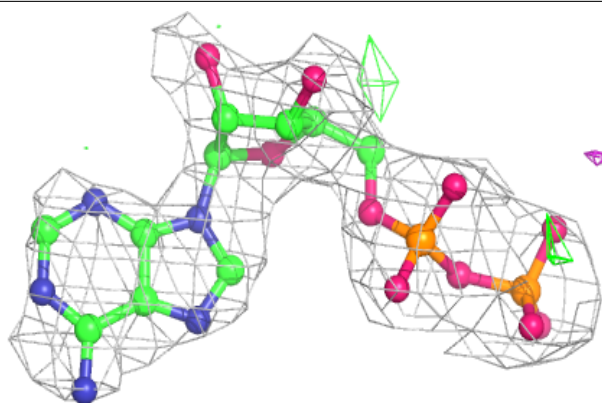
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	601	1/1	0.98	0.10	33,33,33,33	0
8	PO4	M	502	5/5	0.99	0.09	42,43,48,48	0

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.

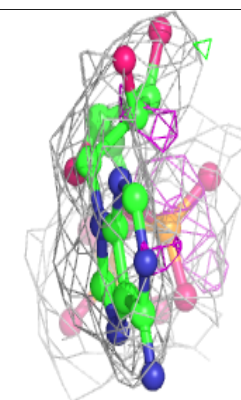
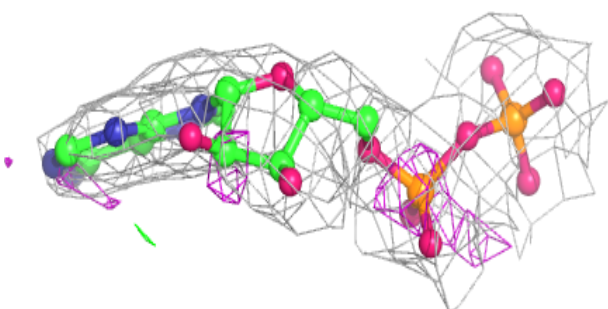
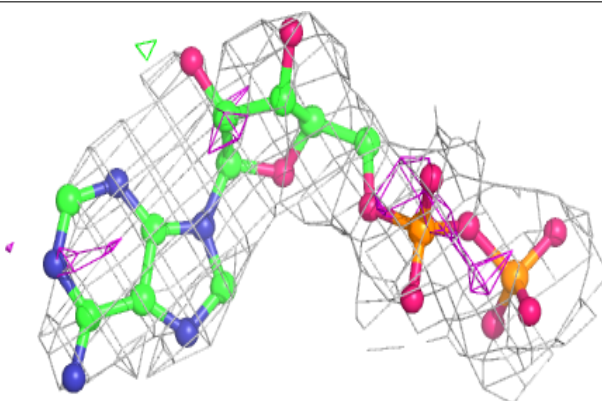


**Electron density around ADP E 501:**

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

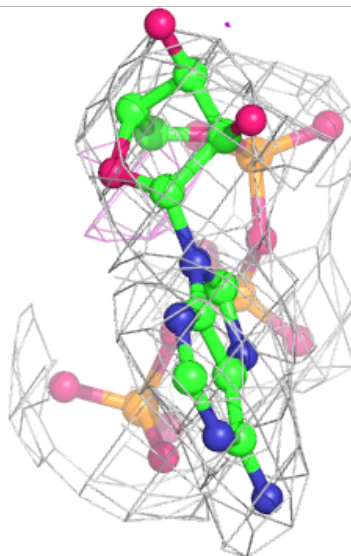
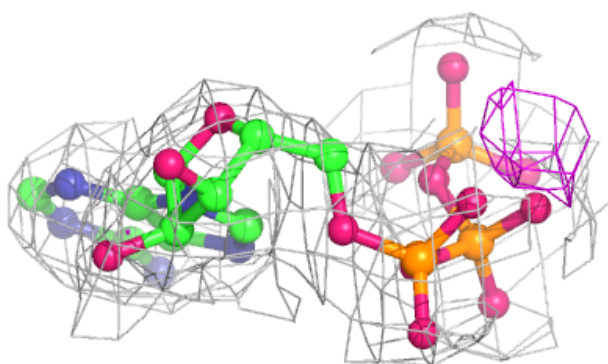
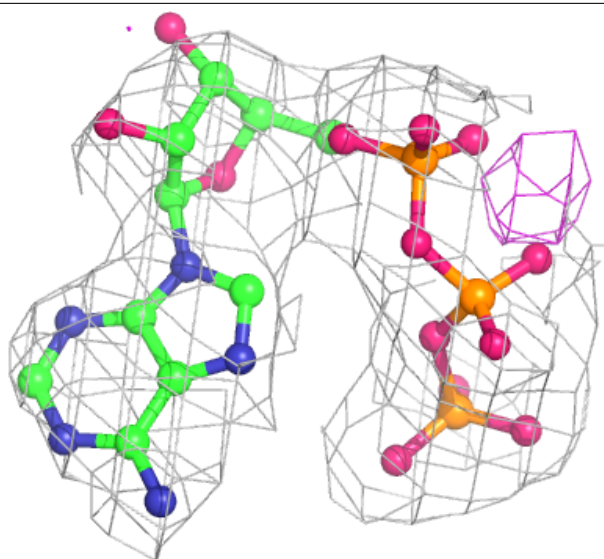
**Electron density around ADP L 600:**

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



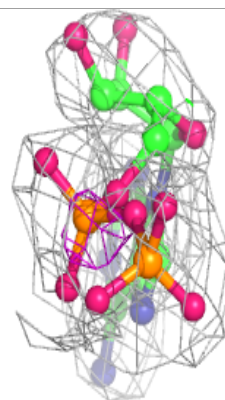
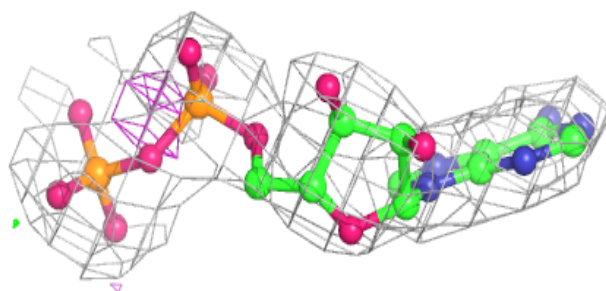
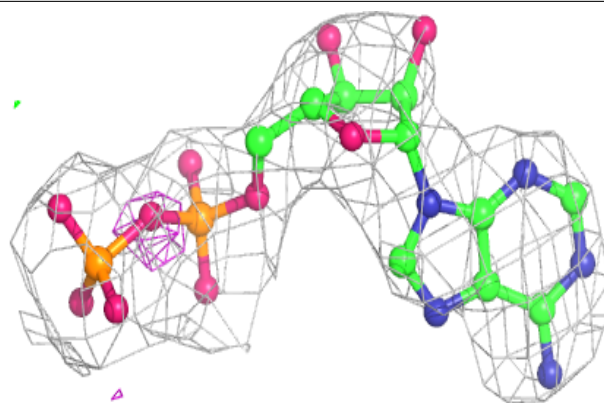
**Electron density around ATP P 201:**

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

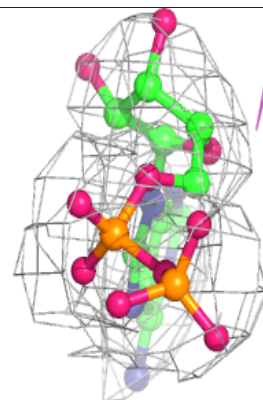
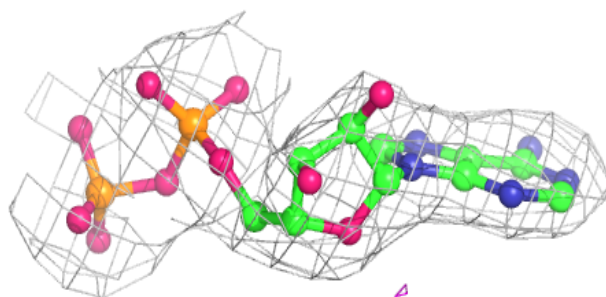
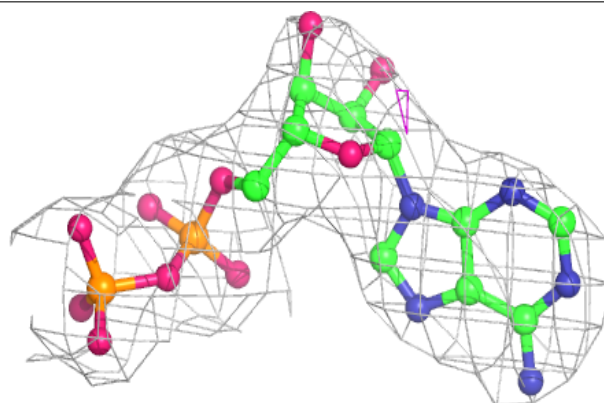


**Electron density around ADP D 600:**

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

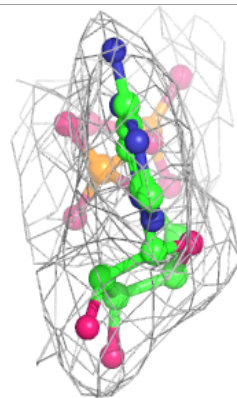
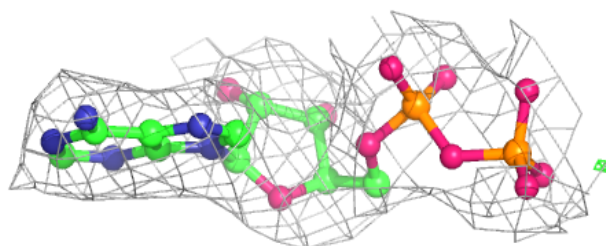
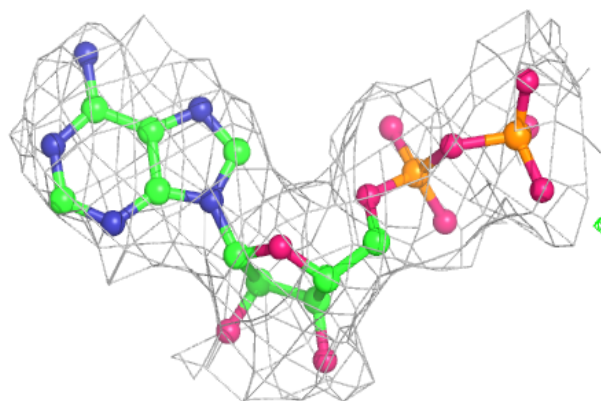
**Electron density around ADP A 601:**

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

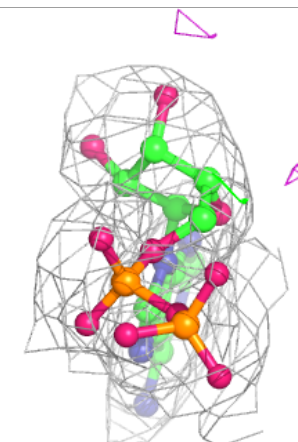
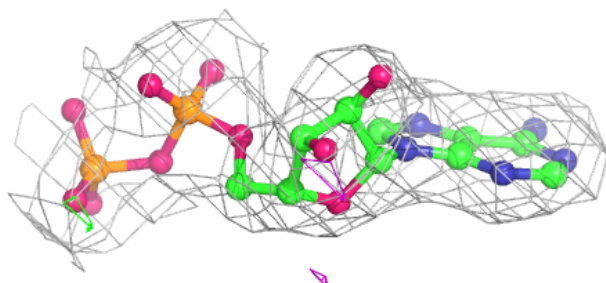
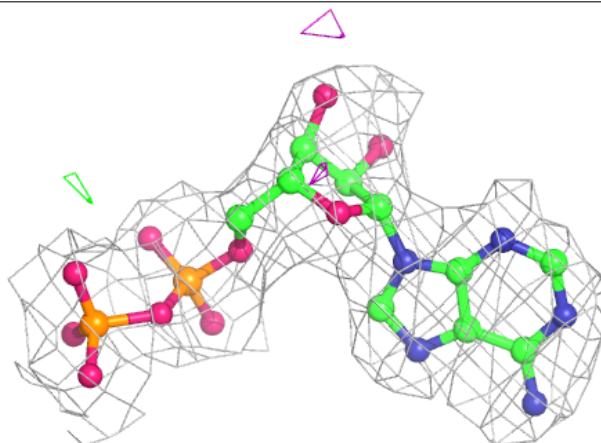


**Electron density around ADP B 600:**

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

**Electron density around ADP K 600:**

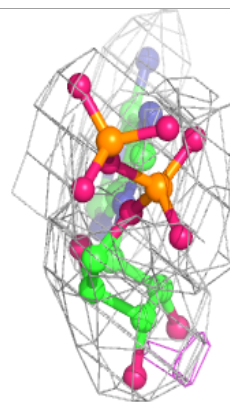
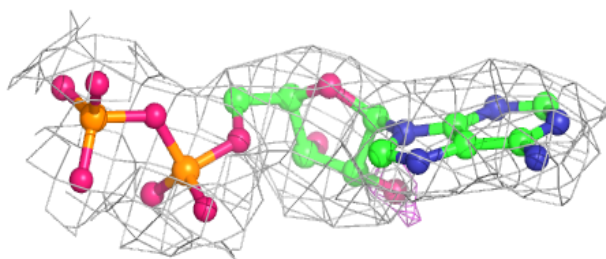
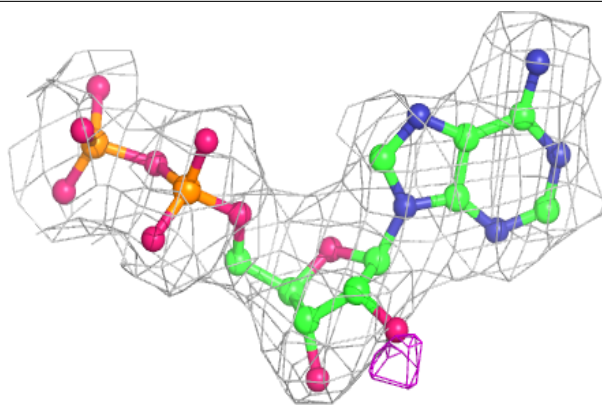
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



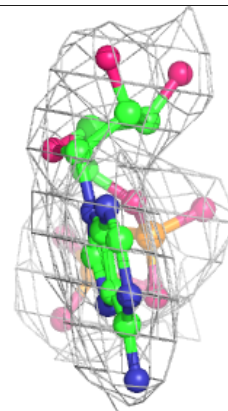
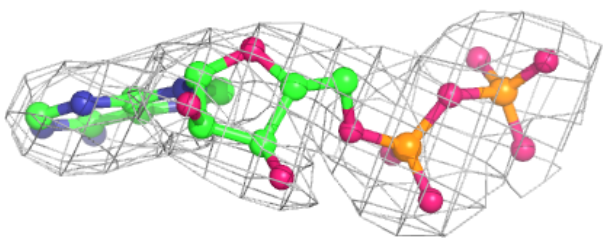
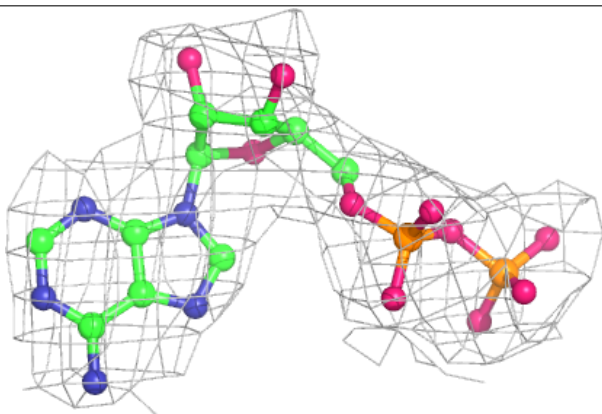


**Electron density around ADP I 600:**

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

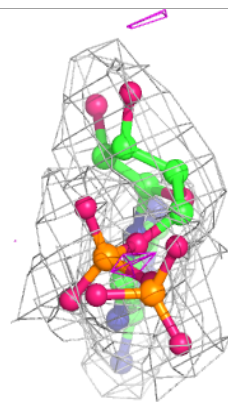
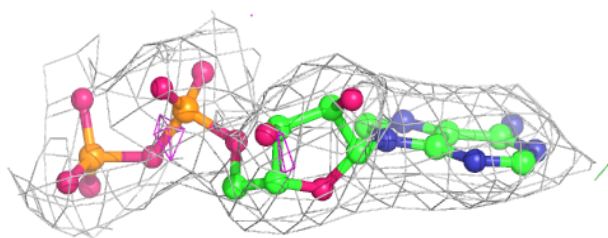
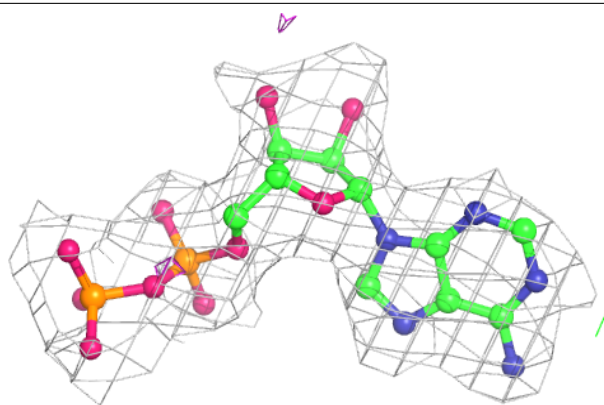
**Electron density around ADP F 600:**

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



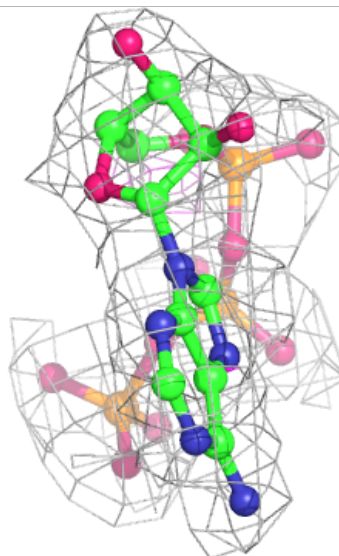
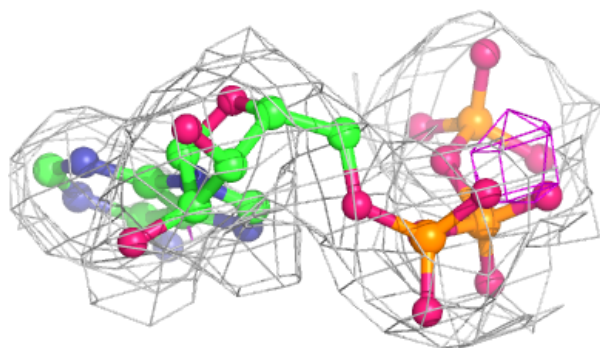
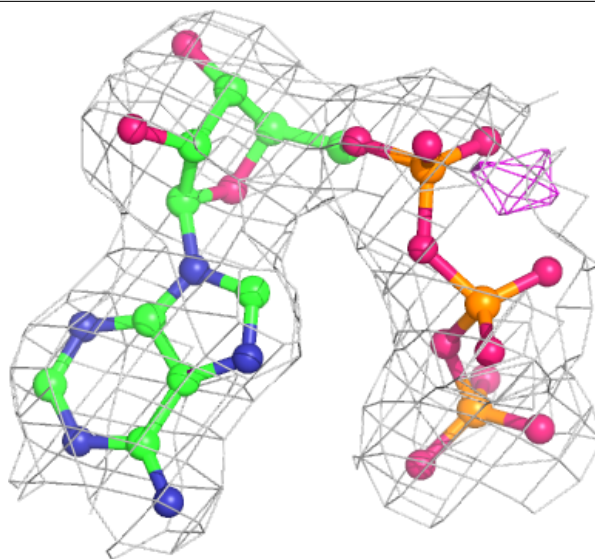
**Electron density around ADP J 600:**

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



**Electron density around ATP H 201:**

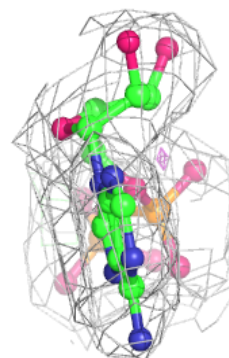
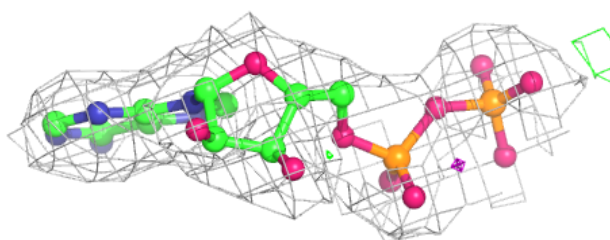
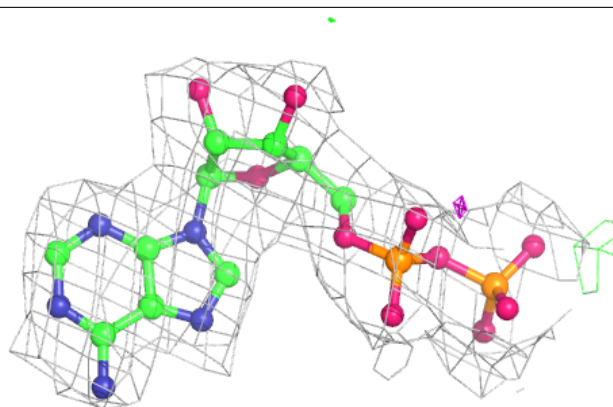
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



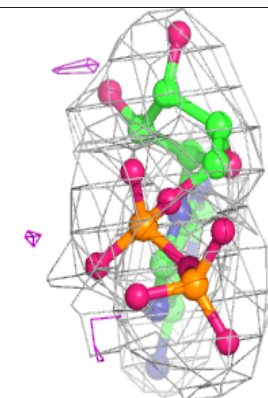
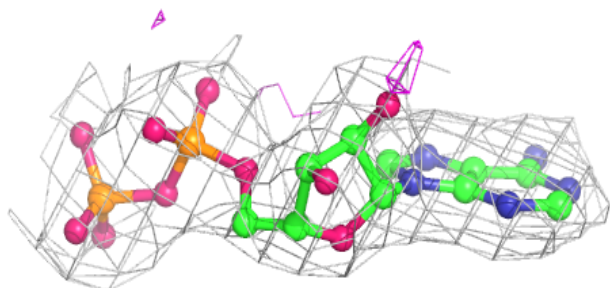
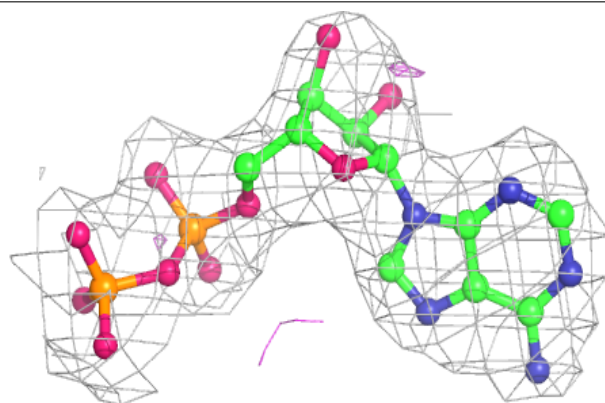


**Electron density around ADP N 600:**

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

**Electron density around ADP C 600:**

$2mF_o-DF_c$  (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.